

Self-consistent Molecular Orbital Methods. XII. Further
Basis Sets for Use in Molecular Orbital Studies of Organic

Journal of Chemical Physics

56, 2257-2261

DOI: 10.1063/1.1677527

Citation Report

#	ARTICLE	IF	CITATIONS
182	Self-consistent Molecular Orbital Methods. XIV. An Extended Gaussian-type Basis for Molecular Orbital Studies of Organic Molecules. Inclusion of Second Row Elements. Journal of Chemical Physics, 1972, 56, 5255-5257.	1.2	188
183	Optimum atomic orbitals for molecular calculations A review. Advances in Physics, 1972, 21, 825-915.	35.9	43
184	Molecular orbital theory of simple carbonium ions. Chemical Physics Letters, 1972, 14, 385-388.	1.2	120
185	The effect of d-functions on molecular orbital energies for hydrocarbons. Chemical Physics Letters, 1972, 16, 217-219.	1.2	1,042
186	Local orbitals for bonding in ethane. Theoretica Chimica Acta, 1973, 29, 75-83.	0.9	19
187	The influence of polarization functions on molecular orbital hydrogenation energies. Theoretica Chimica Acta, 1973, 28, 213-222.	0.9	14,096
188	Structures and stabilities of three-membered rings from ab initio molecular orbital theory. , 1973, , 1-45.		12
189	Even-tempered atomic orbitals. VII. Theoretical equilibrium geometries and reaction energies for carbon suboxide and other molecules containing carbon, oxygen, and hydrogen. Journal of Chemical Physics, 1974, 60, 932-936.	1.2	14
190	Electronic structure and conformational equilibria of phenyl-propylcarbocations. Tetrahedron, 1974, 30, 117-126.	1.0	6
191	Two kinds of wave in an oscillating chemical solution. Faraday Symposia of the Chemical Society, 1974, 9, 38.	0.5	54
192	Accuracy of AHnequilibrium geometries by single determinant molecular orbital theory. Molecular Physics, 1974, 27, 209-214.	0.8	2,038
193	Limit cycles in the plane. An equivalence class of homogeneous systems. Faraday Symposia of the Chemical Society, 1974, 9, 254.	0.5	3
194	Extended basis set studies of hydrocarbon molecular orbital energies. Chemical Physics Letters, 1975, 36, 1-5.	1.2	24
195	Barmer to internal rotation in the methylammonium ion. Journal of Molecular Structure, 1975, 29, 39-45.	1.8	8
196	Gaussian basis sets suitable for accurate valence-shell calculations using the model potential method. Journal of Chemical Physics, 1975, 63, 4678-4684.	1.2	61
197	Self-consistent molecular orbital methods. XV. Extended Gaussian-type basis sets for lithium, beryllium, and boron. Journal of Chemical Physics, 1975, 62, 2921-2923.	1.2	686
198	Ab initio molecular orbital theory. Accounts of Chemical Research, 1976, 9, 399-406.	7.6	1,443
199	Ab initio calculation of the force field of the hydrogen fluoride dimer. Journal of Molecular Spectroscopy, 1976, 61, 1-10.	0.4	93

#	ARTICLE	IF	CITATIONS
200	Beryllium borohydride: C _{3v} or D _{3d} ? Journal of Chemical Physics, 1976, 64, 3080-3081.	1.2	7
201	A nonempirical molecular orbital study on the acidity of the carbon-hydrogen bond. Journal of Chemical Physics, 1977, 67, 517-523.	1.2	36
202	Self-consistent molecular orbital methods. XIX. Split-valence Gaussian-type basis sets for beryllium. Journal of Chemical Physics, 1977, 66, 879-880.	1.2	141
203	Uniform quality Gaussian basis sets. Journal of Chemical Physics, 1977, 66, 964-969.	1.2	43
204	XVIII. On the Relation Between the Spatial Electron Density and the Conformational Properties of Molecular Systems. Israel Journal of Chemistry, 1977, 16, 202-212.	1.0	3
205	Calculations on the inversion of anhydrous and hydrated aziridine. Molecular Physics, 1977, 34, 1429-1436.	0.8	7
206	The electronic structure of peracids. Functional models for cytochrome p-450. Tetrahedron, 1977, 33, 1029-1036.	1.0	29
207	Ab initio computation of the force field and vibrational frequencies of the H ₂ O...HF hydrogen bonded complex. Journal of Molecular Structure, 1977, 39, 295-300.	1.8	23
208	Conformation and electronic structure of oxalic acid by the ab initio method. Journal of Molecular Structure, 1977, 37, 160-163.	1.8	2
209	Structure factors calculated from molecular wavefunctions. Chemical Physics, 1977, 22, 267-271.	0.9	4
210	Relative stability of 1,2-difluoroethylenes. Chemical Physics Letters, 1977, 45, 197-200.	1.2	54
211	A non-empirical molecular orbital study of valence tautomers of C ₂ H ₃ N. International Journal of Quantum Chemistry, 1977, 12, 355-368.	1.0	21
212	Quantum chemical studies on electrophilic addition. Theoretica Chimica Acta, 1977, 44, 385-398.	0.9	32
213	A comparative ab-initio molecular orbital study of ammonia oxide and trifluoramine oxide. Journal of Fluorine Chemistry, 1977, 10, 197-218.	0.9	8
214	On a possible catalytic effect of water on some nucleophilic substitution reactions in inert solvents. Theoretica Chimica Acta, 1978, 47, 133-145.	0.9	21
215	Influence of polarization functions on molecular electrostatic potentials. Theoretica Chimica Acta, 1978, 47, 263-273.	0.9	19
216	Heuristic intermolecular potential function for the methane-water interaction based on ab initio quantum-mechanical calculations. International Journal of Quantum Chemistry, 1978, 14, 319-327.	1.0	12
217	Molecular orbital studies of Al ₂ F ₆ and Al ₂ Cl ₆ using a minimal basis set. International Journal of Quantum Chemistry, 1978, 14, 709-715.	1.0	34

#	ARTICLE	IF	CITATIONS
218	Theoretical study of the structure of azetidine. <i>Journal of Molecular Structure</i> , 1978, 43, 251-257.	1.8	23
219	Isomeric structures of protonated carbon dioxide. <i>Chemical Physics Letters</i> , 1978, 55, 399-403.	1.2	34
220	Harmonic force constants of formic acid: ab initio results and the uniqueness problem of force fields derived from vibrational data. <i>Chemical Physics Letters</i> , 1978, 59, 17-20.	1.2	20
221	Theoretical studies of equilibrium geometries of AH _n molecules. <i>Chemical Physics Letters</i> , 1978, 54, 57-60.	1.2	12
222	An analysis of Gaussian basis sets in terms of molecular one-electron properties. <i>Journal of Chemical Physics</i> , 1978, 68, 2172-2183.	1.2	14
223	Determination of relative intramolecular configuration by nuclear quadrupole double resonance. <i>Faraday Symposia of the Chemical Society</i> , 1978, 13, 93.	0.5	16
224	Molecular symmetry. II. Gradient of electronic energy with respect to nuclear coordinates. <i>Journal of Chemical Physics</i> , 1978, 68, 3998-4004.	1.2	230
225	Finite perturbation calculations of the nuclear spin-spin coupling constant for the hydrogen fluoride molecule. <i>Journal of Chemical Physics</i> , 1978, 69, 943-944.	1.2	7
226	Ion pair and partially hydrated Li+NO ₃ [−] ion pair structures: Correlation of molecular orbital results with matrix isolation data. <i>Journal of Chemical Physics</i> , 1978, 68, 826-831.	1.2	19
227	A comparison between the predictions of vibrational transition moments and force fields using various gaussian basis sets. <i>Molecular Physics</i> , 1979, 38, 145-154.	0.8	12
228	Temporary anions of the fluoroethylenes. <i>Chemical Physics Letters</i> , 1979, 68, 121-126.	1.2	92
229	Ab initio molecular orbital studies of the structure and potential energy surface of the LiAlF ₄ complex. <i>Chemical Physics Letters</i> , 1979, 68, 225-231.	1.2	25
230	A comparative study of H ⁺ and Li ⁺ interactions with oxygen bases. <i>Chemical Physics Letters</i> , 1979, 64, 227-229.	1.2	5
231	Structure factors calculated from molecular wavefunctions. II. Analysis of the molecular charge distribution in diborane. <i>Chemical Physics</i> , 1979, 44, 163-169.	0.9	1
232	A molecular orbital study of lithium ion association with bases. I. The carbonyl bases R ₂ CO. <i>Chemical Physics</i> , 1979, 40, 329-335.	0.9	20
233	A theoretical investigation of the rotational barriers of peroxyformic acid. <i>Tetrahedron</i> , 1979, 35, 1239-1245.	1.0	10
234	Relative stability of the 2 A _{1g} and 2 E _g states of the C ₂ H ₆ ⁺ ion. <i>Theoretica Chimica Acta</i> , 1979, 53, 377-381.	0.9	8
235	Ab initio study of hydrazoic acid. <i>Theoretica Chimica Acta</i> , 1979, 52, 75-88.	0.9	33

#	ARTICLE	IF	CITATIONS
236	Ab initio valence bond calculations. X. Vertical valence ionization potentials of allene and butatriene. <i>International Journal of Quantum Chemistry</i> , 1979, 15, 655-662.	1.0	7
237	Dependence on the geometry and on the basis set of localized orbital energy and moment contributions. <i>Acta Physica Academiae Scientiarum Hungaricae</i> , 1979, 46, 333-340.	0.1	4
238	Bond functions for AB initio calculations on polyatomic molecules hydrocarbons. <i>Chemical Physics Letters</i> , 1979, 66, 358-362.	1.2	38
239	Ab initio Hartree-Fock calculations on acetylene dimer. <i>Chemical Physics Letters</i> , 1979, 67, 508-510.	1.2	42
240	Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole moment derivatives. <i>Journal of the American Chemical Society</i> , 1979, 101, 2550-2560.	6.6	2,034
241	Cubic force constants of the FH ⁻ OH ₂ and FH ⁻ O(CH ₃) ₂ hydrogen-bonded complexes. An analyses of computed Ab initio SCF values. <i>Chemical Physics Letters</i> , 1980, 69, 521-524.	1.2	17
242	MNDO calculations on diazirines. <i>Theoretica Chimica Acta</i> , 1980, 55, 325-331.	0.9	9
243	Exact-exchange Hartree-Fock calculations for periodic systems. II. Results for graphite and hexagonal boron nitride. <i>International Journal of Quantum Chemistry</i> , 1980, 17, 517-529.	1.0	93
244	Ab initio calculations on large molecules using molecular fragments. Generalization of the molecular fragment basis at the minimum basis set level. <i>International Journal of Quantum Chemistry</i> , 1980, 17, 1075-1097.	1.0	22
245	Theoretical study of substituent effects on the acidity of the methyl group: Structure of anions CH ₂ X ⁻ ?. <i>International Journal of Quantum Chemistry</i> , 1980, 18, 1371-1391.	1.0	20
246	On the anisotropy of the intermolecular potential of the CO ₂ -Ne system in the repulsive short-range region. <i>Chemical Physics Letters</i> , 1980, 71, 307-311.	1.2	7
247	Study of localizability for some small molecules. <i>Chemical Physics Letters</i> , 1980, 72, 275-277.	1.2	1
248	Ab initio molecular orbital calculations on beryllium and magnesium atom reactions with water. <i>Chemical Physics Letters</i> , 1980, 75, 69-74.	1.2	28
249	Isomeric structures of protonated ozone: A theoretical study. <i>Journal of Computational Chemistry</i> , 1980, 1, 94-98.	1.5	13
250	An ab initio molecular orbital study of the CH ₂ ⁺ →O ⁺ isomers: The stability of the hydroxymethylene radical cation. <i>International Journal of Mass Spectrometry and Ion Physics</i> , 1980, 33, 87-93.	1.3	20
251	Structural characterization of some substituted azolidine molecules: UPS photoelectron spectroscopic studies. <i>Journal of Molecular Structure</i> , 1980, 69, 151-163.	1.8	22
252	The effect of substituents on the structure of dioxirane. <i>Journal of Molecular Structure</i> , 1980, 69, 217-226.	1.8	10
253	Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. <i>Journal of Chemical Physics</i> , 1980, 72, 650-654.	1.2	14,940

#	ARTICLE	IF	CITATIONS
254	Dependence on the geometry and on the basis set of localized orbital energy and moment contributions. <i>Acta Physica Academiae Scientiarum Hungaricae</i> , 1980, 48, 225-234.	0.1	1
255	Dependence on the geometry and on the basis set of localized orbital energy and moment contributions. <i>Acta Physica Academiae Scientiarum Hungaricae</i> , 1980, 48, 235-241.	0.1	0
256	The use of cubic splines in vibration-rotation problems of diatomic molecules. <i>Molecular Physics</i> , 1980, 41, 759-768.	0.8	7
257	Theoretical studies of positron complexes with atomic anions. <i>Journal of Chemical Physics</i> , 1980, 72, 493-503.	1.2	25
258	On the use of minimal valence basis sets with the coreless Hartree-Fock effective potential. <i>Journal of Chemical Physics</i> , 1980, 73, 5191-5196.	1.2	18
259	Theoretical electronic plus vibrational investigation of some hydrogen-bonded complexes. I. Stretching cubic and quartic force constants of FH ₃ ...OH ₂ . <i>Journal of Chemical Physics</i> , 1980, 73, 2851-2857.	1.2	27
260	Charge distributions and chemical effects. XXII. On the partitioning of molecular energies and the relationships between energy components. <i>Journal of Chemical Physics</i> , 1980, 72, 1013-1017.	1.2	9
261	Affinities of Ammonia and Methylamine for H ⁺ , Li ⁺ , K ⁺ and CH ₃ ⁺ An Ab Initio SCF Study with Large Basis Sets. <i>Israel Journal of Chemistry</i> , 1980, 19, 299-304.	1.0	24
262	Force field, dipole moment derivatives, and vibronic constants of benzene from a combination of experimental and ab initio quantum chemical information. <i>Journal of Chemical Physics</i> , 1981, 74, 3999-4014.	1.2	432
263	Ab initio computation of the quadratic force field of diborane. <i>Computational and Theoretical Chemistry</i> , 1981, 85, 279-283.	1.5	5
264	Equilibrium conformations of higher-energy rotational isomers of vinyl alcohol and methyl vinyl ether. <i>Computational and Theoretical Chemistry</i> , 1981, 85, 185-194.	1.5	40
265	Restricted hartree-fock calculations on C ₆ H ₄ and C ₆ H ₅ . <i>Chemical Physics Letters</i> , 1981, 84, 375-379.	1.2	10
266	New Scale of the Ionic Character of the Chemical Bond Using Multiconfiguration SCF Wave Functions. <i>Bulletin of the Chemical Society of Japan</i> , 1981, 54, 967-970.	2.0	2
267	Nonbonded potential function models for crystalline oxohydrocarbons. The <i>Acta Crystallographica Section A, Crystal Physics, Diffraction and General Crystallography</i> , 1981, 37, 293-301.	0.6	156
268	A molecular orbital study of lithium ion association with bases. The excited carbonyl bases R ₂ CO. <i>Chemical Physics Letters</i> , 1981, 81, 293-296.	1.2	0
269	Study of correlation effects on stretching force constants of the hydrogen-bonded complex F-H ₃ -OH ₂ . <i>Chemical Physics Letters</i> , 1981, 84, 361-364.	1.2	13
270	temporary $\dot{\text{X}}$ and $\dot{\text{I}}$ anions of the chloroethylenes and chlorofluoroethylenes. <i>Chemical Physics Letters</i> , 1981, 82, 270-276.	1.2	105
271	Molecular shapes and crystal structures of cyanogen and benzene. <i>Chemical Physics Letters</i> , 1981, 84, 68-70.	1.2	5

#	ARTICLE	IF	CITATIONS
272	Stretching force constants and derivatives of the dipole moment of the F-HNCH hydrogen-bonded complex. Preliminary results at the SCF level. <i>Chemical Physics Letters</i> , 1981, 84, 91-93.	1.2	16
273	Bond functions for ab initio calculations on polyatomic molecules. Molecules containing C, N, O and H. <i>Chemical Physics Letters</i> , 1981, 78, 147-152.	1.2	27
274	Ab initio calculation of spin-orbit interaction in polyatomic molecules using Gaussian-type wavefunctions. <i>Journal of Computational Chemistry</i> , 1981, 2, 244-250.	1.5	7
275	A reassessment of some restricted Hartree-Fock limit molecular energies and an investigation of the applicability of Ermler and Kern's procedure for their estimation. <i>Journal of Computational Chemistry</i> , 1981, 2, 334-346.	1.5	9
276	Ab initio HF versus semi-empirical results of chemisorption calculations of hydrogen on graphite. <i>Chemical Physics Letters</i> , 1981, 81, 498-502.	1.2	29
277	Can hexazine (N ₆) be stable?. <i>Chemical Physics Letters</i> , 1981, 83, 317-319.	1.2	41
278	A method for molecular correlation energy calculations. Application to the determination of dissociation energies of diatomic and polyatomic molecules. <i>Theoretica Chimica Acta</i> , 1981, 60, 339-353.	0.9	39
279	Calculation of isoelectronic energy differences using perturbation theory. <i>International Journal of Quantum Chemistry</i> , 1981, 19, 179-189.	1.0	0
280	Potential energy surface of the system CO + O: An ab initio study on the O-CO bond formation. <i>International Journal of Quantum Chemistry</i> , 1981, 19, 1139-1145.	1.0	1
281	Ab initio valence bond calculations. XI. Pyridine: Ground and ionized states. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 705-715.	1.0	12
282	Structure moléculaire des dérivés nitrés aromatiques. I. États électroniques singulets du mono et du 1,3,5-trinitrobenzène. <i>Propellants, Explosives, Pyrotechnics</i> , 1981, 6, 126-129.	1.0	4
283	Geometries, energies and polarities of cyanopolynes. <i>Chemical Physics</i> , 1981, 58, 203-210.	0.9	11
284	Theoretical studies of the temperature dependence of magnetic shielding tensors: H ₂ , HF, and LiH. <i>Chemical Physics</i> , 1981, 63, 185-202.	0.9	53
285	The equilibrium geometry of methyl carbamate. <i>Journal of Molecular Structure</i> , 1981, 77, 227-238.	1.8	20
286	An ab initio molecular orbital study of the first two bands in the photoelectron spectrum of hydroxylamine (NH ₂ OH). <i>Journal of Chemical Physics</i> , 1982, 77, 3605-3606.	1.2	4
287	Force in SCF theories. Test of the new method. <i>Journal of Chemical Physics</i> , 1982, 77, 3109-3122.	1.2	31
288	Calculation of correlation energy by a coupled-cluster approach. <i>Physical Review A</i> , 1982, 25, 671-680.	1.0	25
289	An ab initio SCF and CI study of ketene imine. <i>Computational and Theoretical Chemistry</i> , 1982, 87, 355-364.	1.5	20

#	ARTICLE	IF	CITATIONS
290	Electron densities in simple organic molecules. Computational and Theoretical Chemistry, 1982, 89, 83-91.	1.5	21
292	Ab initio study of rotational isomerism in vinylcyclopropane. Computational and Theoretical Chemistry, 1982, 89, 213-225.	1.5	25
293	A mechanistic study of the ion-molecule gas-phase reaction: $\text{CH}_3^+ + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_2^+ + \text{H}_2$. Computational and Theoretical Chemistry, 1982, 88, 343-355.	1.5	12
294	The molecular and electronic structure of bicyclo-[1,1,0]butane, bicyclo[2,1,0]pentane, and bicyclo[3,1,0]-hexane as obtained by ab initio SCF calculations. Computational and Theoretical Chemistry, 1982, 86, 255-265.	1.5	23
295	Theoretical study of ketenimine: Geometry, electronic properties, force constants and barriers to inversion and rotation. Computational and Theoretical Chemistry, 1982, 87, 205-210.	1.5	15
296	An ab initio study of the geometry, energy, and selected force constants for the three planar conformers of carbonic acid, and the bicarbonate ion; and of the energy for the reaction $\text{H}_2\text{O} + \text{CO}_2 \rightarrow \text{H}_2\text{CO}_3$. Journal of Computational Chemistry, 1982, 3, 283-296.	1.5	21
297	The 6-31G++ basis set: An economical basis set for correlated wavefunctions. Journal of Computational Chemistry, 1982, 3, 561-564.	1.5	12
298	Electronic states and barriers to internal rotation in silaallenes. Journal of Computational Chemistry, 1982, 3, 571-579.	1.5	15
300	Bond functions for ab initio calculations. MCSCF results for CH, NH, OH and FH. Chemical Physics Letters, 1982, 89, 228-233.	1.2	15
301	Ab initio molecular orbital studies of the structures and potential energy surfaces of the BeAlF ₅ and MgAlF ₅ complexes. Chemical Physics Letters, 1982, 86, 467-471.	1.2	9
302	A theoretical study on the dissociation reaction of dioxirane $\text{H}_2\text{CO}_2 \rightarrow \text{H}_2 + \text{CO}_2$. Chemical Physics Letters, 1982, 85, 262-265.	1.2	5
303	The additivity of polarization function and electron correlation effects in ab initio molecular-orbital calculations. Chemical Physics Letters, 1982, 89, 497-500.	1.2	73
304	Basis set dependence of protonation reactions of NH ₃ , OH ₂ , and SH ₂ . Chemical Physics Letters, 1982, 93, 540-544.	1.2	8
305	Anharmonic force fields from ab initio calculations. Journal of Molecular Structure, 1982, 79, 13-18.	1.8	2
306	The charge-charge flux-overlap model for the interpretation of atomic polar tensors and infrared intensities. Journal of Molecular Structure, 1982, 80, 297-308.	1.8	19
307	Structure and relative stabilities of isomers of C ₂ H ₂ N ⁺ : an ab initio molecular orbital study. Journal of Molecular Structure, 1982, 91, 313-323.	1.8	2
308	Coupled-cluster approach in electronic structure theory of molecules. Physics Reports, 1982, 90, 159-202.	10.3	49
309	Ab initio calculations as first step towards the structure of free radicals. I. geometries and energies of the ethyl analogs NH ₂ CH ₃ ⁺ and CH ₂ NH ₃ ⁺ . Chemical Physics, 1982, 73, 145-153.	0.9	6

#	ARTICLE	IF	CITATIONS
310	Non-adiabatic interactions in the symmetric ring opening process of dioxirane. <i>Chemical Physics</i> , 1982, 66, 209-215.	0.9	8
311	Energetics and possible mechanisms of ion-beam protein tritiation based on ab initio potential surfaces. <i>Biophysical Chemistry</i> , 1982, 16, 247-251.	1.5	6
312	Bridged and linear dithioacetylenes - Two minima on the potential energy surface?. <i>Tetrahedron Letters</i> , 1982, 23, 4999-5002.	0.7	13
313	Comparative theoretical study of the dissociation process of the isoelectronic molecules BH ₃ CO, CH ₂ CO, HNCO, CO ₂ and BH ₃ N ₂ , CH ₂ N ₂ , HN ₃ , N ₂ O. <i>Theoretica Chimica Acta</i> , 1982, 61, 59-72.	0.9	27
314	Theoretical investigation of the electrophilic attack. IX. Ab initio study of the C ₂ H ₄ ⋅HF molecular complex. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 631-637.	1.0	8
315	Electrostatic potential around halogenated anesthetics. Acidic hydrogen; chlorine vs. fluorine. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 691-707.	1.0	14
316	Nonempirical calculations of the affinity of the acetylene molecule for the lithium cation. <i>Journal of Structural Chemistry</i> , 1983, 24, 474-475.	0.3	0
317	Ab-initio SOS-CI calculations of magnetic properties of the first- and second-row hydrides. <i>Theoretica Chimica Acta</i> , 1983, 63, 35-41.	0.9	29
318	Ring functions, as polarization functions, for ab initio calculations on small rings: Dioxirane. <i>Theoretica Chimica Acta</i> , 1983, 64, 57-64.	0.9	10
319	Restricted Hartree-Fock approximation. II. Computational aspects of the direct minimization procedure. <i>Journal of Computational Chemistry</i> , 1983, 4, 41-47.	1.5	20
320	Uracil-4-Hydroxyuracil tautomerism revisited. <i>Journal of Computational Chemistry</i> , 1983, 4, 345-349.	1.5	12
321	A water-mediated tautomerism mechanism in formamide and amidine. An ab initio study. <i>Journal of Computational Chemistry</i> , 1983, 4, 419-427.	1.5	45
322	Ab initio study of catalyzed and uncatalyzed amide bond formation as a model for peptide bond formation: Ammonia-Glycine reactions. <i>Journal of Computational Chemistry</i> , 1983, 4, 449-460.	1.5	11
323	An ab initio study of the formation and structure of H ₂ CN+⋅N ₂ . <i>Chemical Physics Letters</i> , 1983, 97, 503-507.	1.2	8
324	The vinyloxonium cation (CH ₂ CHOH ₂ ⁺). <i>Chemical Physics Letters</i> , 1983, 99, 107-111.	1.2	11
325	Localizability of dynamic electron correlation. <i>Chemical Physics Letters</i> , 1983, 100, 151-154.	1.2	743
326	Transition atomic basis set for the calculation of core-electron binding energies by a transition operator method. <i>Chemical Physics Letters</i> , 1983, 94, 383-387.	1.2	3
327	Microwave spectrum, dipole moment and ab initio molecular structure of 2-aminopropenenitrile (CH ₂ =C(NH ₂)CN). <i>Chemical Physics Letters</i> , 1983, 97, 135-140.	1.2	11

#	ARTICLE	IF	CITATIONS
328	Correlation and polarization effects in the thermochemical properties of small boron hydrides. Chemical Physics Letters, 1983, 103, 59-62.	1.2	20
329	Green's function ab initio study of the outer valence ionization energies of N ₂ H ₄ , P ₂ H ₄ , As ₂ H ₄ , PH ₂ NH ₂ , PF ₂ NH ₂ and AsH ₂ NH ₂ . Journal of Electron Spectroscopy and Related Phenomena, 1983, 32, 359-369.	0.8	5
331	Theoretical studies of C ₂ H ₄ O isomers. Journal of Molecular Structure, 1983, 92, 239-253.	1.8	9
332	Non-empirical calculations of magnetic properties by the SOS-CI perturbation theory according to Nakatsuji. Journal of Molecular Structure, 1983, 93, 201-206.	1.8	5
333	The reaction pathway for the hydration of ketenimine by water dimer. An Ab initio study. Journal of Molecular Structure, 1983, 93, 329-332.	1.8	3
334	The Ionization of Alkanes. Israel Journal of Chemistry, 1983, 23, 21-36.	1.0	92
335	Ab initio calculations of the potential surface for the 2A ₁ state of CH ₄ ⁺ . Computational and Theoretical Chemistry, 1983, 105, 31-36.	1.5	6
336	Electronic structure and hydrogen bonding of valence-ionized states of \hat{I}^2 -hydroxyacrolein. Computational and Theoretical Chemistry, 1983, 105, 135-142.	1.5	7
338	Structure and relative stabilities of isomers of C ₂ H ₂ N ⁺ : An ab initio molecular orbital study. Computational and Theoretical Chemistry, 1983, 91, 313-323.	1.5	17
339	Non-empirical calculations of magnetic properties by the SOS-CI perturbation theory according to Nakatsuji. Computational and Theoretical Chemistry, 1983, 93, 201-206.	1.5	10
340	The reaction pathway for the hydration of ketenimine by water dimer. An ab initio study.. Computational and Theoretical Chemistry, 1983, 93, 329-332.	1.5	9
341	A comparative ab initio study of the molecular structures and electronic properties of diboron trioxide O(BO) ₂ and dicyanoether O(CN) ₂ . Computational and Theoretical Chemistry, 1983, 104, 353-364.	1.5	28
342	Theoretical studies of C ₂ H ₄ O isomers. Computational and Theoretical Chemistry, 1983, 92, 239-253.	1.5	6
343	A systematic study of the convergence and additivity of correlation and basis set effects on the force constants of small molecules: HF, HCN, and NH ₃ . Journal of Chemical Physics, 1983, 79, 3382-3391.	1.2	105
344	An ab initio study of the reaction Be(3P) + H ₂ (1 \hat{I} g ⁺) $\hat{\rightarrow}$ BeH(2 \hat{I} g ⁺) + H(2S). Journal of Chemical Physics, 1983, 78, 4592-4596.	1.2	19
345	An economical technique for forcing convergence in conventional SCF methods. Journal of Chemical Physics, 1983, 79, 4407-4411.	1.2	20
346	Ab initio studies of weakly bound complexes between some nonpolar molecules and hydrogen fluoride. Journal of Chemical Physics, 1983, 78, 5733-5737.	1.2	29
347	Ab initio studies of the CO ₂ $\hat{\leftarrow}$ HF and N ₂ O $\hat{\leftarrow}$ HF complexes. Journal of Chemical Physics, 1983, 78, 5738-5740.	1.2	39

#	ARTICLE	IF	CITATIONS
348	Theoretical study of Jahn-Teller distortions in C ₆ H ₆ and C ₆ F ₆ . Journal of Chemical Physics, 1983, 79, 1387-1395.	1.2	92
349	On the basis set superposition error in potential surface investigations. I. Hydrogen-bonded complexes with standard basis set functions. Journal of Chemical Physics, 1983, 78, 4606-4611.	1.2	62
350	Chapter 11. Cu, Ag, Au; Zn, Cd, Hg. Annual Reports on the Progress of Chemistry Section A, 1983, 80, 275.	0.8	1
351	Rotational potential surface for alkanes: Basis set and electron correlation effects on the conformations of n-butane. Journal of Chemical Physics, 1984, 81, 1383-1388.	1.2	88
352	The electronic structure of alkali bihalide molecules MX ₂ . I. Ground states of LiF ₂ , NaF ₂ , LiCl ₂ , and NaCl ₂ systems. Journal of Chemical Physics, 1984, 80, 2618-2635.	1.2	14
353	An improved basis set for H ₂ O. Test on Rydberg excited states. Journal of Chemical Physics, 1984, 80, 1937-1942.	1.2	8
354	Basis set dependence of ab initio SCF elastic, Born, electron scattering cross sections for C ₂ H ₄ . Journal of Chemical Physics, 1984, 81, 1940-1942.	1.2	7
355	Diphosphene (HPPH) and phosphino-phosphinidene (H ₂ PP): An ab initio SCF and CI study of stability and electronic structure. Chemical Physics, 1984, 87, 23-29.	0.9	36
356	Theoretical study of the vertical electron affinity and ionization potentials of C ₃ . Chemical Physics, 1984, 89, 245-256.	0.9	34
357	Mechanism of keto-enol tautomerism of ionized vinyl alcohol versus acetaldehyde and their dissociation to C ₂ H ₃ O ⁺ and H ⁺ . An ab initio molecular orbital study. International Journal of Mass Spectrometry and Ion Processes, 1984, 59, 21-37.	1.9	60
358	The ground and excited states of hydrogen sulfide, methanethiol, and hydrogen selenide. Journal of Molecular Spectroscopy, 1984, 105, 438-452.	0.4	44
359	Theoretical study of the conformational dependence of nitrogen and phosphorus magnetic-shielding tensors in hydrazine and diphosphine. Journal of Magnetic Resonance, 1984, 58, 311-314.	0.5	2
360	Theoretical and experimental studies of the charge density in urea. Acta Crystallographica Section B: Structural Science, 1984, 40, 398-404.	1.8	52
361	The nature of the C-C ring-opened form of the ethylene oxide radical cation. Chemical Physics Letters, 1984, 104, 198-202.	1.2	23
362	An ab initio MO study of some aspects of the selective catalytic oxidation of propene to acrolein. Chemical Physics Letters, 1984, 104, 203-209.	1.2	14
363	An ab initio MO study on the thiol-disulphide exchange reaction. Chemical Physics Letters, 1984, 112, 129-132.	1.2	15
364	Linear and bifurcated hydronium ion complexes with electron donors: An AB initio study. Chemical Physics Letters, 1984, 108, 602-608.	1.2	7
365	Structure and harmonic vibrational frequencies of the carbon suboxide molecule using analytic derivative methods. Chemical Physics Letters, 1984, 108, 347-352.	1.2	29

#	ARTICLE	IF	CITATIONS
366	An improved value of the electric quadrupole moment of the ^{14}N nucleus: An ab initio CI calculation on NH_3 . <i>Chemical Physics Letters</i> , 1984, 107, 117-120.	1.2	27
367	Structures and relative energies of gas phase $[\text{C}_3\text{H}_7\text{O}]^+$ ions. <i>Organic Mass Spectrometry</i> , 1984, 19, 385-393.	1.3	32
368	Ab initio calculations on the effect of different basis sets and electron correlation on the transition state for the reactions $\text{HNC} + \text{HCN}$ and $\text{BCN} + \text{BNC}$. <i>Journal of Computational Chemistry</i> , 1984, 5, 1-10.	1.5	19
369	Critical comparison of theoretical and spectroscopic methyl-C-H bond length difference in acetyl compounds, $\text{CH}_3\text{C}(\text{O})\text{X}$. <i>Journal of Computational Chemistry</i> , 1984, 5, 517-522.	1.5	15
370	Substituent effects in second-row molecules: Basis set performance in calculations of normal valency phosphorus and sulfur compounds. <i>Journal of Computational Chemistry</i> , 1984, 5, 612-628.	1.5	32
371	Theoretical conformational studies on unsaturated aldehydes, I. Alkenals. <i>Journal of Biological Physics</i> , 1984, 12, 52-62.	0.7	1
372	Structure moléculaire des dérivés nitro aromatiques. III. Effet de la correction électronique sur le calcul des états singulets à l'équilibre et hors d'équilibre, le long de la liaison $\text{C}=\text{NO}_2$; analyse de populations de charges sur le groupe $\text{C}=\text{NO}_2$. <i>Propellants, Explosives, Pyrotechnics</i> , 1984, 9, 82-90.	1.0	5
373	Ab initio calculations of guanidinium-carboxylate interaction. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 91-99.	1.0	27
374	Ab initio studies of negative ion-molecule(s) clusters present in the atmosphere. II. $\text{OH}^-(\text{H}_2\text{O})_n$ for $n = 0, 2, 3, 4$. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 223-230.	1.0	25
375	Ab initio studies of negative ion-molecule(s) clusters present in the atmosphere. III. $\text{OH}^-(\text{CO}_2)_n$ for $n = 1, 2$. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 231-236.	1.0	2
376	Theoretical study of hydrogen abstraction reactions $\text{CH}_4 + \text{R} \rightarrow \text{CH}_3 + \text{HR}$, geometrical, energetical and kinetical aspects. <i>Theoretica Chimica Acta</i> , 1984, 65, 109-125.	0.9	53
377	Hexacoordinated structures of elements of the second period. <i>Journal of Structural Chemistry</i> , 1984, 24, 847-852.	0.3	0
378	On the barrier and nature of [1.2]-hydrogen migrations in HCN/HNC and their cation radicals. <i>Die Naturwissenschaften</i> , 1984, 71, 473-474.	0.6	20
379	A molecular orbital study of the rotation about the C-C bond in 1,3-butadiene. <i>Theoretica Chimica Acta</i> , 1984, 64, 293-311.	0.9	53
380	Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. <i>Journal of Chemical Physics</i> , 1984, 80, 3265-3269.	1.2	7,488
381	An ab initio SCF study of molecular structures and electronic properties of N-nitrosoamines, $\text{RR}'\text{N}-\text{N}(\text{O})\text{R}''$ ($\text{R}' \rightarrow \text{H}, \text{CH}_3$). <i>Computational and Theoretical Chemistry</i> , 1984, 109, 339-350.	1.5	7
382	Comment on "N ₆ an open-chain molecule?". <i>Computational and Theoretical Chemistry</i> , 1984, 109, 391.	1.5	17
383	Information theory and basis set quality: Automatic classification and systematic improvement of approximate molecular wavefunctions; A study on OH radical. <i>Computational and Theoretical Chemistry</i> , 1984, 110, 107-122.	1.5	14

#	ARTICLE	IF	CITATIONS
384	A molecular orbital study of ethylene and the all-trans conjugated polyenes: C ₄ H ₆ , C ₆ H ₈ , C ₈ H ₁₀ and C ₁₀ H ₁₂ . Computational and Theoretical Chemistry, 1984, 109, 1-16.	1.5	42
385	Quantum chemical investigations of charge transfer interactions in relation to the electronic theory of cancer. Computational and Theoretical Chemistry, 1984, 109, 73-86.	1.5	0
386	Ab initio study of rotational isomerism in 1,3-butadiene. Effect of geometry optimization and basis set size on the barriers to rotation and on the stable rotamers. Computational and Theoretical Chemistry, 1984, 109, 103-126.	1.5	43
387	Conformational analysis of allyl alcohol. An ab initio molecular orbital study. Computational and Theoretical Chemistry, 1984, 108, 229-239.	1.5	14
388	Ab initio hartree-fock investigation of the interaction between hydrogen monolayers and beryllium slabs. Surface Science, 1984, 138, 51-74.	0.8	20
389	First and second derivatives of two electron integrals over Cartesian Gaussians using Rys polynomials. Journal of Chemical Physics, 1984, 80, 1976-1981.	1.2	119
390	Concerning Bent Structures of Cumulenones. Bulletin of the Chemical Society of Japan, 1985, 58, 3025-3026.	2.0	2
391	Application of the electron gas model to the calculation of the geometries of van der Waals complexes. Molecular Physics, 1985, 54, 1437-1452.	0.8	1
392	Ab initio studies of F ₂ (H ₂ O) _n and Cl ₂ (H ₂ O) _n clusters for n = 1, 2. International Journal of Quantum Chemistry, 1985, 27, 281-292.	1.0	18
393	Molecular and electronic structure of the dehydroalanine derivatives. Tetrahedron, 1985, 41, 2015-2018.	1.0	17
394	Substituent effects in second row molecules. Tetrahedron, 1985, 41, 2939-2943.	1.0	10
395	A theoretical study of the force field for carbon trioxide. Chemical Physics, 1985, 95, 373-383.	0.9	26
396	An ab initio study of the ground and excited states of HPO. Chemical Physics, 1985, 98, 447-453.	0.9	12
397	Theoretical and experimental studies on the ground state potential energy surface of C ₂ H ₄ O dications. International Journal of Mass Spectrometry and Ion Processes, 1985, 63, 59-82.	1.9	23
398	Conformation analysis of isomers of imidoyl halides. Theoretical and Experimental Chemistry, 1985, 21, 146-151.	0.2	0
399	Ab initio calculations of potential energy surface for reaction of nucleophilic addition of H ⁺ ion to methylacetylene. Theoretical and Experimental Chemistry, 1985, 21, 290-296.	0.2	0
400	Molecular symmetry in ab initio calculations. II. Acta Physica Hungarica, 1985, 58, 227-232.	0.1	1
401	Theoretical studies of a lithiated mitomycin analog. Journal of Biological Physics, 1985, 13, 39-42.	0.7	2

#	ARTICLE	IF	CITATIONS
402	A Molecular orbital study of the rotation about the C _i -C bond in styrene. <i>Chemical Physics</i> , 1985, 93, 431-443.	0.9	56
403	Deuterium nuclear quadrupole hyperfine coupling in benzene-d ₁ observed by pulsed microwave fourier transform spectroscopy. <i>Chemical Physics Letters</i> , 1985, 115, 317-320.	1.2	27
404	The low-lying electronic states of OCIO and CIOO. <i>Chemical Physics Letters</i> , 1985, 116, 119-124.	1.2	16
405	Infrared intensities of amide modes in N-methylacetamide and poly(glycine I) from ab initio calculations of dipole moment derivatives of N-methylacetamide. <i>Journal of Chemical Physics</i> , 1985, 82, 1631-1641.	1.2	79
406	Calculation of NMR chemical shifts. VI. Gauge invariant and Hermitian condition. <i>Journal of Chemical Physics</i> , 1985, 83, 907-908.	1.2	14
407	Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules. <i>Journal of Chemical Physics</i> , 1985, 82, 2418-2426.	1.2	586
408	Physics of small metal clusters: Topology, magnetism, and electronic structure. <i>Physical Review B</i> , 1985, 32, 2058-2069.	1.1	157
409	Jahn-Teller conformational barriers. <i>Computational and Theoretical Chemistry</i> , 1985, 123, 203-210.	1.5	11
410	A theoretical study of relaxation and reconstruction of the (111) surface of diamond. <i>Surface Science</i> , 1985, 162, 169-174.	0.8	6
411	An ab initio MO study of allene episulfide, cyclopropanethione and thioxyallyl. <i>Computational and Theoretical Chemistry</i> , 1985, 124, 261-268.	1.5	13
412	Structures and relative stabilities of [C ₂ H ₆ N] ⁺ ions: A non-empirical and MNDO study. <i>Computational and Theoretical Chemistry</i> , 1985, 124, 319-324.	1.5	12
413	Ab initio studies of structural features not easily amenable to experiment. <i>Computational and Theoretical Chemistry</i> , 1985, 122, 67-74.	1.5	10
414	Pseudopotential ab initio study of allylcopper complex: Application to propene catalytic partial oxidation mechanism. <i>Computational and Theoretical Chemistry</i> , 1985, 121, 57-67.	1.5	5
415	The distortion of the ring in monosubstituted benzene derivatives: A molecular orbital study. <i>Computational and Theoretical Chemistry</i> , 1985, 122, 155-172.	1.5	82
416	The electronic structure of the monomers, dimers, a trimer, the oxides and the borane complexes of the lithiated ammonias. <i>Computational and Theoretical Chemistry</i> , 1985, 122, 189-204.	1.5	28
417	Gaussian basis sets for nitrogen; Properties of NH ₃ . <i>Computational and Theoretical Chemistry</i> , 1985, 122, 259-268.	1.5	3
418	Hydrogen bonding in salicylaldehyde: A molecular orbital study. <i>Computational and Theoretical Chemistry</i> , 1985, 133, 11-24.	1.5	22
419	Ab initio molecular orbital studies of fluorine dioxide, chlorine dioxide and their isomeric peroxy radical forms. <i>Computational and Theoretical Chemistry</i> , 1985, 133, 25-35.	1.5	9

#	ARTICLE	IF	CITATIONS
420	Theoretical calculations of the hyperfine coupling constants of organic radicals.. Computational and Theoretical Chemistry, 1985, 120, 383-386.	1.5	9
421	Natural bond orbital analysis of molecular interactions: Theoretical studies of binary complexes of HF, H ₂ O, NH ₃ , N ₂ , O ₂ , F ₂ , CO, and CO ₂ with HF, H ₂ O, and NH ₃ . Journal of Chemical Physics, 1986, 84, 5687-5705.	1.2	474
422	Extensive theoretical studies of the hydrogen-bonded complexes (H ₂ O) ₂ , (H ₂ O) ₂ H ⁺ , (HF) ₂ , (HF) ₂ H ⁺ , F ₂ H ⁺ , and (NH ₃) ₂ . Journal of Chemical Physics, 1986, 84, 2279-2289.	1.2	666
423	An ab initio investigation of possible intermediates in the reaction of the hydroxyl and hydroperoxyl radicals. Journal of Chemical Physics, 1986, 84, 5013-5024.	1.2	26
424	The force constants of benzene: Local many-body perturbation theory vs new experiment. Journal of Chemical Physics, 1986, 85, 1703-1704.	1.2	47
425	A quantum chemical study of the cyclic oxocarbon dianions C _n O _n ²⁻ (n = 3,4,5 and 6). Computational and Theoretical Chemistry, 1986, 137, 171-181.	1.5	20
426	The electronic structure of iminoborane, CH ₂ NBH ₂ and some of its derivatives. Computational and Theoretical Chemistry, 1986, 139, 47-62.	1.5	3
427	A molecular orbital study of the changes that accompany rotation of the HO group in phenol, and the barrier height. Computational and Theoretical Chemistry, 1986, 139, 63-74.	1.5	33
428	The electronic structure of CH ₂ NH, CH ₂ NLi and CH ₂ NBeH. Computational and Theoretical Chemistry, 1986, 137, 235-261.	1.5	12
429	The structure and bonding of the lithium metaborate (LiBO ₂) molecule. An ab initio study. Computational and Theoretical Chemistry, 1986, 136, 371-379.	1.5	22
430	Ab initio structures and vibrational analysis of two planar configurations of 1,3,5-hexatriene. Computational and Theoretical Chemistry, 1986, 148, 131-140.	1.5	29
431	A theoretical study of electronic structures and vibrational frequencies of deltic and squaric acids, C _n O _n H ₂ (n = 3 and 4). Computational and Theoretical Chemistry, 1986, 148, 163-174.	1.5	8
433	Basis Set Dependency of Molecular Electronic Structures. Bulletin of the Chemical Society of Japan, 1986, 59, 2729-2733.	2.0	8
434	A High-Resolution Solid-State ²³ Na NMR Study of Sodium Complexes with Solvents, Small Ligand Molecules, and Ionophores. ²³ Na Chemical Shifts as Means for Identification and Characterization of Ion-Ion, Ion-Solvent, and Ion-Ligand Interactions. Bulletin of the Chemical Society of Japan, 1986, 59, 1957-1966.	2.0	26
435	On the accuracy of higher-order force constants calculated at the self-consistent field level of theory. Chemical Physics Letters, 1986, 128, 182-188.	1.2	27
436	Atomic orbital deformation in bond formation: energy effects. Chemical Physics Letters, 1986, 131, 224-229.	1.2	6
437	Deceptive convergence in Møller-plestet perturbation energies. Chemical Physics Letters, 1986, 132, 16-22.	1.2	101
438	Effective-core-potential calculations of sulphur, selenium and tellurium dioxides and dihydrides. Chemical Physics Letters, 1986, 124, 26-30.	1.2	18

#	ARTICLE	IF	CITATIONS
439	Calculation of polarizability derivatives using analytic gradient methods. <i>Chemical Physics Letters</i> , 1986, 124, 376-381.	1.2	271
440	A theoretical study of weak complexes of acetylene: An energy decomposition analysis. <i>Chemical Physics Letters</i> , 1986, 124, 514-516.	1.2	10
441	An ab initio study of ammonia-hydrocarbon complexes. <i>Chemical Physics Letters</i> , 1986, 124, 517-521.	1.2	9
442	On the triplet states of HOCl and HClO. <i>Chemical Physics Letters</i> , 1986, 125, 451-453.	1.2	1
443	The interaction of O ₂ ⁺ with water. <i>Chemical Physics Letters</i> , 1986, 125, 454-458.	1.2	12
444	A minimal multiconfigurational technique. <i>Journal of Computational Chemistry</i> , 1986, 7, 201-207.	1.5	8
445	Substituent Effects on the Low-Lying Singlet and Triplet States of Methylene. <i>Journal of Computational Chemistry</i> , 1986, 7, 428-442.	1.5	15
446	An SCF and CI Study of the 1,3 Shift in the HX-CH ₂ -X-CH ₂ -YH Isoelectronic Series: X, Y=CH ₂ , NH, and O. <i>Journal of Computational Chemistry</i> , 1986, 7, 464-475.	1.5	37
447	On calculations of intermolecular potentials. <i>Journal of Computational Chemistry</i> , 1986, 7, 731-738.	1.5	3
448	A molecular orbital study of pyridine and the rotation about the C _i -C bond in 4-vinylpyridine. <i>Chemical Physics</i> , 1986, 105, 107-116.	0.9	5
449	Ab initio analysis of structure and vibrational spectrum of methyl nitrate. <i>Chemical Physics</i> , 1986, 106, 69-73.	0.9	19
450	A photoelectron spectroscopic and theoretical study of the halogen and hydrogen thiocyanates and isothiocyanates. <i>Chemical Physics</i> , 1986, 109, 289-300.	0.9	23
451	Ab initio quantum-chemical study of the unimolecular pyrolysis mechanisms of acetic acid. <i>Chemical Physics</i> , 1986, 110, 263-274.	0.9	31
452	On the interpretation of the electronic structure and ESR spectrum of CH ₄ ⁺ . <i>Journal of Molecular Structure</i> , 1986, 142, 323-326.	1.8	3
453	The molecular structures of cis- and trans-1,2-dichloroethene: a real-time gas electron diffraction and ab initio study. <i>Journal of Molecular Structure</i> , 1986, 145, 135-142.	1.8	23
454	Distonic radical cations. <i>Tetrahedron</i> , 1986, 42, 6225-6234.	1.0	170
455	Influence of alkyl substituents on the $\dot{\text{C}}\epsilon^*$ negative ion states of benzene and its derivatives. <i>Tetrahedron</i> , 1986, 42, 6269-6276.	1.0	3
456	Ab initio electronic structure calculations of the C ₂ H ₅ B potential energy surface: The stability of borirane. <i>Journal of Organometallic Chemistry</i> , 1986, 317, 1-10.	0.8	27

#	ARTICLE	IF	CITATIONS
457	A molecular orbital study of nitrogen inversion in aniline with extensive geometry optimization. <i>Theoretica Chimica Acta</i> , 1986, 69, 235-245.	0.9	53
458	An ab initio CI study on the rotational barrier of the allyl anion. <i>Theoretica Chimica Acta</i> , 1986, 69, 101-106.	0.9	5
459	An ab initio MO study on the disulfide bond: properties concerning the characteristic S-S dihedral angle. <i>Theoretica Chimica Acta</i> , 1986, 70, 73-80.	0.9	37
460	Energetics of proton transfer between carbon atoms (H3CH ? CH3)?. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 285-292.	1.0	23
461	Bond critical points in the electronic structures of binary hydrides. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 959-973.	1.0	8
462	An ab initio study of intermolecular hydrogen bonding between small peptide fragments. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 1241-1251.	1.0	38
463	On the role of symmetry in the ab initio hartree-fock linear-combination-of-atomic-orbitals treatment of periodic systems. <i>International Journal of Quantum Chemistry</i> , 1986, 29, 1755-1774.	1.0	47
464	Fluorine nonbonded potential parameters derived from crystalline perfluorocarbons. <i>Acta Crystallographica Section B: Structural Science</i> , 1986, 42, 286-295.	1.8	117
465	Nonempirical cluster-model study of the chemisorption of atomic hydrogen on the (111) surface of diamondlike crystals. <i>Physical Review B</i> , 1986, 34, 7203-7208.	1.1	24
466	The second hyperpolarizability of HCl and the effect of basis set variation on this property in hydrogen fluoride by fully coupled Hartree-Fock perturbation theory with a method for circumventing the transformation of two-electron integrals. An ab initio study. <i>Journal of Chemical Physics</i> , 1986, 85, 2831-2835.	1.2	10
467	Improved counterpoise corrections for the ab initio calculation of hydrogen bonding interactions. <i>Journal of Chemical Physics</i> , 1986, 84, 2720-2725.	1.2	72
468	Centrifugal distortions in molecules: An ab initio approach. <i>Journal of Chemical Physics</i> , 1986, 84, 4196-4204.	1.2	12
469	Infrared spectra of HF complexes with methane, silane, and germane. <i>Journal of Chemical Physics</i> , 1987, 86, 3765-3772.	1.2	24
470	ESR and ab initio theoretical studies of the cation radicals $14N^{+4}$ and $15N^{+4}$: The trapping of ion-neutral reaction products in neon matrices at 4 K. <i>Journal of Chemical Physics</i> , 1987, 87, 885-897.	1.2	90
471	Vertical and adiabatic ionization energies of NH_4^+ isomers via electron propagator theory and many body perturbation theory calculations with large basis sets. <i>Journal of Chemical Physics</i> , 1987, 87, 3557-3562.	1.2	42
472	Ab initio calculation of harmonic force fields and vibrational spectra for the methyl, silyl, germyl, and stannyl halides. <i>Journal of Chemical Physics</i> , 1987, 86, 923-936.	1.2	93
473	Photodissociation of $(CO)_2$: Theoretical studies of ground $2B_u$ and excited $2B_g$ potential energy surfaces. <i>Journal of Chemical Physics</i> , 1987, 87, 392-410.	1.2	34
474	Coupled torsional and bending motions in cis methyl vinyl ether. <i>Journal of Chemical Physics</i> , 1987, 86, 1848-1857.	1.2	20

#	ARTICLE	IF	CITATIONS
475	An Ab Initio Molecular Orbital Study of Lithiopyridines. Bulletin of the Chemical Society of Japan, 1987, 60, 3785-3786.	2.0	4
476	A molecular orbital study of 2-,3- and 4-fluoropyridine. Computational and Theoretical Chemistry, 1987, 152, 191-199.	1.5	4
477	A molecular orbit study of the barrier height in benzaldehyde, and the changes in geometry which accompany the rotation of the formyl group. Computational and Theoretical Chemistry, 1987, 152, 201-212.	1.5	34
478	Phosphinodifluorophosphine (H ₂ PPF ₂): Is there a stable gauche conformer? An ab-initio study. Computational and Theoretical Chemistry, 1987, 153, 85-91.	1.5	0
479	Structures, relative stabilities and barriers to internal rotation of isomeric monothioformic acids. Computational and Theoretical Chemistry, 1987, 151, 141-147.	1.5	11
480	Hydrogen bonding in 2-fluorophenol, and rotation about the C—O bond: A molecular orbital study. Computational and Theoretical Chemistry, 1987, 152, 35-53.	1.5	7
481	The electronic structure of CH ₂ NCH ₃ , CH ₂ NNH ₂ , CH ₂ NOH and CH ₂ NF. Computational and Theoretical Chemistry, 1987, 149, 369-389.	1.5	21
482	Infrared spectra and UHF SCF calculations of HF complexes with NO, (NO) ₂ , and NO ₂ . Journal of Chemical Physics, 1987, 86, 6027-6033.	1.2	26
483	Solution of the Hartree-Fock equations for polyatomic molecules by a pseudospectral method. Journal of Chemical Physics, 1987, 86, 3522-3531.	1.2	142
484	Theoretical study of reaction mechanisms for the ketonization of vinyl alcohol in gas phase and aqueous solution. Theoretica Chimica Acta, 1987, 72, 175-195.	0.9	56
485	On the computational realization of planar tetracoordinate carbon. Tetrahedron, 1987, 43, 1019-1026.	1.0	9
486	Hydrated carbonium ions as possible nitrosamine metabolites: An ab initio study. International Journal of Quantum Chemistry, 1987, 32, 123-131.	1.0	2
487	The effect of full and limited counterpoise corrections with different basis sets on the energy and the equilibrium distance of hydrogen bonded dimers. International Journal of Quantum Chemistry, 1987, 32, 207-226.	1.0	44
488	The decomposition of the SCF interaction energy in hydrogen bonded dimers corrected for basis set superposition errors: An examination of the basis set dependence. International Journal of Quantum Chemistry, 1987, 32, 227-248.	1.0	31
489	Scattering of fast electrons and X-rays from CO ₂ molecules. International Journal of Quantum Chemistry, 1987, 32, 217-227.	1.0	6
490	Ab initio calculations on H + C ₂ H ₂ → C ₂ H ₃ using unrestricted Møller-Plesset perturbation theory with spin projection. International Journal of Quantum Chemistry, 1987, 32, 267-282.	1.0	17
491	Centrifugal distortions in molecules: An ab initio approach with application to water. International Journal of Quantum Chemistry, 1987, 32, 407-415.	1.0	7
492	Applying electron propagator theory to electron affinities. International Journal of Quantum Chemistry, 1987, 32, 469-473.	1.0	10

#	ARTICLE	IF	CITATIONS
493	Practical considerations in calculations of the proton transfer in a model active site of papain. International Journal of Quantum Chemistry, 1987, 32, 211-219.	1.0	9
494	A study of the additivity of interactions in cation-water systems. Chemical Physics Letters, 1987, 137, 229-232.	1.2	69
495	The low-lying electronic states of H ₂ CN ⁺ : a preliminary ab initio study. Chemical Physics Letters, 1987, 137, 482-486.	1.2	1
496	A rationalization of unusually late transition structures for dication fragmentations. Chemical Physics Letters, 1987, 136, 294-298.	1.2	40
497	The structure of the C ₂ H ₂ +4 dication. Chemical Physics Letters, 1987, 136, 299-302.	1.2	9
498	Average dipole polarizabilities from the unsold approximation and ab initio data. Chemical Physics Letters, 1987, 136, 575-582.	1.2	11
499	Calculations on the vertical and adiabatic ionization energies of (H ₂ S) ₂ . Chemical Physics Letters, 1987, 134, 366-370.	1.2	9
500	The ionization of ethylene oxide. Chemical Physics Letters, 1987, 135, 78-83.	1.2	38
501	Bond orders and valencies from ab initio wavefunctions: Application to prototypical molecules and to the characterization of solitons in polyenes. Chemical Physics Letters, 1987, 142, 59-66.	1.2	59
502	Mechanism of the isomerization of azirinylidene to ketenimine. Chemical Physics Letters, 1987, 142, 92-95.	1.2	6
503	Polarization counterpoise corrections to correlated hydrogen bond interaction energies. Journal of Computational Chemistry, 1987, 8, 81-83.	1.5	17
504	Centrifugal distortions in molecules: An ab initio approach with application to ozone. Journal of Computational Chemistry, 1987, 8, 307-312.	1.5	9
505	Refined ab initio 6-31G split-valence basis set optimization of the molecular structures of biphenyl in twisted, planar, and perpendicular conformations. Journal of Computational Chemistry, 1987, 8, 1057-1065.	1.5	60
506	Cooperative effects in extended hydrogen bonded systems involving O-H groups. Ab initio studies of the cyclic S ₄ water tetramer. Journal of Computational Chemistry, 1987, 8, 1090-1098.	1.5	70
507	An evaluation of the performance of diffuse function-augmented basis sets for second row elements, Na-Cl. Journal of Computational Chemistry, 1987, 8, 1109-1116.	1.5	203
508	A high-precision Ab initio determination of the equilibrium geometry and force field of HOC ⁺ . Journal of Molecular Spectroscopy, 1987, 121, 440-449.	0.4	11
509	Ab initio structures and vibrational analysis of the isoprene conformers. Journal of Molecular Structure, 1987, 160, 337-346.	1.8	29
510	The analytic evaluation of second-order Møller-plestet (MP2) dipole moment derivatives. Chemical Physics, 1987, 114, 9-20.	0.9	79

#	ARTICLE	IF	CITATIONS
511	X-ray crystallographic and solution studies of the pentamethyldiethylenetriamine and tetramethylethylenediamine adducts of lithium diphenylphosphide. <i>Polyhedron</i> , 1987, 6, 987-993.	1.0	45
512	Structural and energetic parameters of Ca ²⁺ binding to peptides and proteins. <i>Biopolymers</i> , 1988, 27, 1865-1886.	1.2	27
513	Analytical second derivatives for effective core potentials. <i>Chemical Physics Letters</i> , 1988, 153, 76-81.	1.2	31
514	Electronic structure of phenyl cation by MC SCF ab initio calculations. <i>Chemical Physics Letters</i> , 1988, 153, 309-312.	1.2	17
515	Molecular orbital analysis of the XPS spectrum of a fluorine containing polyimide: PMDA- <i>h</i> BDAF. <i>Journal of Polymer Science Part A</i> , 1988, 26, 1199-1205.	2.5	7
516	The complexes of phenyl acetylene with HF, H ₂ O, and NH ₃ : An ab initio study. <i>International Journal of Quantum Chemistry</i> , 1988, 33, 69-76.	1.0	7
517	The nonplanarity of n-doped polyenes and of carbanions with alkali metal counterions. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 51-57.	1.0	4
518	Ab initio electronic structure theory for a cluster model of La _{2-x} Sr _x CuO ₄ . <i>International Journal of Quantum Chemistry</i> , 1988, 34, 237-244.	1.0	23
519	Ab initio mo studies of the decomposition of energetic materials. I. Hydrogen transfer in tnt and in model systems. <i>Chemical Physics</i> , 1988, 124, 39-46.	0.9	16
520	Theoretical ab initio study of the vinylcarbene-CuO complex: application to last step of the propylene partial oxidation mechanism on Cu ₂ O. <i>Journal of Molecular Catalysis</i> , 1988, 44, 323-336.	1.2	1
521	Nonempirical cluster model study of the on-top chemisorption of fluorine and chlorine on C(111) surface. <i>Solid State Communications</i> , 1988, 65, 945-947.	0.9	1
522	An ab initio study of cis/trans isomerization in the XONO systems (X \rightarrow F, Cl). <i>Inorganica Chimica Acta</i> , 1988, 149, 95-99.	1.2	9
523	The anharmonic force fields of silyl fluoride and silyl chloride. <i>Journal of Molecular Spectroscopy</i> , 1988, 132, 193-206.	0.4	39
524	Isolation, characterisation, and solution structures of the bis(pyridine) complex of the n-butyllithium-pyridine adduct, Bun(C ₅ H ₅ N)Li \cdot 2C ₅ H ₅ N, its mode of decomposition, and ab initio calculations on model systems. <i>Journal of Organometallic Chemistry</i> , 1988, 350, 191-205.	0.8	27
525	Ab initio calculations on ring-shaped silica clusters. <i>Catalysis Letters</i> , 1988, 1, 147-154.	1.4	22
526	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. <i>Journal of Chemical Physics</i> , 1988, 88, 5252-5254.	1.2	26
527	Electronic structure of LiBeH ₃ . <i>Physical Review B</i> , 1988, 38, 2380-2387.	1.1	24
528	Thermochemical stabilities and vibrational spectra of isomers of the chlorine oxide dimer. <i>Geophysical Research Letters</i> , 1988, 15, 883-886.	1.5	40

#	ARTICLE	IF	CITATIONS
529	The nonplanarity of the ring and displacement of the substituent group in the orthogonal conformers of toluene, ethylbenzene, styrene and nitrosobenzene: A molecular orbital study. Computational and Theoretical Chemistry, 1988, 180, 37-43.	1.5	14
530	The theoretical study of the heats of formation of organic compounds containing the substituents CH ₃ , CF ₃ , NH ₂ , NF ₂ , NO ₂ , OH and F. Computational and Theoretical Chemistry, 1988, 164, 249-274.	1.5	57
531	Ab initio calculations of amidosulfurous acid, H ₂ N=S ₂ O ₂ H. Computational and Theoretical Chemistry, 1988, 164, 335-342.	1.5	3
532	Analysis of the geometry of the hydroxymethyl radical by the α -different hybrids for different spins α -natural bond orbital procedure. Computational and Theoretical Chemistry, 1988, 169, 41-62.	1.5	1,905
533	Additional standard bond lengths for use in ab initio molecular orbital calculations of neutral species. Computational and Theoretical Chemistry, 1988, 168, 119-124.	1.5	1
534	A preliminary ab initio study of rearrangements in C ₂ B ₃ H ₅ . Computational and Theoretical Chemistry, 1988, 168, 191-203.	1.5	9
535	Reliability of AM1 in conformational analysis of unionized amino acids. Computational and Theoretical Chemistry, 1988, 168, 227-234.	1.5	12
536	Ab initio studies of β -aminobutyric acid (GABA), β -aminobutyric acid imine (GABA imine) and aminoxyacetic acid (AOAA). Computational and Theoretical Chemistry, 1988, 168, 323-333.	1.5	6
537	Dynamics of singlet biradicals. Application of ab initio variational transition state theory to the fragmentation of tetramethylene. Computational and Theoretical Chemistry, 1988, 163, 331-341.	1.5	17
538	Rotational barriers of some CH ₂ X radicalar compounds. Computational and Theoretical Chemistry, 1988, 166, 267-277.	1.5	6
539	The electronic structure of some beryllium amides. Computational and Theoretical Chemistry, 1988, 165, 65-86.	1.5	1
540	Some remarks on nonorthogonal orbitals in quantum chemistry. Computational and Theoretical Chemistry, 1988, 165, 189-202.	1.5	70
541	Extended gaussian-type valence basis sets for calculations involving non-empirical core pseudopotentials. Molecular Physics, 1988, 65, 295-312.	0.8	182
542	Defects in doped polyacetylene: An ab initio infrared and Raman spectroscopy of solitons. Journal of Chemical Physics, 1988, 88, 2859-2860.	1.2	15
543	Ab initio and empirical approaches to the general harmonic force field of methylene chloride. Molecular Physics, 1988, 63, 647-654.	0.8	5
544	Ab initio study of charged polyenes as charge-carrier models in conducting polymers. Physical Review B, 1988, 37, 2520-2528.	1.1	45
545	On the necessity of basis functions for bending frequencies. Journal of Chemical Physics, 1988, 88, 3187-3195.	1.2	174
546	Correlation correction to the Hartree-Fock total energy of solids. II. Physica Scripta, 1988, 38, 194-198.	1.2	31

#	ARTICLE	IF	CITATIONS
547	Structure, vibrational spectra, and IR intensities of polyenes from ab initio SCF calculations. Journal of Chemical Physics, 1988, 88, 1003-1009.	1.2	71
548	Computer modeling of liquid propane using three-site potential models. Journal of Chemical Physics, 1988, 89, 3733-3741.	1.2	29
549	Comment on: Accuracy of ab initio C-H bond length differences and their correlation with isolated C-H stretching frequencies. Journal of Chemical Physics, 1988, 88, 7255-7256.	1.2	24
550	Calculation of the nuclear spin-spin coupling constants. V. Configuration interaction calculation of ^{13}C - and ^{15}N -electron contributions. Journal of Chemical Physics, 1988, 88, 7040-7042.	1.2	5
551	Ab initio calculations of static dipole polarizabilities using improved virtual orbitals and symmetry adapted polarization functions. Molecular Physics, 1988, 65, 925-944.	0.8	9
552	Basis Set Dependency of Energy Components in Hartree-Fock MO Theories. II. Conservability of Virial Ratio between Different Conformations. Bulletin of the Chemical Society of Japan, 1988, 61, 1837-1843.	2.0	4
553	An Ab Initio Molecular Orbital Study of Pyridyl Radicals. Bulletin of the Chemical Society of Japan, 1988, 61, 291-292.	2.0	18
554	Si-P-H complexes in crystal silicon: A theoretical study. Physical Review B, 1989, 39, 12630-12632.	1.1	34
555	Pathologic inversion of core orbitals in approximate Hartree-Fock calculations. Journal of Chemical Physics, 1989, 90, 7313-7316.	1.2	0
556	Analytical gradients for unrestricted Hartree-Fock and second order Møller-Plesset perturbation theory with single spin annihilation. Journal of Chemical Physics, 1989, 90, 2363-2369.	1.2	52
557	Note on the vibrational spectrum of C4 and C5. Journal of Chemical Physics, 1989, 90, 3403-3405.	1.2	51
558	Ab initio study of boron, nitrogen, and boron-nitrogen clusters. I. Isomers and thermochemistry of B3, B2N, BN2, and N3. Journal of Chemical Physics, 1989, 90, 6469-6485.	1.2	120
559	Ionization energies of OH ⁻ 3 isomers. Journal of Chemical Physics, 1989, 91, 7024-7029.	1.2	29
560	Ab initio molecular orbital study on the methylation affinity of N2. Journal of Chemical Physics, 1989, 91, 1376-1377.	1.2	0
561	Interaction energy decomposition and basis set superposition error analysis in hydrogen abstraction from the nitroxyl molecule by atomic hydrogen. Computational and Theoretical Chemistry, 1989, 184, 373-380.	1.5	2
562	An AB initio structural investigation of 1,3-butadiene, isoprene and 2,3-dimethyl-1,3-butadiene rotamers. Computational and Theoretical Chemistry, 1989, 187, 69-82.	1.5	39
563	AB initio force constants: a cautionary tale concerning nitrogen oxides. Computational and Theoretical Chemistry, 1989, 187, 337-357.	1.5	6
564	Ho and hs substituent effect on alkyl radicals: an ab-initio molecular orbital study. Computational and Theoretical Chemistry, 1989, 186, 305-319.	1.5	15

#	ARTICLE	IF	CITATIONS
565	Ab initio SCF and CI study of the cyclopropane/trimethylene radical cations. <i>Chemical Physics</i> , 1989, 139, 293-299.	0.9	19
566	A theoretical study of the dynamics of the reaction $C(3P)+NO(X^2\hat{\sigma}^+)+O(3P)$. <i>Chemical Physics</i> , 1989, 131, 375-390.	0.9	48
567	A computation procedure for the dispersion component of the interaction energy in continuum solute-solvent models. <i>Chemical Physics</i> , 1989, 138, 327-336.	0.9	22
568	Torsional transitions and barrier to internal rotation of 1,2-butadiene. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1989, 45, 479-485.	0.1	5
569	Anharmonic force fields from analytic second derivatives: Method and application to methyl bromide. <i>Chemical Physics Letters</i> , 1989, 157, 367-373.	1.2	333
570	A theoretical study of the $C_3H_4^+$ potential energy surface. <i>Journal of Molecular Structure</i> , 1989, 198, 391-402.	1.8	10
571	Torsional transitions and barrier to internal rotation of 1-butyne. <i>Journal of Molecular Structure</i> , 1989, 196, 101-111.	1.8	23
572	Dilithiation of N,N -diphenylthiourea, $PhNHC(\hat{\sigma}^+S)NPh$, in HMPA: the unexpected structure of the Organometallic Chemistry, 1989, 362, C1-C4.	0.8	12
573	Stationary points on the potential energy surface of O_2^+HF and $O_2^+H_2O$. <i>Journal of Computational Chemistry</i> , 1989, 10, 55-62.	1.5	11
574	The density integration approach to populations. A critical comparison of projection populations to populations defined by the theory of atoms in molecules. <i>Journal of Computational Chemistry</i> , 1989, 10, 118-135.	1.5	15
575	Combined bond polarization function basis sets for accurate ab initio calculation of the dissociation energies of AH_n molecules ($A=Li$ to F). <i>Journal of Computational Chemistry</i> , 1989, 10, 152-162.	1.5	25
576	Basis set dependence, precision, and accuracy of fullab initio gradient optimizations of molecular structures of nonstrained hydrocarbons. I. CC bond lengths. <i>Journal of Computational Chemistry</i> , 1989, 10, 329-343.	1.5	24
577	Ab initio study of the proton affinity of a number of ortho-substituted pyridines. <i>Journal of Computational Chemistry</i> , 1989, 10, 346-357.	1.5	21
578	Combined bond-polarization basis sets for accurate determination of dissociation energies. II. Basis set superposition error as a function of the parent basis set. <i>Journal of Computational Chemistry</i> , 1989, 10, 875-886.	1.5	30
579	A theoretical study of solvation energies of FCH_2COO^+ , FCH_2COOH , and F_2CHCOO^+ . <i>Journal of Computational Chemistry</i> , 1989, 10, 1031-1037.	1.5	9
580	The CH_2Cl torsional barrier of benzyl chloride studied by gas-phase absorption spectroscopy and ab initio calculations. <i>Chemical Physics Letters</i> , 1989, 157, 31-34.	1.2	9
581	On the use of mixed basis sets to compute accurate molecular electrostatic potentials. <i>Chemical Physics Letters</i> , 1989, 160, 305-310.	1.2	17
582	Structures and stabilities of $[C_3H_2]^+ \hat{\sigma}^+$ and $[C_3H_2]_2^+$ ions. <i>Organic Mass Spectrometry</i> , 1989, 24, 539-545.	1.3	10

#	ARTICLE	IF	CITATIONS
583	Ab initio SCF and MP2 calculations of the frequency dependence of the polarizability of cyclohexane. <i>Chemical Physics Letters</i> , 1989, 161, 285-290.	1.2	15
584	Silicon-nitrogen multiple bonding: Theoretical study of silanitriles and silaisonitriles. <i>Chemical Physics Letters</i> , 1989, 159, 21-26.	1.2	9
585	Solute-solvent interactions. a simple procedure for constructing the solvent cavity for retaining a molecular solute. <i>Chemical Physics</i> , 1989, 129, 439-450.	0.9	57
586	Structure and stability of SiB ⁿ⁺ and CB ⁿ⁺ (n = 1-4). <i>Surface Science Letters</i> , 1989, 223, L913-L919.	0.1	1
587	Theoretical studies on the stabilities of 1,2- and 1,3-isomers of cyclic H ₄ A ₂ X ₂ (A=C, Si; X=O,S,CH ₂): the anomeric effect at silicon. <i>Journal of Molecular Structure</i> , 1989, 194, 183-190.	1.8	14
588	Perturbative corrections to basis incompleteness in molecular SCF calculations. <i>Theoretica Chimica Acta</i> , 1989, 75, 129-141.	0.9	0
589	ESCA studies of carbanionic compounds: Butyllithium in heptane solution and dibutylmercury in the gas phase. <i>Journal of Physical Organic Chemistry</i> , 1989, 2, 417-424.	0.9	8
590	A theoretical study of the effect of primary and secondary structure elements on the proton transfer in papain. <i>International Journal of Quantum Chemistry</i> , 1989, 35, 241-252.	1.0	24
591	Theoretical calculation of tautomer equilibria in solution: 4-(5-)methylimidazole. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 1989, 993, 134-136.	1.1	33
592	Through-space interactions in spirenes. <i>Computational and Theoretical Chemistry</i> , 1989, 183, 257-269.	1.5	7
593	Ab initio calculations of nitrogen containing free radicals: The geometrical parameters of HFN ^{•-} , H ₂ CN ^{•-} and HFCN ^{•-} radicals. <i>Computational and Theoretical Chemistry</i> , 1989, 183, 291-300.	1.5	2
594	Ab initio study of neutral O ₂ , SO, S ₂ , C ₂ H ₂ and their mono- and dications. <i>Computational and Theoretical Chemistry</i> , 1989, 183, 103-119.	1.5	28
595	Mechanistic aspects of biological redox reactions involving NADH 1: Ab initio quantum chemical structures of the 1-methyl-nicotinamide and 1-methyl-dihydronicotinamide coenzyme analogues. <i>Computational and Theoretical Chemistry</i> , 1989, 183, 161-174.	1.5	13
596	Ab initio investigations on the energetics of starting reactions during the thermal conversion of acetylene. <i>Computational and Theoretical Chemistry</i> , 1989, 184, 69-78.	1.5	8
597	Structure and stability of SiB ⁿ⁺ AND CB ⁿ⁺ (n = 1-4). <i>Surface Science</i> , 1989, 223, L913-L919.	0.8	11
598	Quasimolecule formation in the calculation of electronic stopping cross sections with the Firsov model. <i>Physical Review A</i> , 1989, 39, 5532-5538.	1.0	0
599	Some Ab initio MO studies relevant to the thermal decomposition of TNT. <i>Journal of Energetic Materials</i> , 1989, 7, 345-354.	1.0	0
600	On the Intrinsic Difference between Topological Aromaticity and So-Called Quasi-Aromaticity. <i>Bulletin of the Chemical Society of Japan</i> , 1989, 62, 2798-2801.	2.0	10

#	ARTICLE	IF	CITATIONS
601	An Ab Initio Molecular Orbital Study on the Ene Reaction of Methyl Acrylate with Propene. Bulletin of the Chemical Society of Japan, 1990, 63, 2246-2251.	2.0	10
602	Parity-Violating Energy Shift of Glycine, Alanine, and Serine in the Zwitterionic Forms: Calculation Using HFO-NG Basis Sets. Bulletin of the Chemical Society of Japan, 1990, 63, 2751-2754.	2.0	25
603	Electron density distribution around hydrogen atoms in linear molecules. Acta Crystallographica Section B: Structural Science, 1990, 46, 23-27.	1.8	5
604	Bonding-deformation and superposition effects in the electron density of tetragonal nickel sulfate hexadeuterate NiSO ₄ .6D ₂ O. Acta Crystallographica Section B: Structural Science, 1990, 46, 27-39.	1.8	14
605	Anisotropy of van der Waals radii of atoms in molecules: alkali-metal and halogen atoms. Acta Crystallographica Section B: Structural Science, 1990, 46, 592-598.	1.8	11
606	Mechanisms of ring contraction, C-H insertion and 1,2-hydrogen migration of cyclobutylidene. Chinese Journal of Chemistry, 1990, 8, 102-109.	2.6	3
607	Effects of heteroatoms on 1,2-rearrangements of 3-membered ring carbenes. Chinese Journal of Chemistry, 1990, 8, 319-324.	2.6	0
608	Thermodynamic stability and reactivity of the antiaromatic heterocycle 1H-azirine. Theoretical and Experimental Chemistry, 1990, 25, 445-450.	0.2	4
609	Oxidative coupling of methane on MgO. ab initio UHF potential energy surface. Computational and Theoretical Chemistry, 1990, 208, 153-162.	1.5	21
610	The theoretical calculation of basicities: an homologous amine series. Computational and Theoretical Chemistry, 1990, 208, 205-221.	1.5	9
611	Ab initio calculation of gas-phase methyl radical formation over Mg ²⁺ and Li ⁺ adsorption model sites. Computational and Theoretical Chemistry, 1990, 210, 323-328.	1.5	13
612	A theoretical approach to the proton transfer between water molecules. Computational and Theoretical Chemistry, 1990, 209, 263-272.	1.5	7
613	Ab initio calculations of structural features not easily amenable to experiment. Computational and Theoretical Chemistry, 1990, 204, 291-300.	1.5	9
614	Anisotropy of electron-density distribution around atoms in molecules: N, P, O and S atoms. Computational and Theoretical Chemistry, 1990, 205, 191-201.	1.5	40
615	An Ab initio study of amino-sulfur compounds. Computational and Theoretical Chemistry, 1990, 206, 335-357.	1.5	9
616	Molecular structure and properties of thioacetic acid. Computational and Theoretical Chemistry, 1990, 207, 67-83.	1.5	33
617	Quantum-chemical study of the Fukui function as a reactivity index: probing the acidity of bridging hydroxyls in zeolite-type model systems. Computational and Theoretical Chemistry, 1990, 207, 115-130.	1.5	63
618	A quantum chemical investigation on the hydrates of Na ⁺ , Mg ²⁺ AND Al ³⁺ . Computational and Theoretical Chemistry, 1990, 208, 45-55.	1.5	10

#	ARTICLE	IF	CITATIONS
619	Theoretical studies on aza-analogs of platonic hydrocarbons. Computational and Theoretical Chemistry, 1990, 208, 63-77.	1.5	18
620	Theoretical and experimental study of the non-S-cis form of unsaturated ethers: Molecular structure and vibrational assignment of cis-methyl-1-propenylether. Journal of Molecular Structure, 1990, 216, 261-278.	1.8	7
621	Molecular orbital calculations on the peroxydimethoxyl dianion, an intermediate of the blank-finkenbeiner reaction. Chemical Physics Letters, 1990, 168, 265-268.	1.2	2
622	Ab initio studies of the structure and thermochemistry of FO radicals. Chemical Physics Letters, 1990, 167, 285-290.	1.2	25
623	An examination of the heats of formation for HFCO and HCICO molecules. Chemical Physics Letters, 1990, 173, 551-556.	1.2	6
624	All ab initio vibrational study of rotational isomerism in oxalyl fluoride, O=C=O, and acryloyl fluoride, O=C=CH ₂ . Chemical Physics, 1990, 147, 65-75.	0.9	17
625	An ab initio study of the CO ₂ -C ₂ H ₂ binary complex. Chemical Physics, 1990, 141, 297-309.	0.9	24
626	A theoretical study of methoxy group rotation in anisole. Chemical Physics, 1990, 140, 35-40.	0.9	34
627	Ab initio studies on L-2,4-diaminobutyric acid (L-DABA). Structural Chemistry, 1990, 1, 379-384.	1.0	3
628	Origin of exo selectivity in norbornene. An ab initio MO study. Journal of Physical Organic Chemistry, 1990, 3, 519-533.	0.9	29
629	Roles of kinetic and potential energies in conjugation II. Aniline and nitrobenzene. Journal of Physical Organic Chemistry, 1990, 3, 587-593.	0.9	6
630	Heats of formation of organic molecules by ab initio calculations. 1. Aliphatic amines. Journal of Physical Organic Chemistry, 1990, 3, 732-736.	0.9	30
631	Computational models for proton transfer in biological systems. International Journal of Quantum Chemistry, 1990, 37, 701-711.	1.0	18
632	Theoretical investigation of the hydration properties for the trans and gauche rotamers of succinonitrile. International Journal of Quantum Chemistry, 1990, 38, 85-92.	1.0	2
633	Gradient optimization of polarization exponents in ab initio MO calculations on H ₂ SO ₄ , HSO ₃ H and CH ₃ SH. Theoretica Chimica Acta, 1990, 77, 281-287.	0.9	23
634	Through-bond and through-space interactions of substituents and the nonlinearity of X-C-Y Linkages. Structural Chemistry, 1990, 1, 179-193.	1.0	15
635	Theoretical studies of the benzene oxide-oxepin valence tautomerism. Structural Chemistry, 1990, 1, 33-39.	1.0	20
636	Molecular structure of nitrobenzene in the planar and orthogonal conformations. Structural Chemistry, 1990, 1, 107-122.	1.0	133

#	ARTICLE	IF	CITATIONS
637	Ab initio self-consistent field and potential-dependent partial equalization of orbital electronegativity calculations of hydration properties of N-acetyl-L-methyl-alanineamide. Biopolymers, 1990, 30, 929-949.	1.2	47
638	[PhLiNCH ₂ CH ₂ NLiPh]·3 HMPA, a Monomeric Dilithiummethylenediamide Complex with N ₂ Li ₂ Double Bridging: Synthesis, Crystal Structure, and Model MO Calculations. Angewandte Chemie International Edition in English, 1990, 29, 410-411.	4.4	18
639	[PhLiNCH ₂ CH ₂ NLiPh]·3 HMPA, ein monomeres Dilithiummethylenediamid mit N ₂ Li ₂ -Doppelbrückung: Synthese, Kristallstruktur und MO-Rechnungen. Angewandte Chemie, 1990, 102, 443-445.	1.6	18
640	A comparison of the IGLO and LORG methods for the calculations of nuclear magnetic shieldings. Journal of Computational Chemistry, 1990, 11, 32-44.	1.5	47
641	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison with ab initio values. Journal of Computational Chemistry, 1990, 11, 159-169.	1.5	157
642	3-P- or 4-P-Coordination in apically oxygenated phosphoranes? An ab initio study of PH ₄ O, PH ₄ O ⁺ . Journal of Computational Chemistry, 1990, 11, 249-264.	1.5	1
643	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. Journal of Computational Chemistry, 1990, 11, 416-430.	1.5	105
644	Diazonium ions. Topological electron density analysis of cyclopropeniumdiazonium dications and of their stability toward dediazonation. Journal of Computational Chemistry, 1990, 11, 663-679.	1.5	15
645	The effect of diffuse functions on minimal basis set superposition errors for H-bonded dimers. Journal of Computational Chemistry, 1990, 11, 930-942.	1.5	28
646	PRODEN: A new program for calculating integrated projected populations. Journal of Computational Chemistry, 1990, 11, 1101-1110.	1.5	4
647	A cautionary note on the use of the frozen-core approximation for correlation energy calculations involving alkali metals. Journal of Computational Chemistry, 1990, 11, 1147-1150.	1.5	33
648	Compact contracted basis sets for third-row atoms: Ga-Kr. Journal of Computational Chemistry, 1990, 11, 1206-1216.	1.5	1,052
649	Accurate determination and analysis of the temperature dependence of long-range spin-spin couplings in 2-chlorobenzaldehyde. Magnetic Resonance in Chemistry, 1990, 28, 939-946.	1.1	12
650	Unusually large effects of single excitations on the geometry of radical species and limiting spin-projection invariance of some correlated methods. Chemical Physics Letters, 1990, 166, 295-302.	1.2	9
651	Ab initio study of proton transfer in [H ₃ N ⁺ H ⁻ NH ₃] ⁺ and [H ₃ N ⁺ H ⁻ OH ₂] ⁺ . Chemical Physics Letters, 1990, 175, 282-288.	1.2	70
652	Molecular mechanics parameters for electronically excited states: The (n, π*) singlet state of formaldehyde. Chemical Physics Letters, 1990, 166, 429-436.	1.2	12
653	Ground and excited states of CaSH through electron propagator calculations. Chemical Physics Letters, 1990, 169, 116-120.	1.2	21
654	Theoretical study of the isomerization of cyanogen. Chemical Physics Letters, 1990, 171, 185-190.	1.2	32

#	ARTICLE	IF	CITATIONS
655	Calculated inversion barriers and proton affinities for P(CH ₃) ₃ and P(C ₆ H ₅) ₃ . Chemical Physics Letters, 1990, 174, 320-324.	1.2	20
656	A simple scheme of estimating substitution or substituent effects in the ab initio MO method based on the shift operator. Chemical Physics Letters, 1990, 172, 243-248.	1.2	22
657	Ab initio investigation of the stationary points on the potential energy surface for the CO ₂ ⋮HCN binary complex. Chemical Physics Letters, 1990, 166, 589-598.	1.2	20
658	Direct analytic SCF second derivatives and electric field properties. Chemical Physics, 1990, 141, 189-196.	0.9	120
659	Low-energy satellite lines in photoelectron spectra-how low is it possible?. Journal of Electron Spectroscopy and Related Phenomena, 1990, 51, 173-181.	0.8	3
660	Some cost-effective approximations to CCSD and QCISD. Chemical Physics Letters, 1990, 172, 354-360.	1.2	8
661	Sum rules for Cartesian polarizability derivative tensors. Chemical Physics Letters, 1990, 174, 511-516.	1.2	15
662	The anharmonic force fields of PH ₃ , PHF ₂ , PF ₃ , PH ₅ , and H ₃ PO. Journal of Molecular Spectroscopy, 1990, 140, 226-236.	0.4	20
663	Ab initio vibrational analysis of trans- and gauche-2,3-dimethylbuta-1,3-diene. Journal of Molecular Structure, 1990, 221, 159-167.	1.8	12
664	Transferability of quantum mechanical force field scale factors between conjugated hydrocarbons. Journal of Molecular Structure, 1990, 222, 415-429.	1.8	16
665	Ab initio studies on the dimer of sulfur dioxide and hydrogen cyanide. Journal of Chemical Physics, 1990, 93, 4187-4191.	1.2	11
666	High-resolution rotation-vibration spectroscopy of difluorophosphorane: A combined theoretical and experimental study. Journal of Chemical Physics, 1990, 93, 4603-4614.	1.2	20
667	On decomposition of second-order Møller-Plesset supermolecular interaction energy and basis set effects. Journal of Chemical Physics, 1990, 92, 4357-4363.	1.2	187
668	Heats of formation of SiH _m F _n calculated by ab initio molecular orbital methods. Journal of Chemical Physics, 1990, 92, 5404-5416.	1.2	35
669	An examination of the heats of formation for formyl and fluoroformyl radicals calculated by ab initio molecular orbital methods. Journal of Chemical Physics, 1990, 93, 9203-9205.	1.2	14
670	A theoretical investigation of HSO/HOS and their positive ions. Journal of Chemical Physics, 1990, 92, 6627-6634.	1.2	29
671	Pseudospectral Hartree-Fock calculations on glycine. Journal of Chemical Physics, 1990, 92, 1163-1173.	1.2	43
672	Ground and excited states of CaCH ₃ , CaNH ₂ , CaOH, and CaF through electron propagator calculations. Journal of Chemical Physics, 1990, 92, 6728-6731.	1.2	47

#	ARTICLE	IF	CITATIONS
673	Theory of multicenter partitioning of molecular energies. <i>Journal of Chemical Physics</i> , 1990, 92, 6620-6626.	1.2	6
674	Local electron momentum anisotropy in molecules. <i>Journal of Chemical Physics</i> , 1990, 92, 2943-2952.	1.2	13
675	Accurate configuration interaction calculations of the hyperfine interactions in the benzene cation. <i>Journal of Chemical Physics</i> , 1990, 92, 6081-6083.	1.2	33
676	Structures, barriers for internal rotation, vibrational frequencies, and thermodynamic functions of CH ₂ FCH ₂ , CHF ₂ CH ₂ , and CF ₃ CH ₂ radicals: An ab initio study. <i>Journal of Chemical Physics</i> , 1990, 93, 6620-6629.	1.2	27
677	Theoretical study of bicyclo[2.2.0]hexaplumbane. A more flexible and less strained Pb skeleton compared with C, Si, Ge, and Sn skeletons. <i>Journal of the Chemical Society Chemical Communications</i> , 1990, , 630.	2.0	9
678	Parallel and cross cycloaddition of triplet penta-1,4-diene. An ab initio MO study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1990, , 735.	0.9	3
679	Amidines. Part 33. Full ab initio 3-21G optimization of the molecular structures of fluoro derivatives of formamidine and their protonation products. Quantitative structure–basicity relations of amidines. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1990, , 1551-1557.	0.9	12
680	Floppy structure of the benzene dimer: Ab initio calculation on the structure and dipole moment. <i>Journal of Chemical Physics</i> , 1990, 93, 5893-5897.	1.2	147
681	Pseudospectral Hartree–Fock theory: Applications and algorithmic improvements. <i>Journal of Chemical Physics</i> , 1990, 93, 3397-3407.	1.2	93
682	Histamine tautomerism and its mode of action. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 1990, 1036, 158-161.	1.1	12
683	Natural Bond Orbital Analysis of Internal Rotation Barriers and Related Phenomena. <i>Israel Journal of Chemistry</i> , 1991, 31, 277-285.	1.0	179
684	Ab initio molecular orbital calculations of conformational energies of ethyl methyl ether: basis set and electron correlation effects. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1991, 87, 3207.	1.7	14
685	Basis set and electron correlation effects on the internal rotational barrier heights of formamide and acetamide. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1991, , 1255.	0.9	27
686	Lithiations of mercaptoamines containing $\text{NC}(\text{S})\text{NH}$, $\text{NHC}(\text{S})$ and $\text{NHC}(\text{S})\text{NH}$ units: syntheses, crystal structures and model molecular-orbital calculations. <i>Journal of the Chemical Society Dalton Transactions</i> , 1991, , 765-776.	1.1	14
687	An ab initio study of the structure and infrared spectrum of Si ₂ C. <i>Journal of Chemical Physics</i> , 1991, 95, 5609-5611.	1.2	54
688	The Effect of a Protein Environment on the Proposed Activation Mechanism of the Histamine H ₂ Receptor. <i>Israel Journal of Chemistry</i> , 1991, 31, 409-421.	1.0	2
689	A computational evaluation of the CO ₂ -HCN associating system thermodynamics: considerable low temperature isomerism manifestations. <i>Thermochimica Acta</i> , 1991, 186, 35-42.	1.2	1
690	Vibrational spectra and structure of methyl trans-crotonate. <i>Vibrational Spectroscopy</i> , 1991, 2, 107-123.	1.2	12

#	ARTICLE	IF	CITATIONS
691	Conformational stability for methyl acrylate: a vibrational spectroscopic and ab initio MO study. <i>Vibrational Spectroscopy</i> , 1991, 2, 43-60.	1.2	32
692	Changes in electronically excited states and photochemistry of troponoids on complexation with acids. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1991, 61, 329-342.	2.0	7
693	Analytical potential energy surface for methane in terms of interatomic forces. <i>Chemical Physics</i> , 1991, 154, 425-435.	0.9	14
694	The vibrational spectra of the monohalogenated cyclopropanes: Ab initio calculations and an experimental study of fluorocyclopropane. <i>Chemical Physics</i> , 1991, 156, 85-93.	0.9	3
695	Ab initio study of the infrared photoconversion in the water-hydrogen iodide system. <i>Chemical Physics</i> , 1991, 154, 23-32.	0.9	11
696	The vibrational spectrum of H ₄ SiO ₄ calculated using ab initio molecular orbital methods. <i>Journal of Molecular Structure</i> , 1991, 246, 179-184.	1.8	10
697	Atomic charges and charge fluxes in cis and trans-C ₂ H ₂ X ₂ (X=F, Cl): an ab initio study. <i>Journal of Molecular Structure</i> , 1991, 248, 281-288.	1.8	13
698	Theoretical and experimental study of the non-s-cis form of unsaturated ethers. Molecular structure and vibrational assignment of the high-energy isomer of methylvinylether. <i>Journal of Molecular Structure</i> , 1991, 249, 343-363.	1.8	19
699	Molecular similarity indices in electron propagator theory. <i>Chemical Physics Letters</i> , 1991, 185, 270-275.	1.2	24
700	Time-dependent Hartree-Fock second-order molecular properties with a moderately sized basis set. II. Dispersion coefficients. <i>Journal of Chemical Physics</i> , 1991, 94, 1295-1305.	1.2	38
701	Time-dependent Hartree-Fock second-order molecular properties with a moderately sized basis set. I. The frequency dependence of the dipole polarizability. <i>Journal of Chemical Physics</i> , 1991, 94, 1288-1294.	1.2	55
702	Application of quantum chemistry to geochemistry and geophysics. <i>Computational and Theoretical Chemistry</i> , 1991, 226, 129-145.	1.5	9
703	The use of MIDI basis set at the correlated level. <i>Computational and Theoretical Chemistry</i> , 1991, 236, 219-230.	1.5	2
704	A refined theoretical investigation of the oxygen-electrode processes of an alkaline hydrogen-oxygen fuel cell. <i>Computational and Theoretical Chemistry</i> , 1991, 233, 185-207.	1.5	3
705	CO ₂ -HCN complex system: temperature-dependent coexistence of linear and T-shaped structures. <i>Computational and Theoretical Chemistry</i> , 1991, 235, 51-56.	1.5	5
706	A novel interpretation of Hund's rule for two-electron molecular systems. <i>Computational and Theoretical Chemistry</i> , 1991, 235, 115-122.	1.5	5
707	The effect of basis set variation and correlation on the second hyperpolarizability of H ₂ O. <i>Computational and Theoretical Chemistry</i> , 1991, 235, 137-146.	1.5	4
708	A refined theoretical investigation of the hydrogen-electrode processes of an acidic hydrogen-oxygen fuel cell. <i>Computational and Theoretical Chemistry</i> , 1991, 230, 313-321.	1.5	3

#	ARTICLE	IF	CITATIONS
709	Ab initio calculations of the equilibrium geometries and vibrational frequencies of carbonyl cyanide, thiocarbonyl cyanide and thiopropynal. Computational and Theoretical Chemistry, 1991, 231, 87-94.	1.5	7
710	A refined theoretical investigation of the hydrogen-electrode processes of an alkaline hydrogen-oxygen fuel cell. Computational and Theoretical Chemistry, 1991, 232, 225-238.	1.5	3
711	The Lewis acidity scale of boron trihalides. Computational and Theoretical Chemistry, 1991, 236, 75-84.	1.5	26
712	The vibrational spectra of the boron halides and their molecular complexes. Computational and Theoretical Chemistry, 1991, 236, 135-159.	1.5	8
713	A computational molecular orbital study of the oxide and oxepin valence tautomers of naphthalene. Computational and Theoretical Chemistry, 1991, 234, 227-246.	1.5	9
714	Nonempirical calculations of dipole moments of molecules in semifloating gaussian basis sets. Theoretical and Experimental Chemistry, 1991, 26, 455-459.	0.2	0
715	The stabilisation of water as a ligand in lithiated organic compounds: intra- and inter-molecular hydrogen bonding in the structures of the aquo complexes $[\text{Li}\cdot\text{HMPAA}\cdot\text{H}_2\text{O}]_2$ and $[\text{Li}\cdot\text{HMPA}]_2\cdot\text{H}_2\text{O}$. Inorganica Chimica Acta, 1991, 185, 163-167.	1.2	29
716	An examination of the heats of formation for CH_3CO and CF_3CO radicals. Chemical Physics Letters, 1991, 187, 354-359.	1.2	16
717	Structure and infrared spectroscopy of the C_{11} molecule. Chemical Physics Letters, 1991, 187, 367-374.	1.2	45
718	The potential energy surface of H_4SiO_4 . Chemical Physics Letters, 1991, 178, 483-487.	1.2	8
719	On the crucial importance of polarization functions for the calculation of molecules with third-row elements: the conformations of chlorocarbonyl isocyanate $\text{ClC}(\text{O})\text{NCO}$ and the equilibrium of 1,2-dithioglyoxal with its cyclic isomer 1,2-dithiete. Chemical Physics Letters, 1991, 177, 175-183.	1.2	73
720	A combined theoretical and experimental approach to the unimolecular loss of molecular hydrogen from protonated formaldehyde: Determination of the average internal energy of metastable $[\text{CH}_2\text{OH}]^+$ ions. Organic Mass Spectrometry, 1991, 26, 67-73.	1.3	33
721	A critical comparison of MINDO/3, MNDO, AM1, and PM3 for a model problem: Carbon clusters C_2 - C_{10} . An ad hoc reparametrization of MNDO well suited for the accurate prediction of their spectroscopic constants. Journal of Computational Chemistry, 1991, 12, 52-70.	1.5	76
722	On a proposed radiation-induced polaronic hole in silicon dioxide. Journal of Computational Chemistry, 1991, 12, 254-265.	1.5	13
723	Splicing I: Using mixed basis sets in ab initio calculations. Journal of Computational Chemistry, 1991, 12, 421-426.	1.5	12
724	Parametrization of calcium binding site in proteins and molecular dynamics simulation on phospholipase A2. Journal of Computational Chemistry, 1991, 12, 717-730.	1.5	13
725	A general procedure for obtaining wave functions obeying the virial theorem. Journal of Computational Chemistry, 1991, 12, 1089-1096.	1.5	19
726	A New Look at Electron Localization. Angewandte Chemie International Edition in English, 1991, 30, 409-412.	4.4	587

#	ARTICLE	IF	CITATIONS
727	Ein neuer Blick auf die Elektronenlokalisierung. <i>Angewandte Chemie</i> , 1991, 103, 421-424.	1.6	119
728	Chromophore Systeme, 1. Konformation und Lichtabsorption von Hexaä ^{1,5} dienä ^{3,4} dion (Divinylglyoxal). <i>Chemische Berichte</i> , 1991, 124, 821-826.	0.2	11
729	Theoretical study of the reaction of OH with HNO. <i>Chemical Physics</i> , 1991, 153, 415-426.	0.9	23
730	The structure and stability of the O ₂ +2 dication: a dramatic failure of MÅllerâ€”Plesset perturbation theory. <i>Chemical Physics Letters</i> , 1991, 182, 216-224.	1.2	78
731	A semi-empirical and ab-initio analysis of fluoroketones as reactive electrophiles. <i>Journal of Fluorine Chemistry</i> , 1991, 53, 79-91.	0.9	39
732	On the origin of Î€-facial diastereoselectivity in nucleophilic additions to chiral carbonyl compounds. 1. Rotational profiles of propionaldehyde 1, chloroacetaldehyde 2, and 2-chloropropionaldehyde 3.. <i>Tetrahedron</i> , 1991, 47, 8991-9004.	1.0	31
733	Evaluation of solvent effects on the dissociation of aliphatic carboxylic acids in aqueousN,N-dimethylformamide mixtures according to the scaled particle theory. <i>Journal of Physical Organic Chemistry</i> , 1991, 4, 87-95.	0.9	11
734	A contracted bromine basis set for use in calculation of molecular energies. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 781-787.	1.0	11
735	Papain in aqueous solution and the role of Asp-158 in the mechanism: AnAb InitioSCF +DRF +BEM study. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 49-59.	1.0	17
736	Renormalized ground states in electron propagator theory. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 35-42.	1.0	9
737	The ring opening of cyclopropylidene to allene: global features of the reaction surface. <i>Theoretica Chimica Acta</i> , 1991, 78, 287-326.	0.9	56
738	Polarization correction to the electrostatic potential at the CNDO and theab initio level. Influence of the basis set expansion. <i>Theoretica Chimica Acta</i> , 1991, 79, 141-152.	0.9	13
739	On the structure dependence of the static longitudinal linear electric polarizability of infinite polyenes: An ab-initio uncoupled perturbed Hartree-Fock crystal orbital study. <i>Molecular Engineering</i> , 1991, 1, 115-129.	0.2	3
740	Calculation of the nuclear spinâ€”spin coupling constants. VI. Manyâ€”body perturbation theoretic calculation of electron correlation effect. <i>Journal of Chemical Physics</i> , 1991, 94, 533-536.	1.2	17
741	Abinitio study of the structure, infrared spectra, and heat of formation of C ₄ . <i>Journal of Chemical Physics</i> , 1991, 94, 3753-3761.	1.2	66
742	Calculation of the dispersion interaction energy by using localized molecular orbitals. <i>Journal of Chemical Physics</i> , 1991, 94, 5565-5573.	1.2	31
743	Pseudospectral Hartreeâ€”Fock gradient calculations. <i>Journal of Chemical Physics</i> , 1991, 94, 8152-8157.	1.2	26
744	Structure and vibrational properties of water hydrogen halide complexes. <i>Journal of Chemical Physics</i> , 1991, 94, 2915-2922.	1.2	34

#	ARTICLE	IF	CITATIONS
745	Microwave spectrum and ab initio calculations of ethylbenzene: potential energy surface of the ethyl group torsion. <i>Molecular Physics</i> , 1991, 74, 885-895.	0.8	59
746	An ab initio molecular orbital study of protonated water clusters, $H(H_2O)_n$, $n = 1$ to 5, at the SCF and MP2 levels. <i>Molecular Physics</i> , 1991, 73, 375-405.	0.8	56
747	Ab Initio Quantum Chemistry for Combustion. , 1991, , 3-35.		0
748	Ab initio second- and fourth-order Møller-Plesset study on structure, stabilization energy, and stretching vibration of benzene- \dots -X (X=He,Ne,Ar,Kr,Xe) van der Waals molecules. <i>Journal of Chemical Physics</i> , 1992, 97, 335-340.	1.2	105
749	Pseudospectral full configuration interaction. <i>Journal of Chemical Physics</i> , 1992, 97, 1876-1880.	1.2	45
750	Some molecular orbital calculations on the conformational behavior of 1,4-dihydronaphthalene. <i>Journal of Chemical Physics</i> , 1992, 96, 1653-1654.	1.2	3
751	Spin-orbit coupling constants in a multiconfiguration linear response approach. <i>Journal of Chemical Physics</i> , 1992, 96, 2118-2126.	1.2	90
752	Ab initio study of the structure, cooperativity, and vibrational properties of the $H_2O:(HF)_2$ hydrogen bonded complex. <i>Journal of Chemical Physics</i> , 1992, 97, 1911-1918.	1.2	23
753	An examination of substituent effects on the reaction of OH radicals with $HXCO$ (where X=H, F, and Cl). <i>Journal of Chemical Physics</i> , 1992, 96, 1921-1927.	1.2	57
754	An ab initio study of the structure and infrared spectrum of Si_3C . <i>Journal of Chemical Physics</i> , 1992, 96, 6768-6772.	1.2	56
755	Dipole oscillator strength properties and dispersion energies for acetylene and benzene. <i>Molecular Physics</i> , 1992, 75, 311-324.	0.8	76
756	A theoretical investigation of the ground and low-lying excited states of butadiene radical cation. <i>Journal of Chemical Physics</i> , 1992, 96, 3745-3755.	1.2	9
757	Ab initio studies of dissociation pathways on the ground state potential energy surface for $HFCO$ and $HCICO$. <i>Journal of Chemical Physics</i> , 1992, 96, 7587-7596.	1.2	42
758	The reaction of sulfur atoms with carbon disulfide: Potential energy surface features. <i>Journal of Chemical Physics</i> , 1992, 96, 7449-7457.	1.2	14
759	Anisotropic repulsive potential energy surfaces from Hartree-Fock calculations for $HeCO_2$ and $HeOCS$. <i>Journal of Chemical Physics</i> , 1992, 96, 6621-6628.	1.2	25
760	Intramolecular and dissociation dynamics of the CF_2Br radical. <i>Journal of Chemical Physics</i> , 1992, 97, 6432-6442.	1.2	7
761	Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes. <i>Molecular Physics</i> , 1992, 77, 381-396.	0.8	26
762	Ground and excited state properties of many-body energies in $Li_n + nF$ -ions. <i>Molecular Physics</i> , 1992, 75, 1365-1374.	0.8	6

#	ARTICLE	IF	CITATIONS
763	The polarizabilities of species present in ionic solutions. <i>Molecular Physics</i> , 1992, 76, 353-372.	0.8	94
764	Quantum-chemical studies of hydrogen bonding involving thioxoketones, thienols, thioformaldehyde and hydrogen sulfide with specific reference to the strength of intramolecular hydrogen bonds. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 2315.	1.7	42
765	Pyramidal inversion energies of hypervalent selenoxides. An ab initio MO study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 1925.	0.9	7
766	Theoretical studies of the structure and thermochemistry of FO ₂ radical: Comparison of Møller-Plesset perturbation, complete active space self-consistent field, and quadratic configuration interaction methods. <i>Journal of Chemical Physics</i> , 1992, 96, 2861-2867.	1.2	29
767	Lithiation and dethiacarbonylation of a heterocyclic thioamide C ₆ H ₄ O-C(=S)NH by reaction with solid Li ₂ S in the presence of hexamethylphosphoramide: synthesis and crystal structure of [C ₆ H ₄ O-C(=S)NLi-HMPA] ₂ ·C ₆ H ₄ (OH)NH ₂ . <i>Journal of the Chemical Society Chemical Communications</i> , 1992, , 1492-1494.	2.0	12
768	Surprisingly high accuracy of ECP methods for predicting Fe-C bond dissociation energies of FeCH ₃ ⁺ , FeCH ₂ ⁺ and FeCH ⁺ . <i>Journal of the Chemical Society Chemical Communications</i> , 1992, , 118-120.	2.0	7
769	Intramolecular effects in the cycloaddition of three ethylenes vs. the Diels-Alder reaction. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 2101-2108.	0.9	28
770	Isolation, structure and MO calculational investigations of a highly stable, hydrogen-bonded primary amine-phosphine oxide adduct, 2-aminobenzothiazole-HMPA, C ₆ H ₄ SC(=N)NH ₂ O=P(NMe ₂) ₃ ; a possible model to explain the carcinogenicity of HMPA (HMPA = hexamethylphosphoramide). <i>Journal of the Chemical Society Chemical Communications</i> , 1992, , 262-264.	2.0	14
771	Predicted structures for Ti ₈ C ₁₂ and Si ₈ C ₁₂ dodecahedron molecules. <i>Journal of the Chemical Society Chemical Communications</i> , 1992, , 1222.	2.0	37
772	The vibrational spectrum of FBrCO. <i>Molecular Physics</i> , 1992, 77, 1187-1195.	0.8	8
773	Ab initio study of the geometry, stretching, vibrations, and assignment of the observed frequencies of the ground state C ₆ H (hexatriynyl) radical. <i>Journal of Chemical Physics</i> , 1992, 97, 1602-1605.	1.2	15
774	Ab initio molecular orbital calculated stationary points on the potential energy surface of H ₄ AlO ₄ ³⁻ similarities with H ₄ SiO ₄ . <i>Computational and Theoretical Chemistry</i> , 1992, 257, 305-312.	1.5	3
775	Calculation of nuclear magnetic shieldings. VIII. Gauge invariant many-body perturbation method. <i>Journal of Chemical Physics</i> , 1992, 96, 2039-2043.	1.2	25
776	Theoretical and neon matrix electron spin resonance studies of the methanol cation: CH ₃ OH ⁺ , CH ₃ OD ⁺ , CH ₂ DOH ⁺ , and ¹³ CH ₃ OH ⁺ . <i>Journal of Chemical Physics</i> , 1992, 97, 5363-5376.	1.2	44
777	Ab initio calculations of many-body energy expansion in Linn+ <i>F</i> ? clusters. <i>International Journal of Quantum Chemistry</i> , 1992, 41, 281-292.	1.0	13
778	Ab initio CPHF calculations of the static polarizability and second hyperpolarizability of small molecules: Comparisons between standard and moderately large basis sets augmented with diffuse functions. <i>International Journal of Quantum Chemistry</i> , 1992, 42, 1577-1594.	1.0	24
779	The accurate calculation of dipole moments and dipole polarizabilities using Gaussian-based density functional methods. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 463-479.	1.0	59
780	On the role of polarization functions in SCF calculations of glycine and related systems with intramolecular hydrogen bonding. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 15-26.	1.0	25

#	ARTICLE	IF	CITATIONS
781	Modeling of coupled proton transfers by analytic functions. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 109-124.	1.0	12
782	Ab-initioSCF investigation of glycolic acid. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 505-515.	1.0	14
783	Attempts to calculate the electron affinity of acrylonitrile. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 563-573.	1.0	4
784	Calculation of barriers to proton transfer using a variety of electron correlation methods. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 817-835.	1.0	10
785	Heats of formation of organic molecules byab initio calculations. Aldehydes and ketones. <i>Journal of Physical Organic Chemistry</i> , 1992, 5, 225-229.	0.9	21
786	Relative Stability of cis and trans conformers of 2- and 3-fluorostyrene: An ab initio SCF-MO study. <i>Structural Chemistry</i> , 1992, 3, 95-101.	1.0	7
787	An ab initio structural and vibrational analysis of gauche,trans,trans- and gauche,cis,trans-hexa-1,3,5-trienes. <i>Structural Chemistry</i> , 1992, 3, 15-26.	1.0	27
788	Basis set validation for polyatomic cation-water interactions. <i>Molecular Engineering</i> , 1992, 2, 137-152.	0.2	5
789	The spin polarization model for hyperfine coupling constants. <i>Theoretica Chimica Acta</i> , 1992, 82, 93-115.	0.9	120
790	A detailed analysis of pseudorotation in PH ₄ F. <i>Theoretica Chimica Acta</i> , 1992, 83, 21-30.	0.9	21
791	MCSCF study of polaron- and bipolaron-like defects in small all-trans conjugated polyenes. <i>Theoretica Chimica Acta</i> , 1992, 83, 155-163.	0.9	14
792	Electronic structure and the unimolecular reactions of imine peroxide HNOO. <i>Theoretica Chimica Acta</i> , 1992, 82, 299-308.	0.9	26
793	Second-order Green's function calculations of the ionization potential of a (H ₂) ₇ chain embedded in a homogeneous electric field. <i>Theoretica Chimica Acta</i> , 1992, 82, 309-319.	0.9	11
794	On the optimisation of exponents of d and f polarisation functions for first row atoms. <i>Theoretica Chimica Acta</i> , 1992, 84, 115-124.	0.9	6
795	Pseudopotential Periodic Hartree-Fock Study of the Cristobalite Phases of Silica and Germanium Dioxide. <i>Journal of the American Ceramic Society</i> , 1992, 75, 1239-1246.	1.9	15
796	Experimental and ab initio theoretical vibrational Raman optical activity of tartaric acid. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1992, 48, 1051-1066.	0.1	41
797	The harmonic force fields of dimethyl zinc, cadmium and mercury: A joint theoretical and experimental study. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1992, 48, 1067-1082.	0.1	10
798	Inverse isotopic shifts in the vibrational spectra of the isotopomers of methanimine, H ₂ C=NH. <i>Journal of Molecular Structure</i> , 1992, 272, 161-177.	1.8	16

#	ARTICLE	IF	CITATIONS
799	An ab initio examination of the harmonic frequencies of ethylene and its isotopomers. Journal of Molecular Structure, 1992, 272, 179-186.	1.8	16
800	A comparison of ab initio, NMR and diffraction results for a strong OHF hydrogen bond. Journal of Molecular Structure, 1992, 271, 149-154.	1.8	2
801	Analytic functions fit to proton transfer potentials. Journal of Molecular Structure, 1992, 270, 173-185.	1.8	56
802	Satellite lines at the ionization threshold in charge transfer systems. Chemical Physics, 1992, 159, 11-27.	0.9	4
803	The proton position in amine-HX (X $\hat{\rightarrow}$ Br, I) complexes. Chemical Physics, 1992, 166, 85-96.	0.9	19
804	Fully optimized contracted Gaussian basis sets for atoms Li to Kr. Journal of Chemical Physics, 1992, 97, 2571-2577.	1.2	8,555
805	A theoretical model investigation of the oxygen-electrode processes of an acidic hydrogen-oxygen fuel cell. Computational and Theoretical Chemistry, 1992, 276, 97-115.	1.5	2
806	A study of the stable conformations of methylvinyl sulfoxide and sulfone by ab initio calculations. Computational and Theoretical Chemistry, 1992, 276, 167-173.	1.5	15
807	Ab initio characterization of possible dissociation pathways for multiphoton ionization of the water dimer in supersonic free jets. Computational and Theoretical Chemistry, 1992, 254, 453-463.	1.5	6
808	Efficient new methods for the determination of integrated atomic properties via atom specific electron density functions based on subsets of selected localized molecular orbitals and the reduction of the space of the primitives. Computational and Theoretical Chemistry, 1992, 255, 45-91.	1.5	2
809	Ab initio study of the effect of external perturbations in the dissociation of CH ₃ Cl. Computational and Theoretical Chemistry, 1992, 255, 283-296.	1.5	8
810	An ab initio molecular orbital study of the potential energy surface for the orthosilicate anion, [H ₃ SiO ₄] ⁻ . Computational and Theoretical Chemistry, 1992, 258, 379-387.	1.5	3
811	Quantum-chemical study of the Fukui function as a reactivity index. Computational and Theoretical Chemistry, 1992, 259, 317-330.	1.5	50
812	Ab initio study of the basis set dependence of the structural parameters, relative energies and fundamental frequencies of glyoxal. Computational and Theoretical Chemistry, 1992, 253, 199-216.	1.5	8
813	A quantum chemical study of the binding energies in the hydrates of Zn ²⁺ , Cd ²⁺ and Hg ²⁺ . Computational and Theoretical Chemistry, 1992, 253, 275-285.	1.5	21
814	Comparative ab initio study of (CH ₃) ₂ CHX (X = F, Cl) and (CH ₃) ₂ CX ₂ -type molecules (X = H, F, Cl). Computational and Theoretical Chemistry, 1992, 257, 157-166.	1.5	5
815	Ab initio calculation of anharmonic force fields for the methyl, silyl, germyl, and stannyl halides. Chemical Physics, 1992, 159, 49-66.	0.9	67
816	Intermolecular potential function for methanol dimer interactions from ab initio calculations. Chemical Physics, 1992, 166, 341-360.	0.9	26

#	ARTICLE	IF	CITATIONS
817	A re-examination of the infrared and ultraviolet spectroscopy of trifluoroacetyl fluoride and trifluoroacetyl chloride: An experimental and theoretical study. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1992, 48, 1115-1126.	0.1	8
818	Infrared, raman, microwave and ab initio study of dimethyl disulfide: structure and force field. <i>Journal of Molecular Structure</i> , 1992, 273, 99-121.	1.8	38
819	Non-Arrhenius temperature dependence of the rate constant for the H + H ₂ S reaction. <i>Chemical Physics Letters</i> , 1992, 189, 199-204.	1.2	41
820	Van der Waals and charge-transfer complexes of molecular oxygen and water. <i>Chemical Physics Letters</i> , 1992, 192, 213-216.	1.2	19
821	A 1 : 1 Adduct of 2-Aminobenzothiazole and a Urea Derivative, and Its Spatial Arrangement. <i>Angewandte Chemie International Edition in English</i> , 1992, 31, 1634-1636.	4.4	6
822	Ab initio study of proton transfer between methylnitroamine and trimethylamine. <i>Chemical Physics Letters</i> , 1992, 199, 55-61.	1.2	5
823	Ï€* negative ion resonance states of (E)- and (Z)-1,3,5-hexatriene. Prediction of electron affinities near threshold. <i>Chemical Physics Letters</i> , 1992, 200, 527-533.	1.2	4
824	Ab initio calculation of harmonic force fields and vibrational spectra for trichloromethyltitanium and related compounds. <i>Chemical Physics Letters</i> , 1992, 189, 105-111.	1.2	9
825	Ab initio CPHF calculations of first hyperpolarizabilities of nitrogen-containing polyenes with donor-acceptor substituents. <i>Chemical Physics Letters</i> , 1992, 190, 533-538.	1.2	10
826	The role of CF ₃ C(O)Ox radicals in atmospheric chemical processes. <i>Chemical Physics Letters</i> , 1992, 191, 7-12.	1.2	17
827	The structure, stability, and infrared spectrum of B ₂ N, B ₂ N ⁺ , B ₂ N ⁺ , BO, B ₂ O and B ₂ N ₂ .. <i>Chemical Physics Letters</i> , 1992, 193, 243-250.	1.2	49
828	Large discrepancies between the theoretically predicted and experimentally observed vibrational frequencies of ONCl ₂ and ONClF. <i>Chemical Physics Letters</i> , 1992, 197, 330-334.	1.2	6
829	Molecular structure of ethyl nitrate from gas-phase electron diffraction and ab initio MO calculations. <i>Chemical Physics Letters</i> , 1992, 197, 489-494.	1.2	19
830	Energy hypersurface local properties of the O ₂ HF ⁺ rearrangement. <i>Chemical Physics Letters</i> , 1992, 195, 189-193.	1.2	0
831	Gas-phase chemistry of the methyl carbamate radical cation, H ₂ NCOOCH ₃ ⁺ . A test case for ion structure assignment. <i>Organic Mass Spectrometry</i> , 1992, 27, 126-134.	1.3	11
832	Deacetylation of gaseous amidoalkylating reagents (N-acyliminium ions) via iminium/ketene complexes: An unprecedented isotope effect. <i>Organic Mass Spectrometry</i> , 1992, 27, 398-405.	1.3	7
833	A systematic ab initio study of the group V trihalides MX ₃ and pentahalides MX ₅ (M = P?Bi, X = F?I). <i>Journal of Computational Chemistry</i> , 1992, 13, 165-176.	1.5	39
834	Ab initio evidence for the stepwise mechanism of the McLafferty rearrangement of the butanal radical cation. <i>Journal of Computational Chemistry</i> , 1992, 13, 183-186.	1.5	11

#	ARTICLE	IF	CITATIONS
835	Pauli repulsion in the open shell species BeH and Co+. Journal of Computational Chemistry, 1992, 13, 268-274.	1.5	3
836	Conformational analysis of carbonyl and thiocarbonyl ethyl esters: The HC(?X) (X,Y = O or S) internal rotation. Journal of Computational Chemistry, 1992, 13, 799-809.	1.5	12
837	Heats of formation of organic molecules by Ab Initio calculations: Carboxylic acids and esters. Journal of Computational Chemistry, 1992, 13, 838-841.	1.5	22
838	Theoretical studies of organometallic compounds. I. All electron and pseudopotential calculations of Ti(CH ₃) _n Cl _{4-n} (n = 0-4). Journal of Computational Chemistry, 1992, 13, 919-934.	1.5	70
839	Theoretical studies of organometallic compounds. II. All electron and pseudopotential calculations of M(CH ₃) _n Cl _{4-n} (M = C, Si, Ge, Sn, Pb; n = 0-4). Journal of Computational Chemistry, 1992, 13, 935-943.	1.5	21
840	Theoretical studies of organometallic compounds. III. Structures and bond energies of FeCH _n and FeCH _n ⁺ (n = 1, 2, 3). Journal of Computational Chemistry, 1992, 13, 1184-1198.	1.5	19
841	Ab Initio computed molecular structures and energies of the conformers of glucose. Journal of Computational Chemistry, 1992, 13, 1255-1261.	1.5	111
842	Ab-initio-Studien an N-Acyliminium-Ionen. Helvetica Chimica Acta, 1992, 75, 1095-1110.	1.0	24
843	Ein 1:1-Addukt aus 2-Aminobenzothiazol und einem Harnstoffderivat sowie seine Anordnung im Raum. Angewandte Chemie, 1992, 104, 1662-1664.	1.6	0
844	Sequence-ion studies in peptides: The generation of C ³⁺ ions" part 2. Organic Mass Spectrometry, 1993, 28, 1059-1063.	1.3	3
845	Isomerization and dissociation processes of protonated Î ² -propiolactone and related C ₃ H ₅ O ₂ ⁺ isomers: A combined experimental and theoretical study. Organic Mass Spectrometry, 1993, 28, 1270-1283.	1.3	1
846	Ab initio study of the structure and dipole moment of azulene. Chemical Physics Letters, 1993, 201, 67-74.	1.2	48
847	A photoelectron and ab initio study of the CH ₃ SCH ₂ radical. Chemical Physics Letters, 1993, 213, 257-261.	1.2	17
848	External polarization functions and polarizability calculations for H ₂ . Chemical Physics Letters, 1993, 203, 578-582.	1.2	4
849	Theoretical study of the (H ₂ O) ₆ cluster. Chemical Physics Letters, 1993, 213, 181-188.	1.2	219
850	Structures of PhX (X Î O and N). Importance of polarization functions in the basis set. Chemical Physics Letters, 1993, 207, 185-189.	1.2	13
851	Use of approximate integrals in ab initio theory. An application in MP2 energy calculations. Chemical Physics Letters, 1993, 208, 359-363.	1.2	1,116
852	Five-membered ring intermediates in the gas-phase CN ⁺ + N ₂ O reaction. A theoretical study. Chemical Physics Letters, 1993, 209, 161-166.	1.2	1

#	ARTICLE	IF	CITATIONS
853	The molecular structure of phosphabenzene. A theoretically predicted correction to the experimentally determined C ⁺ -C bond lengths. <i>Chemical Physics Letters</i> , 1993, 210, 211-215.	1.2	24
854	Benzene ⁺ O ₂ interaction potential from ab initio calculations. <i>Chemical Physics Letters</i> , 1993, 205, 331-336.	1.2	31
855	The keto/enol tautomerism of selenoformamide and telluroformamide. <i>Chemical Physics Letters</i> , 1993, 205, 337-342.	1.2	17
856	Multireference CI study of the electron affinity of C ₃ . <i>Chemical Physics Letters</i> , 1993, 204, 320-322.	1.2	3
857	Quantum ⁺ Mechanical ab initio Investigation of the Transition ⁺ Metal Compounds OsO ₄ , OsO ₃ F ₂ , OsO ₂ F ₄ , OsOF ₆ , and OsF ₈ . <i>Chemische Berichte</i> , 1993, 126, 1325-1330.	0.2	36
858	Derivate des Imidazols, VI. Stabile Carben ⁺ Borane. <i>Chemische Berichte</i> , 1993, 126, 2041-2045.	0.2	140
859	D-Gluconhydroximo-1,5-lactam and Related N-Arylcarbamates Theoretical Calculations, Structure, Synthesis, and Inhibitory Effect on α -Glucosidases. <i>Helvetica Chimica Acta</i> , 1993, 76, 2666-2686.	1.0	51
860	Use of effective core potentials for ab initio calculations on molecular siloxanes and silicates. <i>Journal of Computational Chemistry</i> , 1993, 14, 216-225.	1.5	17
861	Ab initio calculations on phosphorus compounds. II. Effects of disubstitution on ligand apicophilicity in phosphoranes. <i>Journal of Computational Chemistry</i> , 1993, 14, 522-529.	1.5	22
862	Conformational analysis of 2,3,6,7-tetrahydroazepines with implications for D ₁ -selective benzazepines. <i>Journal of Computational Chemistry</i> , 1993, 14, 571-578.	1.5	7
863	Quantitative comparison of molecular electrostatic potential distributions from several semiempirical and ab initio wave functions. <i>Journal of Computational Chemistry</i> , 1993, 14, 922-927.	1.5	24
864	Ab initio study of hydrogen bonding in the phenol-water system. <i>Journal of Computational Chemistry</i> , 1993, 14, 1027-1035.	1.5	103
865	Ab initio CI study of the laser radiation effect on pyrolysis of 1,2-dichloroethane. <i>Chemical Physics</i> , 1993, 169, 305-315.	0.9	7
866	An ab initio study of the molecular structures of 1,4,5,8-naphthalenetetrone and 5,8-dihydroxy-1,4-naphthoquinone. <i>Journal of Molecular Structure</i> , 1993, 297, 235-241.	1.8	19
867	Wavenumbers and intensities of the fundamental vibrational modes of HNSi and DNSi from quantum-chemical computations. <i>Journal of Molecular Structure</i> , 1993, 297, 243-253.	1.8	1
868	Ab initio molecular orbital studies of the vibrational spectra of nitrosyl fluoride and chloride monomers and dimers. <i>Journal of Molecular Structure</i> , 1993, 297, 255-264.	1.8	6
869	Ab initio study of the force field, geometry and vibrational assignment of urea. <i>Journal of Molecular Structure</i> , 1993, 295, 245-258.	1.8	25
870	Ab initio studies of the dipole polarizabilities of conjugated molecules Part 1. Ethene and benzene. <i>Journal of Molecular Structure</i> , 1993, 300, 1-7.	1.8	16

#	ARTICLE	IF	CITATIONS
871	AM1 and PM3 semiempirical molecular orbital study of silatranes III. 1-Chlorosilatrane. <i>Journal of Organometallic Chemistry</i> , 1993, 454, 15-23.	0.8	20
872	Ab initio infrared and Raman spectra of the H ₃ SiO ⁻ monomeric anionic species. <i>Vibrational Spectroscopy</i> , 1993, 5, 325-335.	1.2	6
873	Theoretical study on crown compounds as building blocks of functional molecules I. The relation between the hole size and the number of atoms in the ring of cyclic ethers and amines. <i>Tetrahedron</i> , 1993, 49, 3959-3970.	1.0	14
874	Pseudopotential periodic Hartree-Fock study of Mg ₂ SiO ₄ polymorphs: Olivine, modified spinel and spinel. <i>Physics and Chemistry of Minerals</i> , 1993, 20, 333.	0.3	5
875	Aktivierung von CO ₂ an d-bergangsmetallzentren: Zum Ablauf der CO ₂ -Reduktion an Nickel(O)-Fragmenten. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 1993, 619, 1105-1110.	0.6	25
876	Ab initio study of the electronic properties of potential antagonists of the glycine receptor: 1. Transition state of the 2-pyridone · H ₂ O/2-hydroxypyridine · H ₂ O tautomeric equilibrium. <i>International Journal of Quantum Chemistry</i> , 1993, 46, 183-190.	1.0	7
877	Intrinsic reaction coordinate of perturbed potential energy surfaces: Construction of perturbed energy profiles. <i>International Journal of Quantum Chemistry</i> , 1993, 47, 307-317.	1.0	1
878	Modeling proton transfer potentials in angularly deformed hydrogen bonds. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 77-87.	1.0	8
879	Behavior of interaction energy and intramolecular bond stretch in linear and bifurcated hydrogen bonds. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 181-190.	1.0	7
880	Basis set dependence of ab-initio calculated vibration frequencies. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 331-341.	1.0	4
881	Comparison of ground and triplet state geometries of malonaldehyde. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 419-429.	1.0	7
882	Efficient computation of electron-repulsion integrals in ab initio studies of polymeric systems. <i>International Journal of Quantum Chemistry</i> , 1993, 48, 793-806.	1.0	9
883	Active site dynamics of acyl-chymotrypsin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1993, 16, 172-194.	1.5	40
884	Heats of formation of organic molecules by ab initio calculations: Alkyl radicals. <i>Journal of Physical Organic Chemistry</i> , 1993, 6, 551-554.	0.9	11
885	A study of the gas-phase reaction of carbonyl fluoride with water. <i>Journal of Atmospheric Chemistry</i> , 1993, 16, 285-292.	1.4	9
886	Energy analysis on small to medium sized H-bonded complexes. <i>Theoretica Chimica Acta</i> , 1993, 85, 409-421.	0.9	36
887	Comparison of the Hartree-Fock, Møller-Plesset, and Hartree-Fock-Slater method with respect to electrostatic properties of small molecules. <i>Theoretica Chimica Acta</i> , 1993, 86, 391-416.	0.9	10
888	On the origin of π -facial diastereoselectivity in nucleophilic additions to chiral carbonyl compounds 3. Rotational profiles of 2-methoxypropanal and 2-N,N-dimethylaminopropanal. <i>Tetrahedron</i> , 1993, 49, 3971-3982.	1.0	21

#	ARTICLE	IF	CITATIONS
889	Basis set effects on the intermolecular interaction of the H ₂ -H ₂ system obtained using ab initio molecular orbital calculations with the Møller-Plesset perturbation correction. Computational and Theoretical Chemistry, 1993, 280, 273-281.	1.5	8
890	On the structural and electronic properties of methylenemalondehyde. Computational and Theoretical Chemistry, 1993, 281, 15-20.	1.5	2
891	Molecular structure of methyl acrylate: the high energy s-trans-(C=C ₁ -O) conformer. Computational and Theoretical Chemistry, 1993, 282, 123-129.	1.5	14
892	Structure-stability relationships in unsaturated sulfur compounds. Computational and Theoretical Chemistry, 1993, 285, 71-75.	1.5	7
893	An ab initio study of the ¹⁹ F nuclear magnetic resonance chemical shielding tensor in the hydrogen difluoride ion FHF ⁻ and its variation with bond length and angle deformation. Computational and Theoretical Chemistry, 1993, 285, 229-233.	1.5	1
894	An ab initio study on the structure of cyanuric fluoride. Computational and Theoretical Chemistry, 1993, 280, 21-24.	1.5	2
895	AM1 and PM3 semiempirical molecular orbital study of silatranes.. Computational and Theoretical Chemistry, 1993, 283, 251-259.	1.5	17
896	Ab initio calculations of isotropic hyperfine coupling constants in $\dot{\text{I}}^2$ -ketoenolyl radicals. Computational and Theoretical Chemistry, 1993, 287, 89-92.	1.5	8
897	Abinitioelectron density distributions in molecules containing sulfur-sulfur bonds. Journal of Chemical Physics, 1993, 99, 1837-1843.	1.2	11
898	Ab initio study of the stability of [n]paracyclophanes and their Dewar benzene-type isomers. Theoretica Chimica Acta, 1993, 85, 43-59.	0.9	15
899	Quantum mechanical study of the structure and stability of molecular van der Waals' clusters I: hydrates of SO ₂ . Zeitschrift für Physik D-Atoms Molecules and Clusters, 1993, 26, 326-328.	1.0	1
900	Measured and calculated double-ionization energies of the chlorofluoroethane molecules CF ₃ CF ₂ Cl, CF ₃ CFCl ₂ , CF ₃ CCl ₃ , CF ₂ ClCF ₂ Cl, CF ₂ ClCFCl ₂ , CF ₂ ClCCl ₃ , CFCI ₂ CFCI ₂ and CFCI ₂ CCl ₃ . International Journal of Mass Spectrometry and Ion Processes, 1993, 124, 251-257.	1.9	4
901	Ab initio and semiempirical investigations of the complexation of methyl pyruvate by ammonia and the ammonium cation. Journal of Molecular Structure, 1993, 297, 285-293.	1.8	41
902	Vibrational spectra of end-capped thiophenes: a combined experimental and theoretical study. Journal of Molecular Structure, 1993, 298, 65-86.	1.8	14
903	Endothermicity or exothermicity of water/alcohol mixtures. Journal of Molecular Structure, 1993, 300, 539-550.	1.8	41
904	MNDO, AM1 and PM3 semiempirical molecular orbital study of 1-fluorosilatrane. Journal of Organometallic Chemistry, 1993, 446, 99-106.	0.8	22
905	H ⁺ +H, He, and H ₂ scattering using a new time-dependent method for electron nuclear dynamics. Journal of Chemical Physics, 1993, 99, 4554-4565.	1.2	25
906	Practical schemes for distributed polarizabilities. Molecular Physics, 1993, 78, 1267-1291.	0.8	79

#	ARTICLE	IF	CITATIONS
907	A theoretical investigation of the geometries, vibrational frequencies, and binding energies of several alkali halide dimers. <i>Journal of Chemical Physics</i> , 1993, 98, 2182-2190.	1.2	29
908	Theoretical reaction pathways for the formation of $[\text{Si}(\text{OH})_5]^{1-}$ and the deprotonation of orthosilicic acid in basic solution. <i>Geochimica Et Cosmochimica Acta</i> , 1993, 57, 3847-3853.	1.6	53
909	The History and Evolution of Gaussian Basis Sets. <i>Israel Journal of Chemistry</i> , 1993, 33, 357-367.	1.0	51
910	Ab initio and electron correlation corrected energy band structure of polymeric five-membered heterocycles. <i>Synthetic Metals</i> , 1993, 59, 97-110.	2.1	33
911	Theoretical studies of the M-CO bond lengths and first dissociation energies of the transition metal hexacarbonyls $\text{Cr}(\text{CO})_6$, $\text{Mo}(\text{CO})_6$ and $\text{W}(\text{CO})_6$. <i>Journal of the Chemical Society Chemical Communications</i> , 1993, , 1709-1711.	2.0	39
912	The low lying electronic states of O^{2-} . <i>Journal of Chemical Physics</i> , 1993, 99, 1271-1277.	1.2	37
913	Conformers, vibrational spectra and laser-induced rotamerization of CH_2ClCOOH . <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 3235.	1.7	12
914	Model calculations of chemical interactions. Part 6. "Origin of diastereofacial selectivity in 1,3-dipolar cycloaddition of formonitrile oxide with bicyclo[2.1.0]pent-2-ene and 2,3-dioxabicyclo[2.2.2]oct-5-ene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 3913-3920.	1.7	7
915	An ab initio investigation of the molecular structure and vibrational spectrum of the silanol-hydrogen molecular complex. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 983-989.	1.7	4
916	Model calculations of chemical interactions. Part 5. "Diastereofacial selectivity in 1,3-dipolar cycloaddition of formonitrile oxide to norbornene and cis-3,4-dichlorocyclobutene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 29-36.	1.7	8
917	Triplet-singlet intersystem crossing as the second step of the cycloaddition of triplet penta-1,4-diene. An ab initio MO study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 71-74.	0.9	2
918	The singlet-triplet gap of the halonitrenium ions NHX^+ , NX_2^+ and the halocarbenes CHX , CX_2 ($\text{X} = \text{F}, \text{Cl}$). <i>J. Phys. Chem.</i> 1993, 97, 10784-10791.	1.0	47
919	Binding properties of carbohydrate O-sulfate esters based on ab initio 6-31 +G** calculations on methyl and ethyl sulfate anions. <i>Journal of the American Chemical Society</i> , 1993, 115, 9648-9654.	6.6	31
920	Ab initio studies of the lowest singlet and triplet potential energy surfaces of CO_2S . <i>Molecular Physics</i> , 1993, 79, 685-697.	0.8	4
921	Spin-orbit interactions from self consistent field wavefunctions. <i>Molecular Physics</i> , 1993, 80, 479-502.	0.8	19
922	Pseudopotential periodic hartree-fock investigation of potassium dihydrogen phosphate. <i>Ferroelectrics</i> , 1993, 150, 303-311.	0.3	13
923	Reactions of pulsed laser produced boron and nitrogen atoms in a condensing argon stream. <i>Journal of Chemical Physics</i> , 1993, 98, 922-931.	1.2	79
924	Calculation of the interaction energy in a localized representation for several diatomic systems. <i>Molecular Physics</i> , 1993, 80, 1059-1065.	0.8	2

#	ARTICLE	IF	CITATIONS
925	The vibrational spectrum of H ₂ O ₃ : An ab initio investigation. Journal of Chemical Physics, 1993, 99, 5768-5779.	1.2	16
926	Does chlorine peroxide exhibit a strong ultraviolet absorption near 250 nm?. Journal of Chemical Physics, 1993, 98, 9335-9339.	1.2	53
927	The COSY potential energy surface: Aspects of the lowest singlet and triplet potential energy surfaces for the reaction of oxygen atoms with carbon disulfide. Journal of Chemical Physics, 1993, 98, 5566-5578.	1.2	7
928	Pseudospectral double excitation configuration interaction. Journal of Chemical Physics, 1993, 98, 7081-7085.	1.2	29
929	A theoretical investigation of the geometries, vibrational frequencies, and binding energies of several mixed alkali halide dimers. Journal of Chemical Physics, 1993, 99, 9764-9769.	1.2	7
930	Multi-Reference CI Calculation of Potential Energy Curves for cis-trans Isomerization of Stilbene Cation Radical. Bulletin of the Chemical Society of Japan, 1993, 66, 1622-1626.	2.0	8
931	Theoretical Studies on Hydrogen Bonding Interactions between Peptide Units. Bulletin of the Chemical Society of Japan, 1993, 66, 3423-3429.	2.0	13
932	The Lowest Lying Singlet and Triplet States of the Halonitrenium Ions NX ₂ ⁺ and NHX ⁺ and a Comparison with the Carbon Analogues CX ₂ and CHX (X = F, Cl, Br, I). A Theoretical Study. Bulletin of the Chemical Society of Japan, 1993, 66, 3153-3165.	2.0	23
933	Theoretical Study of the Rates and Mechanism of the Gas-Phase Reaction H + HN ₃ ⁺ → NH ₂ + N ₂ . Bulletin of the Chemical Society of Japan, 1993, 66, 1944-1948.	2.0	2
934	Ab Initio Triplet Potential Energy Curves of Methyl-Substituted Arylethylenes along the Double Bond Twisting. Bulletin of the Chemical Society of Japan, 1993, 66, 2754-2757.	2.0	8
935	A study of the large amplitude motions of indoline through microwave spectroscopy and ab initio calculations. Molecular Physics, 1993, 78, 1561-1574.	0.8	18
936	The molecular structure of the benzene-ClF complex. Molecular Physics, 1993, 78, 1351-1364.	0.8	5
937	Theoretical Studies on Molecular Determinants for Recognition at H ₃ Histamine Receptors. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1994, 49, 471-475.	0.6	9
938	Localization methods for distributed polarizabilities. Molecular Physics, 1994, 83, 293-307.	0.8	61
939	Accurate prediction of static dipole polarizabilities with moderately sized basis sets. Molecular Physics, 1994, 82, 193-209.	0.8	57
940	Ab Initio Calculations of the Hydrogen Peroxide-Hydrogen Halide Complexes (HOOH...n...n...n.XH, X = F, Cl). The Journal of Physical Chemistry, 1994, 98, 7819-7822.	2.9	20
941	The S ₀ → S ₁ transition of trans-β-methyl styrene. Journal of Chemical Physics, 1994, 101, 11082-11083.	1.2	5
942	Effect of solvation on the shapes, sizes, and anisotropies of polyatomic anions via molecular electrostatic potential topography: An ab initio self-consistent reaction field approach. Journal of Chemical Physics, 1994, 100, 6718-6726.	1.2	33

#	ARTICLE	IF	CITATIONS
943	Variation of interatomic distances in ice VIII to 10 GPa. <i>Physical Review B</i> , 1994, 49, 12540-12550.	1.1	116
944	Electronic structure and potential energy surfaces of the ethylene radical cation at and in the vicinity of the 90°-twisted form. <i>Journal of Chemical Physics</i> , 1994, 100, 1350-1352.	1.2	9
945	Vibrational spectroscopy of NO+(H ₂ O) _n : Evidence for the intracuster reaction NO+(H ₂ O) _n +H ₃ O+(H ₂ O) _{n-2} (HONO) at n=4. <i>Journal of Chemical Physics</i> , 1994, 100, 7153-7165.	1.2	76
946	An ab initio molecular orbital study of the unimolecular dissociation reactions of dia- and trichloroethylene. <i>Journal of Chemical Physics</i> , 1994, 101, 5942-5956.	1.2	36
947	Ab initio potential and variational transition state theory rate constant for H atom association with the diamond (111) surface. <i>Journal of Chemical Physics</i> , 1994, 101, 2476-2488.	1.2	32
948	Chemistry of Higher Group 14 Homologues of Thioketones R ₁ R ₂ M[S] (M=Si, Ge, Sn, Pb). Phosphorus, Sulfur and Silicon and the Related Elements, 1994, 95, 21-33.	0.8	6
949	Theoretical study of the mechanism of recombinative hydrogen desorption from the monohydride phase of Si(100): The role of defect migration. <i>Journal of Chemical Physics</i> , 1994, 101, 8073-8081.	1.2	87
950	The vibrational spectra of krypton and xenon difluoride: High-resolution infrared studies and ab initio calculations. <i>Journal of Chemical Physics</i> , 1994, 101, 1-14.	1.2	88
951	An ab initio molecular orbital study of the unimolecular dissociation reactions of vinylchloride. <i>Journal of Chemical Physics</i> , 1994, 100, 8976-8990.	1.2	64
952	Ab initio calculations on monohalogenophosphanes PH ₂ X (X=F,Cl,Br,I), and experimental detection and characterization of PH ₂ F and PH ₂ Cl by high resolution infrared spectroscopy. <i>Journal of Chemical Physics</i> , 1994, 101, 5585-5595.	1.2	20
953	A computational study of the reaction of the FO radical with H ₂ . <i>Journal of Chemical Physics</i> , 1994, 100, 2896-2899.	1.2	14
954	Gas phase substitution reactions by radical cations. Part 3. Methylene transfer of the C ₁ -C ring-opened oxirane radical cation to pyrazole and imidazole. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1994, 134, 1-10.	1.9	5
955	Spin correlation in ĩ-electron systems from spin-coupled wavefunctions. II. Further applications. <i>Chemical Physics</i> , 1994, 186, 251-273.	0.9	13
956			

#	ARTICLE	IF	CITATIONS
961	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. <i>Journal of Molecular Structure</i> , 1994, 311, 45-53.	1.8	2
962	Electronic structure of the disilyl radical anion. <i>Journal of Physical Organic Chemistry</i> , 1994, 7, 251-255.	0.9	8
963	Ab initio calculations of isotropic hyperfine coupling constants in α -ketoenol radicals. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 97-108.	1.0	11
964	Recent developments in the theoretical design of low-gap polymers and their nonlinear optical properties. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 353-364.	1.0	13
965	Symmetry breaking and its influence on the correlation energy for CF_4^+ and CF_3^+ ions. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 947-956.	1.0	8
966	On the dimerization process of nitroso compounds. <i>Theoretica Chimica Acta</i> , 1994, 87, 321-333.	0.9	18
967	Rotation and inversion states in thermal E/Z isomerization of aromatic azo compounds. <i>Chemical Physics Letters</i> , 1994, 217, 430-435.	1.2	56
968	Vibrational frequency shifts of diatomic molecules in interaction with a Na^+ cation by ab initio calculations. Comparison with experiment on H_2 and N_2 adsorbed in NaA zeolite. <i>Chemical Physics Letters</i> , 1994, 217, 544-550.	1.2	35
969	Theoretical calculation of the height of the barrier for OH rotation in phenol. <i>Chemical Physics Letters</i> , 1994, 218, 261-269.	1.2	25
970	A numerical study of molecular information entropies. <i>Chemical Physics Letters</i> , 1994, 219, 15-20.	1.2	53
971	Full valence complete active space SCF, multireference CI, and density functional calculations of $1A_1 \rightarrow 3B_1$ singlet-triplet gaps for the valence-isoelectronic series BH_2 , CH_2 , NH_2 , AlH_2 , SiH_2 , PH_2 , GaH_2 , GeH_2 , and AsH_2 . <i>Chemical Physics Letters</i> , 1994, 218, 387-394.	1.2	96
972	Quantum chemical models for electrified interfaces. <i>Chemical Physics Letters</i> , 1994, 222, 101-106.	1.2	16
973	Transition state structure of the formic acid isomeric reaction in solution. <i>Chemical Physics Letters</i> , 1994, 223, 23-26.	1.2	7
974	The $Cu-C$ bond dissociation energy of $CuCH_3$. A dramatic failure of the QCISD(T) method. <i>Chemical Physics Letters</i> , 1994, 224, 195-199.	1.2	42
975	Kinetics and thermochemistry of the reversible gas phase reaction $HONO + NH_3 \rightleftharpoons CEH_3H + HONO$ studied by infrared diode laser spectroscopy. <i>Chemical Physics Letters</i> , 1994, 227, 6-12.	1.2	16
976	Vibrational frequencies of AlF_3 . <i>Chemical Physics Letters</i> , 1994, 230, 196-202.	1.2	13
977	The structure of hydridogallium and hydridoaluminium bis(tetrahydroborates). <i>Chemical Physics Letters</i> , 1994, 230, 306-312.	1.2	5
978	Heat of formation determination of the ground and excited state of cyanomethylene ($HCCN$) radical. <i>Chemical Physics Letters</i> , 1994, 230, 372-376.	1.2	13

#	ARTICLE	IF	CITATIONS
979	Ab initio investigation of the stationary points on the potential energy surface for the ethylene-sulfur dioxide complex. <i>Chemical Physics Letters</i> , 1994, 231, 283-288.	1.2	2
980	Proton transfer in model hydrogen-bonded systems by a density functional approach. <i>Chemical Physics Letters</i> , 1994, 231, 295-300.	1.2	99
981	On the use of quantum energy surfaces in the derivation of molecular force fields. <i>Computer Physics Communications</i> , 1994, 84, 131-155.	3.0	82
982	Basis set effects on the direct calculation of intermolecular coupling elements for electron transfer reactions. <i>Inorganica Chimica Acta</i> , 1994, 226, 237-245.	1.2	4
983	On the gas-phase reaction of C ₃ O ₂ ⁺ with C ₃ O ₂ . <i>Organic Mass Spectrometry</i> , 1994, 29, 540-546.	1.3	5
984	Ab initio molecular orbital study of 1-fluorosilatrane. <i>Journal of Computational Chemistry</i> , 1994, 15, 385-394.	1.5	28
985	Optimization of solute cavities and van der Waals parameters in ab initio MST-SCRF calculations of neutral molecules. <i>Journal of Computational Chemistry</i> , 1994, 15, 446-454.	1.5	135
986	Force field for computation of conformational energies, structures, and vibrational frequencies of aromatic polyesters. <i>Journal of Computational Chemistry</i> , 1994, 15, 752-768.	1.5	386
987	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. <i>Journal of Computational Chemistry</i> , 1994, 15, 847-857.	1.5	73
988	Structure of disiloxane: A semiempirical and Post-Hartree-Fock study. <i>Journal of Computational Chemistry</i> , 1994, 15, 925-936.	1.5	21
989	On the calculation of ab initio quantum molecular similarities for large systems: Fitting the electron density. <i>Journal of Computational Chemistry</i> , 1994, 15, 1113-1120.	1.5	46
990	Heats of formation of organic molecules calculated from ab initio theory and a group equivalent scheme: Alkenes. <i>Journal of Computational Chemistry</i> , 1994, 15, 1437-1445.	1.5	11
991	The imidic acids H ₂ C=N-OH and CH ₃ C=N-OH and their tautomeric carbenes H ₂ N=C-OH and CH ₃ C=N(OH): stable species in the gas phase formed by one-electron reduction of their cations. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1994, 136, 191-208.	1.9	55
992	Molecular polarization maps as a tool for studies of intermolecular interactions and chemical reactivity. <i>Journal of Molecular Graphics</i> , 1994, 12, 3-13.	1.7	27
993	Ab initio studies on the mixed heterodimers of ammonia and hydrogen cyanide. <i>Chemical Physics</i> , 1994, 182, 39-51.	0.9	7
994	Quantum chemical study of the adsorption of an H ₂ O molecule on an uncharged mercury surface. <i>Journal of Electroanalytical Chemistry</i> , 1994, 369, 227-231.	1.9	57
995	Variation of geometry, vibrational frequencies and zero-point energies with internal rotation. <i>Journal of Molecular Structure</i> , 1994, 320, 125-146.	1.8	13
996	Ab initio study of molecular conformations, ground state force field and vibrational spectra of S-methyl dithiocarbamate. <i>Journal of Molecular Structure</i> , 1994, 327, 181-191.	1.8	0

#	ARTICLE	IF	CITATIONS
997	Crystal and molecular structure of the lithium p-nitrosophenolate dihydrate dimer: an example of a strong dependence of the I€-electron cooperative substituent effect on the hydrogen-bonding network in the crystal lattice. <i>Journal of Molecular Structure</i> , 1994, 324, 251-259.	1.8	4
998	Correlation of frequency shifts with other properties in ice: a periodic Hartree-€Fock study. <i>Journal of Molecular Structure</i> , 1994, 325, 77-84.	1.8	3
999	Theoretical study of stable silylenes and germylenes. <i>Journal of Organometallic Chemistry</i> , 1994, 475, 73-84.	0.8	73
1000	Ab initio geometry optimisation of the C1i-S(H)OHi-Cl uneven sulfurane with the inclusion of electron correlation. <i>Computational and Theoretical Chemistry</i> , 1994, 315, 29-33.	1.5	1
1001	An ab initio study of anticonvulsants. <i>Computational and Theoretical Chemistry</i> , 1994, 315, 245-251.	1.5	8
1002	Bonding in carbonyl and thiocarbonyl compounds: an ab initio charge density study of H2Ci-€X and HC(i-€X)YH (X,Y i-€ O or S). <i>Computational and Theoretical Chemistry</i> , 1994, 315, 123-136.	1.5	38
1003	The relation between hydrogen-bond strengths and vibrational frequency shifts: a theoretical study of complexes of oxygen and nitrogen proton acceptors and water. <i>Computational and Theoretical Chemistry</i> , 1994, 314, 1-8.	1.5	9
1004	Small clusters between water and alcohols. <i>Computational and Theoretical Chemistry</i> , 1994, 314, 39-47.	1.5	18
1005	Cooperativity in hydrogen bonded clusters: an improved ab initio SCF study on the structure and energetics of neutral, protonated and deprotonated chains and of neutral, cyclic hydrogen fluoride oligomers. <i>Computational and Theoretical Chemistry</i> , 1994, 314, 211-227.	1.5	38
1006	Computational study of imidazole and methyl imidazoles. <i>Computational and Theoretical Chemistry</i> , 1994, 304, 45-51.	1.5	15
1007	A simplified scheme of atom equivalents to relate ab initio energies to enthalpies of formation. <i>Computational and Theoretical Chemistry</i> , 1994, 304, 93-99.	1.5	16
1008	Basis set effects on the intermolecular interaction of hydrocarbon molecules obtained by an ab initio molecular orbital method: evaluation of dispersion energy. <i>Computational and Theoretical Chemistry</i> , 1994, 307, 107-118.	1.5	89
1009	Ab initio Hartree- Fock calculations of the interaction energy of bimolecular complexes. <i>Computational and Theoretical Chemistry</i> , 1994, 307, 239-259.	1.5	9
1010	Conformational effects on vibrational frequencies of cysteine and serine: an ab initio study. <i>Computational and Theoretical Chemistry</i> , 1994, 305, 205-224.	1.5	41
1011	A comparative molecular mechanics, semiempirical and ab initio study of saturated five-membered rings. <i>Computational and Theoretical Chemistry</i> , 1994, 303, 205-212.	1.5	23
1012	Ab initio studies of the dipole polarizabilities of conjugated molecules Part 4. The dipole polarizability and first hyperpolarizability of o-benzyne and related molecules. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 265-273.	1.5	11
1013	Ab initio calculations on the 2,3-dihydro-1,4-diazepinium cation. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 291-298.	1.5	0
1014	Structure-€stability relationships in unsaturated sulfur compounds Part V. An ab initio study of the stable conformations of (E)- and (Z)-methyl-l-propenyl sulfide, sulfoxide and sulfone. <i>Computational and Theoretical Chemistry</i> , 1994, 313, 313-320.	1.5	6

#	ARTICLE	IF	CITATIONS
1015	Reaction of Si ⁺ (2P) with acetylene and with ethylene. Examination of the potential energy surfaces for adducts SiC ₂ H ₂ ⁺ and SiC ₂ H ₄ ⁺ . Computational and Theoretical Chemistry, 1994, 313, 1-17.	1.5	10
1016	Ab initio calculations on H ₃ X ₂ SiLi and H ₃ X ₂ Si ⁺ (X = N, P). Computational and Theoretical Chemistry, 1994, 313, 55-72.	1.5	1
1017	The structure of methimazole and its consequences for current therapeutic models of graves' disease.. Bioorganic and Medicinal Chemistry Letters, 1994, 4, 1357-1360.	1.0	25
1018	Ab initio theoretical study of the monomer-dimer equilibrium in lithium and sodium gem-dichloro allyl and methyl systems. Tetrahedron, 1994, 50, 12511-12520.	1.0	7
1019	Ab initio studies of the dipole polarizabilities of conjugated molecules. Computational and Theoretical Chemistry, 1994, 312, 57-67.	1.5	7
1020	A preliminary study of monomer geometry effects in theoretical calculations of the interaction energy for weak molecular complexes. Computational and Theoretical Chemistry, 1994, 312, 109-114.	1.5	2
1021	Guanine, 6-thioguanine and 6-selenoguanine: ab initio HF/DZP and MP2/DZP comparative studies. Computational and Theoretical Chemistry, 1994, 311, 37-44.	1.5	35
1022	Theoretical studies on specific interactions between biological molecules: interaction of cationic arginine with anionic glutamic acid. Computational and Theoretical Chemistry, 1994, 311, 45-53.	1.5	2
1023	Ab initio studies of crystal field effects. Computational and Theoretical Chemistry, 1994, 304, 101-107.	1.5	16
1024	Metal/conjugated polymer interfaces: A local density functional study of aluminum/polyene interactions. Journal of Chemical Physics, 1994, 100, 9258-9264.	1.2	15
1025	Theoretical reaction pathways for the formation of [Si(OH) ₅] ⁻ and the deprotonation of orthosilicic acid in basic solution. Geochimica et Cosmochimica Acta. Geochimica Et Cosmochimica Acta, 1994, 58, 2755-2756.	1.6	2
1026	Estimation of standard partial molal entropies of aqueous ions at 25°C and 1 bar. Geochimica et Cosmochimica Acta. Geochimica Et Cosmochimica Acta, 1994, 58, 2756-2758.	1.6	10
1027	Molecular structures of cis- and trans-S-Ethyl thiocrotonate. A combined vibrational spectroscopic and ab initio SCF-MO study. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 3491.	1.7	21
1028	Vibrational polarizability of polyacetylene chains. Journal of Chemical Physics, 1994, 101, 10796-10807.	1.2	55
1029	Studies on the boron-nitrogen bond length of the classical donor-acceptor complex H ₃ N-BF ₃ . Journal of the Chemical Society Chemical Communications, 1994, , 1489-1490.	2.0	39
1030	Vibrational Raman optical activity calculations using London atomic orbitals. Faraday Discussions, 1994, 99, 165-180.	1.6	225
1031	An ab initio study of the structure and infrared spectrum of Si ₂ C ₃ . Journal of Chemical Physics, 1994, 100, 175-180.	1.2	52
1032	Structure and fundamental vibrations of phenoxyl radical. Journal of Chemical Physics, 1994, 100, 5023-5035.	1.2	83

#	ARTICLE	IF	CITATIONS
1033	Pseudospectral Møller-Plesset perturbation theory through third order. Journal of Chemical Physics, 1994, 100, 3631-3638.	1.2	70
1034	Theoretical study on the mechanism of ester hydrolysis in micellar catalysis using model systems. Journal of the Chemical Society Perkin Transactions II, 1994, , 2053.	0.9	8
1035	Ab initio quantum chemistry study of the gas-phase reaction of ClO with HO ₂ . Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1811.	1.7	23
1036	Millimeter- and submillimeter-wave spectroscopy of dibridged Si ₂ H ₂ isotopomers: Experimental and theoretical structure. Journal of Chemical Physics, 1994, 100, 8614-8624.	1.2	55
1037	The calculation of molecular response properties using perturbed spin-coupled wave functions. II. Polarizability and magnetic susceptibility of H ₂ and LiH as functions of internuclear distance. Journal of Chemical Physics, 1994, 100, 4417-4431.	1.2	18
1038	Reaction of H ₂ S with OH and a study of the HSO and SOH isomers. High-level ab initio calculations. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 3051.	1.7	36
1039	Hydroxylamine-water: intermolecular potential function and simulation of hydrated NH ₂ OH. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2337-2344.	1.7	10
1040	Ab initio potential energy curves for low-lying states of carbon disulfide. Journal of Chemical Physics, 1994, 100, 7481-7486.	1.2	23
1041	EPR study of NaCl: CO ₂ ? and NaCl : SO ₂ ?. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 3261.	1.7	4
1042	Ab Initio Investigation of the Acetaldehyde-to-Acetaldehyde Enolate Proton Transfer. Journal of the American Chemical Society, 1994, 116, 5400-5404.	6.6	44
1043	Ab initio SCF and force-field calculations on low-energy conformers of 2-acetylamino-2,N-dimethylpropanamide. Journal of the Chemical Society Perkin Transactions II, 1994, , 563-568.	0.9	29
1044	Hydrogen and Halogen Bonding on The Diamond (100)2 Å ⁻¹ Surface: An Ab Initio Study. Materials Research Society Symposia Proceedings, 1994, 349, 439.	0.1	0
1045	An ab Initio MO Study on Gas-Phase Adsorptive Interactions of Aromatic Compounds onto the Surface of Silica Gel. Chemistry Letters, 1994, 23, 2151-2154.	0.7	15
1046	[(PhCH ₂) ₂ NLi ⁺ CH ₂ PPh ₃] ₂ der erste eindeutig charakterisierte Komplex zwischen einem neutralen Phosphorlid und einer Lithiumverbindung: Isolierung, Struktur und ab-initio-Rechnungen. Angewandte Chemie, 1995, 107, 514-516.	1.6	3
1047	Relative carbonyl isocyanate cation [OCNCO] ⁺ affinities of pyridines determined by the kinetic method using multiple-stage (MS ₃) mass spectrometry. Journal of Mass Spectrometry, 1995, 30, 807-816.	0.7	45
1048	Proton-transfer reactions within ionized methanol clusters: Mass spectrometric and molecular orbital studies. Journal of Mass Spectrometry, 1995, 30, 969-976.	0.7	40
1049	The isomers of ionized dimethyl sulfoxide (C ₂ H ₆ OS ⁺) and their CH ₃ OS ⁺ fragments. An ab initio and multiple-stage mass spectrometric (MS _n) study. Journal of Mass Spectrometry, 1995, 30, 1553-1561.	0.7	19
1050	Structure and Bonding of Transition Metal Dihydrogen Complexes[M(CO) ₅ (H ₂)](M= Cr, Mo, W). Angewandte Chemie International Edition in English, 1995, 34, 354-357.	4.4	59

#	ARTICLE	IF	CITATIONS
1051	The First Unambiguous Characterization of a Neutral Phosphorus Ylide-Lithium Complex: Isolation, Structure, and Ab Initio Investigations of $[(\text{PhCH}_2)_2\text{N}=\text{C}(\text{Li}^+\text{CH}_2\text{PPh}_3)]_2$. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 478-481.	4.4	49
1052	Relative stability of alternative chair forms and hydroxymethyl conformations of $^2\text{-D}$ -glucopyranose. <i>Carbohydrate Research</i> , 1995, 276, 219-251.	1.1	184
1053	The photoelectron spectrum of thiazyl cyanide, NSCN. <i>Chemical Physics Letters</i> , 1995, 233, 33-35.	1.2	7
1054	Electron correlation and the structure of 1- and 2-hydrotrioxy. An ab initio and density functional approach. <i>Chemical Physics Letters</i> , 1995, 233, 111-114.	1.2	16
1055	Critical assessment of density functional methods for study of proton transfer processes. <i>Chemical Physics Letters</i> , 1995, 234, 159-164.	1.2	82
1056	On the barrier to molecular axial rotation in crystalline benzene. <i>Chemical Physics Letters</i> , 1995, 239, 267-272.	1.2	4
1057	The solvent effect on the acidities of haloacetic acids in aqueous solution. A RISM-SCF study. <i>Chemical Physics Letters</i> , 1995, 240, 199-204.	1.2	21
1058	Vinylidenecarbenoid. The importance of solvation and electron correlation effects on its structure. <i>Chemical Physics Letters</i> , 1995, 241, 21-25.	1.2	8
1059	Pseudospectral correlation methods on distributed memory parallel architectures. <i>Chemical Physics Letters</i> , 1995, 241, 490-496.	1.2	8
1060	A REMPI study of indene and its clusters with argon and krypton. <i>Chemical Physics Letters</i> , 1995, 242, 139-146.	1.2	16
1061	The calculation of bond dissociation energies of transition metal complexes using isostructural reactions. <i>Chemical Physics Letters</i> , 1995, 242, 521-526.	1.2	48
1062	A theoretical study on the photochemical reaction of ICN in liquid Ar. <i>Chemical Physics Letters</i> , 1995, 245, 469-474.	1.2	18
1063	Ab initio predictions of the lowest electronic states, structures vibrational frequencies of phenylphosphinidene. <i>Chemical Physics Letters</i> , 1995, 246, 59-65.	1.2	16
1064	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding: vibrational consequences of proton position in 1:1 complexes of HCl and 4-X-pyridines. <i>Chemical Physics Letters</i> , 1995, 247, 89-94.	1.2	38
1065	Dipole moment of the water molecule in the condensed phase: a periodic Hartree-Fock estimate. <i>Chemical Physics Letters</i> , 1995, 247, 135-141.	1.2	50
1066	X-Ray spectral determination of the effective charges on phosphorus, sulfur, and chlorine atoms in chemical compounds with a nonempirical charge scale. <i>Heteroatom Chemistry</i> , 1995, 6, 553-557.	0.4	5
1067	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. <i>Journal of Computational Chemistry</i> , 1995, 16, 563-575.	1.5	94
1068	Potential energy function for cation-peptide interactions: An ab initio study. <i>Journal of Computational Chemistry</i> , 1995, 16, 690-704.	1.5	56

#	ARTICLE	IF	CITATIONS
1069	On the existence of SH ₃ , SeH ₃ , and TeH ₃ : Discrepancies between all-electron and pseudopotential calculations. <i>Journal of Computational Chemistry</i> , 1995, 16, 1055-1066.	1.5	54
1070	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. <i>Journal of Computational Chemistry</i> , 1995, 16, 1357-1377.	1.5	944
1071	C ⁺ -H ⁻ O and O ⁻ -H ⁻ O bonded intermediates in the dissociation of low energy methyl glycolate radical cations. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1995, 146-147, 305-322.	1.9	11
1072	Bond functions and the topological properties of the bonds. <i>Structural Chemistry</i> , 1995, 6, 333-337.	1.0	0
1073	Ab-initio SCF investigation of β -aminobutyric acid. <i>Amino Acids</i> , 1995, 8, 271-289.	1.2	6
1075	Silicon carbide in circumstellar environment. <i>Astrophysics and Space Science</i> , 1995, 226, 149-163.	0.5	6
1076	Class IV charge models: A new semiempirical approach in quantum chemistry. <i>Journal of Computer-Aided Molecular Design</i> , 1995, 9, 87-110.	1.3	309
1077	Strain and structural effects on rates of formation and stability of tertiary carbenium ions in the light of molecular mechanics calculations. <i>Journal of Physical Organic Chemistry</i> , 1995, 8, 507-528.	0.9	24
1078	Large basis sets and geometry optimizations in embedded cluster calculations. <i>International Journal of Quantum Chemistry</i> , 1995, 54, 73-81.	1.0	3
1079	Theoretical energies of representative carbon-carbon bonds. <i>International Journal of Quantum Chemistry</i> , 1995, 55, 469-476.	1.0	8
1080	ADFT study of the ground state of the N ₃ radical. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 655-661.	1.0	7
1081	Proton transfer in small model systems: A density functional study. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 697-705.	1.0	27
1082	Systematic ab initio SCF conformational analysis of indol-3-ylacetic acid phytohormone (auxin): Comparison with experiment and molecular mechanics calculations. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 75-81.	1.0	12
1083	Contour integrals in electron propagator theory. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 331-337.	1.0	6
1084	Stable structures of Na(H ₂ O) _n (n = 1-3) clusters by ab initio simulated annealing. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 669-674.	1.0	6
1085	The diagnostic value of the m/z 102 peak in the positive-ion fast-atom bombardment mass spectra of peptides. <i>Rapid Communications in Mass Spectrometry</i> , 1995, 9, 845-850.	0.7	10
1086	Localized charge distributions in stable n-hexane radical cations. <i>Rapid Communications in Mass Spectrometry</i> , 1995, 9, 1115-1119.	0.7	0
1087	The ionized methylene transfer from the distonic radical cation CH-O-CH to heterocyclic compounds. A pentaquadrupole mass spectrometric study. <i>Journal of the American Society for Mass Spectrometry</i> , 1995, 6, 554-563.	1.2	25

#	ARTICLE	IF	CITATIONS
1088	Hydrogen bonds in small water clusters: A theoretical point of view. <i>Journal of Molecular Liquids</i> , 1995, 67, 49-61.	2.3	19
1089	Identification of multiple transition structures on the potential energy hypersurface for [2+2] electrocyclization of the pentadienyl cation bearing a phosphorus in the 3-position. <i>Journal of Molecular Graphics</i> , 1995, 13, 283-286.	1.7	2
1090	Dissociation of acetyl bromide: an experimental and theoretical study. <i>Chemical Physics</i> , 1995, 196, 59-67.	0.9	5
1091	Na ⁺ in liquid hydroxylamine: pair potential function from ab initio calculations and Monte Carlo computer simulation of a 0.36 M NaCl solution (2 NaCl/200 NH ₂ OH). <i>Chemical Physics</i> , 1995, 199, 129-144.	0.9	2
1092	Vibrational frequencies of cysteine and serine zwitterions—an ab initio assignment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1995, 51, 925-928.	2.0	51
1093	Hydrogen bond patterns in solid state carboxylic acids. Vibrational study of the hydrogen bond patterns in oxamic, malonamic and succinamic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1995, 51, 1601-1615.	2.0	22
1094	FT-IR identification, characterization and ab initio vibrational analysis of phosgene, oxalyl chloride and 1,2-dichlorocyclobutene-3,4-dione trapped in argon cryogenic matrices. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1995, 51, 349-362.	2.0	13
1095	Theoretical structure investigations of N-acetyl-L-proline amide. <i>Journal of Molecular Structure</i> , 1995, 352-353, 59-70.	1.8	25
1096	Synthetic and theoretical MO calculational studies of lithiotriazine intermediates produced during alkyllithium-induced cyclotrimerisation reactions of organic nitriles, and comparison of their structures with that of a methylmagnesiatriazine derivative. <i>Journal of Organometallic Chemistry</i> , 1995, 486, 79-93.	0.8	29
1097	A theoretical investigation of the N-oxide moiety. <i>Tetrahedron Letters</i> , 1995, 36, 699-702.	0.7	5
1098	Basis set superposition errors for Slater vs. gaussian basis functions in H-bond interactions. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 77-83.	1.5	15
1099	Geometrical consequences of intermolecular hydrogen bond formation in the formic acid and acetic acid dimers from ab initio MO calculations. <i>Computational and Theoretical Chemistry</i> , 1995, 332, 161-169.	1.5	34
1100	Structure and energetics of SO ₂ —X ⁺ (X = F, Cl, Br, and I) complexes. <i>Computational and Theoretical Chemistry</i> , 1995, 333, 291-296.	1.5	1
1101	Influence of polarization functions on atomic properties of bridge N and H atoms of HCN — HCN. <i>Computational and Theoretical Chemistry</i> , 1995, 335, 11-23.	1.5	10
1102	A generalized multistructural description of the ground state of ozone and water molecules. <i>Computational and Theoretical Chemistry</i> , 1995, 335, 51-57.	1.5	14
1103	Theoretical studies on the substituent effect of the thermal cycloaddition of ethylene and formaldehyde. <i>Computational and Theoretical Chemistry</i> , 1995, 336, 91-100.	1.5	3
1104	Anti van't Hoff/Le Bel geometries of boron compounds. A theoretical study of classical and nonclassical isomers of B ₂ CH ₄ , B ₂ NH ₃ and B ₂ OH ₂ . <i>Computational and Theoretical Chemistry</i> , 1995, 338, 117-130.	1.5	16
1105	Bond angles around tetrahedrally bonded carbon, and distortion of the tetrahedron in CH ₃ -X structures. <i>Computational and Theoretical Chemistry</i> , 1995, 338, 155-173.	1.5	5

#	ARTICLE	IF	CITATIONS
1106	Enthalpies of formation from theoretical methods: a new approach based on density functional theory plus semiempirical corrections. <i>Computational and Theoretical Chemistry</i> , 1995, 337, 25-30.	1.5	15
1107	An ab initio study of the molecular complexes formed between H ₂ S and the acid sites of zeolites. <i>Computational and Theoretical Chemistry</i> , 1995, 341, 237-251.	1.5	12
1108	Theoretical study of the N ₂ O molecule. <i>Computational and Theoretical Chemistry</i> , 1995, 340, 143-148.	1.5	13
1109	Molecular packing analysis. Part 3. The prediction of m-nitroaniline crystal structure. <i>Computational and Theoretical Chemistry</i> , 1995, 357, 1-8.	1.5	9
1110	Variational calculation of the dynamic third-order susceptibility of water. <i>Computational and Theoretical Chemistry</i> , 1995, 357, 199-205.	1.5	3
1111	The effect of substituents on the deprotonation energy of selected primary, secondary and tertiary alcohols. <i>Computational and Theoretical Chemistry</i> , 1995, 358, 229-249.	1.5	8
1112	Elucidation of Primary Radiation Damage in DNA through Application of <i>Ab Initio</i> Molecular Orbital Theory. <i>International Journal of Radiation Biology</i> , 1995, 67, 627-645.	1.0	158
1113	Theoretical study of the vibrational spectra of the transition metal carbonyls M(CO) ₆ [M=Cr, Mo, W], M(CO) ₅ [M=Fe, Ru, Os], and M(CO) ₄ [M=Ni, Pd, Pt]. <i>Journal of Chemical Physics</i> , 1995, 102, 8474-8484.	1.2	395
1114	Systematic study of the static electrical properties of the CO molecule: Influence of the basis set size and correlation energy. <i>Journal of Chemical Physics</i> , 1995, 102, 7573-7583.	1.2	24
1115	On the structure and stability of geometrical isomers of N ₃ F. <i>Journal of Chemical Physics</i> , 1995, 103, 7983-7989.	1.2	7
1116	Bidimensional tunneling splitting in the A ¹ and X ¹ states of tropolone. <i>Journal of Chemical Physics</i> , 1995, 103, 353-359.	1.2	58
1117	Validation of self-consistent hybrid density functionals for the study of structural and electronic characteristics of organic $\dot{\text{C}}$ radicals. <i>Journal of Chemical Physics</i> , 1995, 102, 384-393.	1.2	138
1118	Paramagnetic defects induced by mechanical stress in calcium sulfide phosphor. <i>Journal of Applied Physics</i> , 1995, 78, 876-892.	1.1	11
1119	Gauge-invariant basis sets for magnetic property calculations. <i>Journal of Chemical Physics</i> , 1995, 102, 285-293.	1.2	30
1120	Vibronic activity in trans,trans-1,3,5,7 octatetraene: The S ₀ ⁺ S ₁ spectrum. <i>Journal of Chemical Physics</i> , 1995, 103, 10492-10501.	1.2	29
1121	Mode-selective photoisomerization in 5-hydroxytropolone. II. Theory. <i>Journal of Chemical Physics</i> , 1995, 102, 5260-5270.	1.2	29
1122	Barriers for hydrogen atom diffusion on the Si(100)-1 surface. <i>Journal of Chemical Physics</i> , 1995, 102, 8249-8254.	1.2	45
1123	Ab initio study of styrene and $\dot{\text{C}}$ -methyl styrene in the ground and in the two lowest excited singlet states. <i>Journal of Chemical Physics</i> , 1995, 103, 20-36.	1.2	68

#	ARTICLE	IF	CITATIONS
1124	Pseudospectral multireference single and double excitation configuration interaction. <i>Journal of Chemical Physics</i> , 1995, 102, 7564-7572.	1.2	39
1125	An extended basis set ab initio study of alkali metal cation-water clusters. <i>Journal of Chemical Physics</i> , 1995, 103, 3526-3542.	1.2	223
1126	S ₀ →S ₁ transition of trans- <i>p</i> -methyl styrene: Vibronic structure and dynamics. <i>Journal of Chemical Physics</i> , 1995, 103, 37-47.	1.2	24
1127	Si adatom binding and diffusion on the Si(100) surface: Comparison of ab initio, semiempirical and empirical potential results. <i>Journal of Chemical Physics</i> , 1995, 102, 1044-1056.	1.2	71
1128	van der Waals complexes between COCl ₂ , COFCl, COF ₂ , and chlorine molecule: An infrared matrix isolation and ab initio study. <i>Journal of Chemical Physics</i> , 1995, 102, 1731-1739.	1.2	27
1129	Calculation and interpretation of total energies in electron propagator theory. <i>Journal of Chemical Physics</i> , 1995, 103, 5630-5639.	1.2	14
1130	¹⁹ F nuclear magnetic shielding tensor of CH ₃ F. <i>Molecular Physics</i> , 1995, 86, 235-249.	0.8	13
1131	Carbon-13 chemical shift tensors of carboxylic acids: GIAO calculations in acetic acid + methylamine dimer. <i>Molecular Physics</i> , 1995, 86, 865-872.	0.8	37
1132	Ab Initio Comparison of Identity-Reaction Proton Transfers from Carbon Acids Yielding Localized vs. Delocalized Conjugate Bases. <i>Journal of Organic Chemistry</i> , 1995, 60, 3452-3458.	1.7	36
1133	Ab initio study of the HCO ₃ ⁻ /H ₂ O exchange in the (NH ₃) ₃ ZnII(HCO ₃ ⁻) complex. <i>Theoretica Chimica Acta</i> , 1995, 91, 333-351.	0.9	1
1134	Magnetic Hyperfine Coupling Constants in Free Radicals. , 1995, , 109-138.		15
1135	Structure, epr parameters, and reactivity of organic free radicals from a density functional approach. <i>Theoretica Chimica Acta</i> , 1995, 91, 113-128.	0.9	84
1136	Potential energy profiles of the geometric isomerization and the thermal decomposition of diphosphene HP=PH in the ground and excited electronic states. <i>Theoretica Chimica Acta</i> , 1995, 92, 1-12.	0.9	2
1137	The thioformamidyl group as an $\hat{\iota}$ -substituent in carbocations. <i>Canadian Journal of Chemistry</i> , 1995, 73, 1468-1477.	0.6	11
1138	Theoretical and experimental barriers to internal rotation in 2,6-difluorobenzaldehyde and 2,4,6-trifluorobenzaldehyde. Relatively low barriers. <i>Canadian Journal of Chemistry</i> , 1995, 73, 106-112.	0.6	3
1139	Static vibrational polarizability of all-trans polyethylene and polysilane. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 1641-1646.	1.7	20
1140	Orbiting of the lithium atom in the [Me ₂ Si(NSiMe ₃) ₂] ₂ InLi molecule: theoretical confirmation. <i>Journal of the Chemical Society Chemical Communications</i> , 1995, , 443-444.	2.0	10
1141	Rotational isomerism in acrylic acid. A combined matrix-isolated IR, Raman and ab initio molecular orbital study. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 1571.	1.7	72

#	ARTICLE	IF	CITATIONS
1142	On the C ₂ H ₂ +potential energy hypersurface. An ab initio study. Journal of the Chemical Society Chemical Communications, 1995, , 143-144.	2.0	4
1143	UV-induced isomerization of (E)-crotonic acid. Combined matrix-isolated IR and ab initio MO study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3755.	1.7	25
1144	The resonance Raman spectrum of cyclobutene. Journal of Chemical Physics, 1995, 103, 5911-5918.	1.2	21
1145	Nonequilibrium solvent effects on the S _N 2 reaction using a self-consistent reaction field continuum model based on multipole expansions. Journal of Chemical Physics, 1995, 103, 9249-9260.	1.2	24
1146	Theoretical Approaches to Anharmonic Resonances. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 514-519.	0.9	9
1147	Struktur und Bindungsverhältnisse der Übergangsmetall-Diwasserstoffkomplexe [M(CO) ₅ (H ₂)] (M = Cr, Mo, W). Angewandte Chemie, 1995, 107, 383-386.	1.6	38
1148	Ab initio calculations on electron-transfer catalysis by metal ions. Topics in Current Chemistry, 1996, , 1-24.	4.0	8
1149	Ab Initio Study of Reactions of sym-Triazine. The Journal of Physical Chemistry, 1996, 100, 5681-5689.	2.9	21
1150	Local treatment of electron correlation in coupled cluster theory. Journal of Chemical Physics, 1996, 104, 6286-6297.	1.2	703
1151	The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. Theoretica Chimica Acta, 1996, 93, 281-301.	0.9	298
1152	Structure and Bonding of the Transition-Metal Carbonyl Complexes M(CO) ₅ L (M = Cr, Mo, W) and M(CO) ₃ L (M = Ni, Pd, Pt; L = CO, SiO, CS, N ₂ , NO ⁺ , CN ⁻ , NC ⁻ , HCCH, CCH ₂ , CH ₂ , CF ₂ , H ₂). Organometallics, 1996, 15, 105-117.	1.1	193
1153	A theoretical study of the ionic dissociation of HF, HCl, and H ₂ S in water clusters. Journal of Chemical Physics, 1996, 104, 7081-7085.	1.2	148
1154	Ab Initio Molecular Orbital Analysis of Dimers of cis-Formic Acid. Implications for Condensed Phases. The Journal of Physical Chemistry, 1996, 100, 11285-11291.	2.9	79
1155	Bent's Rule and the Structure of Transition Metal Compounds. Inorganic Chemistry, 1996, 35, 2097-2099.	1.9	44
1156	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. Molecular Physics, 1996, 89, 1313-1325.	0.8	49
1157	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Bicyclic Nonalternant Hydrocarbons: The Pentalenoid and Heptalenoid Systems. The Journal of Physical Chemistry, 1996, 100, 2100-2106.	2.9	23
1158	Formic Acetic Anhydride in the Gas Phase, Studied by Electron Diffraction and Infrared Spectroscopy, Supplemented with ab-Initio Calculations of Geometries and Force Fields. The Journal of Physical Chemistry, 1996, 100, 11620-11629.	2.9	19
1159	Conformers, Energetics, and Basicity of 2,2'-Bipyridine. Journal of the American Chemical Society, 1996, 118, 10269-10274.	6.6	123

#	ARTICLE	IF	CITATIONS
1160	$\hat{\Gamma}^2$ -Cyanoethyl Anion: $\hat{\Lambda}$ Lusus Naturae. Journal of the American Chemical Society, 1996, 118, 4462-4468.	6.6	11
1161	Theoretical Studies of Regioselectivity in the Photochemical Cycloaddition of Allene to Cyclopentenone. Journal of Organic Chemistry, 1996, 61, 952-961.	1.7	15
1162	Structure of the Soluble Lewis Acid Poly(p-phenylenebenzobisthiazole) and Poly(p-phenylenebenzobisoxazole) Complexes. Chemistry of Materials, 1996, 8, 54-59.	3.2	10
1163	Origins of the Exalted b_{2u} Frequency in the First Excited State of Benzene. Journal of the American Chemical Society, 1996, 118, 666-671.	6.6	91
1164	Interplay of Theory and Experiment: $\hat{\Lambda}$ Reversal of the Torquoselectivity of the Electrocyclic Ring Opening of 3-Acetylcyclobutene by a Lewis Acid. Journal of Organic Chemistry, 1996, 61, 640-646.	1.7	13
1165	Ab Initio Study of Some Phenyl- and (Halophenyl)alkali Compounds. Journal of Organic Chemistry, 1996, 61, 3151-3154.	1.7	13
1166	Molecular Structures of Methyl difluoroarsine, CH_3AsF_2 , and Dimethylfluoroarsine, $(\text{CH}_3)_2\text{AsF}$, in the Gas Phase As Determined by Electron Diffraction and Ab Initio Calculations. Inorganic Chemistry, 1996, 35, 6952-6958.	1.9	6
1167	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes $[(\text{C}_5\text{H}_5)_2\text{MH}_3]_{n+}$ ($M = \text{Mo}, \text{W}, n = 1; M = \text{Nb}, \text{Ta}, n = 0$). Journal of the American Chemical Society, 1996, 118, 4617-4621.	6.6	60
1168	Ab Initio Studies of Proton Sponges. 3. 4,5-Bis(dimethylamino)fluorene and 4,5-Bis(dimethylamino)phenanthrene. Journal of Organic Chemistry, 1996, 61, 4480-4482.	1.7	35
1169	Barrier to Rotation in Thioformamide: Implications for Amide Resonance. Journal of the American Chemical Society, 1996, 118, 1737-1742.	6.6	94
1170	Ab Initio Studies of the $\text{GaH}_3 \cdot \text{H}_2\text{O}$, $\text{GaF}_3 \cdot \text{H}_2\text{O}$, and $\text{GaCl}_3 \cdot \text{H}_2\text{O}$ Molecular Complexes. The Journal of Physical Chemistry, 1996, 100, 5672-5675.	2.9	11
1171	Ab Initio Studies of the Exocyclic Hydroxymethyl Rotational Surface in $\hat{\Gamma}^{\pm}$ -d-Glucopyranose. Journal of the American Chemical Society, 1996, 118, 1190-1193.	6.6	54
1172	The Dimerization of Cyclobutadiene. An ab Initio CASSCF Theoretical Study. Journal of the American Chemical Society, 1996, 118, 880-885.	6.6	50
1173	Unexpected Coexistence of Isomeric Forms and Unusual Structures of $\text{Ru}(\text{CO})_2\text{L}_3^-$. Inorganic Chemistry, 1996, 35, 7468-7469.	1.9	16
1174	Ab Initio Molecular Orbital Study on Hyperpolarizabilities of an Interacting 2-Methyl-4-nitroaniline Molecular Pair: $\hat{\Lambda}$ A Molecular Study on the Oriented-Gas Approximation. The Journal of Physical Chemistry, 1996, 100, 8777-8781.	2.9	34
1175	Ligand Effects in Transition Metal Dihydrogen Complexes: $\hat{\Lambda}$ A Theoretical Study 1. Organometallics, 1996, 15, 4547-4551.	1.1	64
1176	Isomers on the Si_2CH_4^+ Potential Energy Surface. Organometallics, 1996, 15, 5391-5398.	1.1	5
1177	Does 4-Iodoniacyclopentene Exist?. Journal of Organic Chemistry, 1996, 61, 8664-8666.	1.7	1

#	ARTICLE	IF	CITATIONS
1178	Structure of a Model Transient Peroxide Intermediate of Peroxidases by ab Initio Methods. <i>Journal of the American Chemical Society</i> , 1996, 118, 10584-10587.	6.6	53
1179	Small and Medium-Sized Bridgehead Bicyclic Lactams: A Systematic ab Initio Molecular Orbital Study. <i>Journal of the American Chemical Society</i> , 1996, 118, 8658-8668.	6.6	131
1180	Theoretical Studies of <i>o</i> -, <i>m</i> -, and <i>p</i> -Benzyne Negative Ions. <i>Journal of the American Chemical Society</i> , 1996, 118, 11872-11883.	6.6	52
1181	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding 2. A theoretical study of distances, force constants, and vibrational frequencies in complexes of hydrogen halides and 4-substituted pyridines. <i>Molecular Physics</i> , 1996, 89, 47-59.	0.8	38
1182	Carbohydrates: A United Atom AMBER* Parameterization of Pyranoses and Simulations Yielding Anomeric Free Energies. <i>Journal of the American Chemical Society</i> , 1996, 118, 2078-2086.	6.6	97
1183	Inductive and Conjugative σ^+ C Polarizations in π -Trithiocarbenium Ions $[C(SH)_3]^+$ and $[C(SH)_3]^{2+}$. Potential Energy Surface Analysis, Electronic Structure Motif, and Spin Density Distribution. <i>Journal of the American Chemical Society</i> , 1996, 118, 11617-11628.	6.6	9
1184	Substituent Effects in the Hetero-Diels-Alder Reaction of Thiocarbonyl Compounds with Butadiene. <i>Journal of Organic Chemistry</i> , 1996, 61, 5121-5129.	1.7	19
1185	Generation of Covalent and Electrostatic Complexes in Association Reactions of tert-Butyl Cation with Small Organics. <i>Journal of the American Chemical Society</i> , 1996, 118, 2449-2457.	6.6	28
1186	Theoretical Study of Metal-Tetrahydroborato Ligand Interactions in $[Y(THF)_4(BH_4)_2]^+$. <i>Inorganic Chemistry</i> , 1996, 35, 3964-3966.	1.9	9
1187	Low Symmetry in $P(NR_2)_3$ Skeletons and Related Fragments: An Inherent Phenomenon. <i>Journal of the American Chemical Society</i> , 1996, 118, 12673-12682.	6.6	37
1188	π -Aromaticity of Substituted 1H-Phosphirenium Cations and Substituted Silacyclopropenes. <i>Journal of Organic Chemistry</i> , 1996, 61, 5840-5846.	1.7	83
1189	Photolysis of Matrix-Isolated 4-R-1,2,4-triazoline-3,5-diones: Identification of Aziridine-2,3-dione Transients. <i>Journal of Organic Chemistry</i> , 1996, 61, 666-670.	1.7	15
1190	Oxidative Addition of Group 14 Element Hydrido Compounds to $OsH_2(\eta^2-CH_2CH_2)(CO)(P^iPr_3)_2$: A Synthesis and Characterization of the First Trihydrido-Silyl, Trihydrido-Germyl, and Trihydrido-Stannyl Derivatives of Osmium(IV). <i>Inorganic Chemistry</i> , 1996, 35, 1250-1256.	1.9	52
1191	Doubly Bridgedansa-Zirconocenes Based on the Norbornadiene Skeleton: A Quantum Mechanical and Molecular Mechanics Study. <i>Organometallics</i> , 1996, 15, 2254-2263.	1.1	19
1192	Hartree-Fock static longitudinal (hyper)polarizability of polyynes. <i>Journal of Chemical Physics</i> , 1996, 104, 8586-8592.	1.2	68
1193	Theory of CO adsorption on MgO(100): the influence of intermolecular interactions on the CO orientation. <i>Surface Science</i> , 1996, 346, 283-293.	0.8	52
1194	Cluster and band structure ab initio calculations on the adsorption of CO on acid sites of the TiO ₂ (110) surface. <i>Surface Science</i> , 1996, 350, 159-175.	0.8	125
1195	Orientation and periodicity in the $c(4 \times 8)$ and $p(2 \times 1)$ structures of 3-thiophene carboxylic acid on Cu(110). <i>Surface Science</i> , 1996, 352-354, 238-247.	0.8	21

#	ARTICLE	IF	CITATIONS
1196	CF ₃ radicals as growth precursors and halogen-assisted growth on diamond (100)2 Å ⁻¹ : an ab initio study. <i>Surface Science</i> , 1996, 359, 213-226.	0.8	12
1197	Topological analysis of the electron localization function applied to delocalized bonds. <i>Canadian Journal of Chemistry</i> , 1996, 74, 1088-1096.	0.6	585
1198	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. <i>Advances in Quantum Chemistry</i> , 1996, , 71-162.	0.4	137
1199	Origin of depressed dipole moments in five-membered, unsaturated heterocycles. <i>Canadian Journal of Chemistry</i> , 1996, 74, 1215-1220.	0.6	14
1200	Ab Initio Study of the Effect of Fluorination upon the Structure and Configurational Stability of I [±] -Sulfonyl Carbanions: The Role of Negative Hyperconjugation. <i>Journal of the American Chemical Society</i> , 1996, 118, 4622-4630.	6.6	84
1201	Design of optimized photorefractive polymers: A novel class of chromophores. <i>Journal of Chemical Physics</i> , 1996, 105, 10637-10647.	1.2	102
1202	Theoretical study of the vibrational spectra of the transition-metal carbonyl hydrides HM(CO) ₅ (M=Mn, Re), H ₂ M(CO) ₄ (M=Fe, Ru, Os), and HM(CO) ₄ (M=Co, Rh, Ir). <i>Journal of Chemical Physics</i> , 1996, 105, 3636-3648.	1.2	87
1203	Factors Controlling Regioselectivity in the Reduction of Polynitroaromatics in Aqueous Solution. <i>Environmental Science & Technology</i> , 1996, 30, 3028-3038.	4.6	80
1204	Why Do Cationic Carbon Monoxide Complexes Have High C=O Stretching Force Constants and Short C=O Bonds? Electrostatic Effects, Not π -Bonding. <i>Journal of the American Chemical Society</i> , 1996, 118, 12159-12166.	6.6	271
1205	Structure of the Transition States and Intermediates Formed in the Water-Exchange of Metal Hexaaqua Ions of the First Transition Series. <i>Journal of the American Chemical Society</i> , 1996, 118, 6760-6766.	6.6	142
1206	Molecular Geometry of Benzaldehyde and Salicylaldehyde: A Gas-Phase Electron Diffraction and ab Initio Molecular Orbital Investigation. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7426-7434.	2.9	111
1207	Intramolecular Hydrogen Bonding and Molecular Structure of 2,5-Dihydroxyterephthalaldehyde and 4,6-Dihydroxyisophthalaldehyde: A Gas-Phase Electron Diffraction and ab Initio Molecular Orbital Study. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19303-19309.	2.9	16
1208	Pyrrolidiazines. 2. Structure and Chemistry of Pyrrolo[1,2-a]pyrazine and 1,3-Dipolar Cycloaddition of Its Azomethine Ylides. <i>Journal of Organic Chemistry</i> , 1996, 61, 4655-4665.	1.7	38
1209	Comparative Study of Nonlocal Density Functional Theory and ab Initio Methods: The Potential Energy Surface of sym-Triazine Reactions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15368-15382.	2.9	18
1210	Structure Analysis Restrained by ab Initio Calculations: The Molecular Structure of 2,5-Dichloropyrimidine in Gaseous and Crystalline Phases. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12280-12287.	2.9	178
1211	Low-Frequency Raman Scattering and the Fast Relaxation Process in Glycerol. <i>Science</i> , 1996, 273, 480-483.	6.0	36
1212	Ab Initio Study of the Interaction of Guanine and Adenine with Various Mono- and Bivalent Metal Cations (Li ⁺ , Na ⁺ , K ⁺ , Rb ⁺ , Cs ⁺ ; Cu ⁺ , Ag ⁺ , Au ⁺ ; Mg ²⁺ , Ca ²⁺ , Sr ²⁺ , Ba ²⁺ ; Zn ²⁺ , Cd ²⁺ , and Hg ²⁺). <i>The Journal of Physical Chemistry</i> , 1996, 100, 7250-7255.	2.9	214
1213	Electronic Structure of Stable Carbenes, Silylenes, and Germylenes. <i>Journal of the American Chemical Society</i> , 1996, 118, 2039-2046.	6.6	403

#	ARTICLE	IF	CITATIONS
1214	Linear and Cyclic Clusters of Hydrogen Cyanide and Cyanoacetylene: A Comparative ab Initio and Density Functional Study on Cooperative Hydrogen Bonding. The Journal of Physical Chemistry, 1996, 100, 13474-13486.	2.9	52
1215	Environmental Effects on the Formation of the Primary and Secondary Ozonides of Ethylene at Cryogenic Temperatures. Journal of the American Chemical Society, 1996, 118, 3687-3693.	6.6	28
1216	A theoretical evaluation of steric and electronic effects on the structure of [OSO4 (NR3)] (NR3 =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.9	1
1217	Density Functional Theory (DFT) Study of Enthalpy of Formation. 1. Consistency of DFT Energies and Atom Equivalents for Converting DFT Energies into Enthalpies of Formation. The Journal of Physical Chemistry, 1996, 100, 14665-14671.	2.9	77
1218	Two different co-ordination modes of hydrazide ligands in silicon and germanium compounds. Journal of the Chemical Society Dalton Transactions, 1996, , 2095.	1.1	13
1219	Rearrangements of the water trimer. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2505.	1.7	91
1220	Proximity effects on nuclear spin-spin coupling constants. Part 2. The electric field effect on $^1\text{J}(\text{CH})$ couplings. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3029-3033.	1.7	46
1221	N,N-dimethylhydroxylamine: structural studies of the free molecule and of hydrogen-bonding in the solid state. Journal of the Chemical Society Perkin Transactions II, 1996, , 2727.	0.9	16
1222	Geometry distorting intramolecular interactions to an alkyne group in 1-(2-aminophenyl)-2-(2-nitrophenyl)ethyne: a joint experimental? theoretical study. Journal of the Chemical Society Perkin Transactions II, 1996, , 1849.	0.9	11
1223	Copper Coordination in Zeolite-Supported Lean NOx Catalysts. The Journal of Physical Chemistry, 1996, 100, 19518-19524.	2.9	39
1224	UV Photoelectron and ab Initio Quantum Mechanical Evaluation of Nucleotide Ionization Potentials in Water Counterion Environments: Polarization Effects on DNA Alkylation by Carcinogenic Methylating Agents. Journal of the American Chemical Society, 1996, 118, 3694-3707.	6.6	53
1225	Theoretical Evaluation of Steric Effects in [ReH5(PR3)2(SiR3)2] Complexes with the IMOMM Method. Inorganic Chemistry, 1996, 35, 6401-6405.	1.9	29
1226	Electronically Excited States of 1,4:5,8-Bismethano-1,4,4a,5,8,8a-hexahydronaphthalene, a Nonconjugated Diene: Comparison of Theory and Experiment. Journal of the American Chemical Society, 1996, 118, 1235-1240.	6.6	7
1227	The structure and binding energy of K+ ether complexes: A comparison of MP2, RI-MP2, and density functional methods. Journal of Chemical Physics, 1996, 105, 1940-1950.	1.2	58
1228	Local weak pairs spectral and pseudospectral singles and doubles configuration interaction. Journal of Chemical Physics, 1996, 105, 6455-6470.	1.2	53
1229	A comparative study of the energetics, structures, and mechanisms of the HCN-HNC and LiCN-LiNC isomerizations. Canadian Journal of Chemistry, 1996, 74, 1072-1077.	0.6	18
1230	Density functional theory study of ethene and acetylene addition to oxazole and protonated oxazole. Journal of the Chemical Society Perkin Transactions II, 1996, , 1021.	0.9	39
1231	$\hat{\pi}$ -Bond cleavage upon electronic excitation of acetyl chloride study of Cl single surfaces by full geometry optimization. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 373-375.	1.7	9

#	ARTICLE	IF	CITATIONS
1232	The generation, stability, dissociation and ion/molecule chemistry of sulfinyl cations in the gas phase. Journal of the Chemical Society Perkin Transactions II, 1996, , 587.	0.9	19
1233	Tetraborane(10), B ₄ H ₁₀ : structures in gaseous and crystalline phases. Journal of the Chemical Society Dalton Transactions, 1996, , 4589.	1.1	96
1234	Volume 1 References. , 1996, , 1215-1369.		0
1235	Three-membered Rings with One Selenium or Tellurium Atom. , 1996, , 259-276.		1
1236	Conformational Analysis of 1,4-Disilabutane and 1,5-Disilapentane by Combined Application of Gas-Phase Electron Diffraction and ab Initio Calculations and the Crystal Structure of 1,5-Disilapentane at Low Temperatures. The Journal of Physical Chemistry, 1996, 100, 9339-9347.	2.9	56
1237	Computation of the Infrared Spectrum of an Acidic Zeolite Proton Interacting with Acetonitrile. The Journal of Physical Chemistry, 1996, 100, 9282-9291.	2.9	30
1238	Ab Initio MO Calculations of NMR ¹⁵ N- ⁶ Li Coupling Constants in Lithium Amide Monomers, Oligomers, and Mixed Aggregates with LiCl. Bulletin of the Chemical Society of Japan, 1996, 69, 305-309.	2.0	38
1239	Theoretical Study on Metal NMR Chemical Shifts. Electronic Mechanism of the Xe Chemical Shift. Bulletin of the Chemical Society of Japan, 1996, 69, 953-959.	2.0	20
1240	A Theoretical Study of the Structural Isomers of Phosphaazarine. Main Group Chemistry, 1996, 1, 189-196.	0.4	1
1241	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	1.2	578
1242	A Density Functional Study of Acidic Hydroxyl Groups in Zeolites and Their Interaction with Carbon Monoxide. The Journal of Physical Chemistry, 1996, 100, 1814-1819.	2.9	33
1243	A theoretical study of the lowest-energy singlet and triplet electronic states p-iminophosphaalkyne and nitrilimine. Computational and Theoretical Chemistry, 1996, 360, 41-54.	1.5	6
1244	Modelling the vibrational behaviour of the cyclic carboxylic acid dimer. SQM force field of the formic acid dimer. Computational and Theoretical Chemistry, 1996, 360, 81-97.	1.5	41
1245	Prediction of geometrical parameters for silatranes: an ab initio molecular orbital and density functional theory study. Computational and Theoretical Chemistry, 1996, 362, 199-208.	1.5	26
1246	An assessment of density functional theory on evaluating activation barriers for small organic gas-phase rearrangement reactions. Computational and Theoretical Chemistry, 1996, 362, 163-173.	1.5	27
1247	A pseudorotation model and ring-puckering of cyclopentane. Computational and Theoretical Chemistry, 1996, 362, 243-255.	1.5	36
1248	Electronic structure of hydroxylated derivatives of the flavylum cation. Computational and Theoretical Chemistry, 1996, 363, 87-96.	1.5	22
1249	Benzyl, 9-fluorenyl and diphenylmethyl cations: structures and relative stabilities based on hydride transfer reactions. Computational and Theoretical Chemistry, 1996, 363, 131-138.	1.5	16

#	ARTICLE	IF	CITATIONS
1250	Cycloaddition extrusion reactions in the preparation of pyrroles. A DFT-AM1 theoretical study. Computational and Theoretical Chemistry, 1996, 365, 55-61.	1.5	37
1251	Semiempirical and ab initio study of closed and open shell derivatives of 10-methylisoalloxazine: a model of flavin redox states. Computational and Theoretical Chemistry, 1996, 364, 139-149.	1.5	22
1252	Comparison of atomic charge distributions obtained from different procedures: basis set and electron correlation effects. Computational and Theoretical Chemistry, 1996, 365, 81-88.	1.5	28
1253	Ab initio and semiempirical (AM1) structural studies of O-(2,2,2-trichloro-1-hydroxyethyl)-benzamidoxime and its hydrogen bonded dimer. Computational and Theoretical Chemistry, 1996, 375, 267-272.	1.5	0
1254	Theoretical and experimental studies of F ₃ SiCO ⁺ and F ₃ SiOC ⁺ . International Journal of Mass Spectrometry and Ion Processes, 1996, 153, 161-172.	1.9	7
1255	The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine. Chemical Physics, 1996, 204, 239-249.	0.9	31
1256	Vapour pressures of fluorocarbons in polyols, polyamines and polycarboxyls. Journal of Fluorine Chemistry, 1996, 78, 167-175.	0.9	1
1257	An infrared and raman spectroscopic study of crystalline trans-crotonic acid. Journal of Molecular Structure, 1996, 377, 181-192.	1.8	11
1258	An unusually small muon-electron coupling constant $\hat{\epsilon}^{\mu}$ muonium addition to biacetyl. Chemical Physics Letters, 1996, 259, 103-112.	1.2	10
1259	The interaction of water with sulfonium ions and the effects of hydration on the energetics of methyl group transfer: An ab initio molecular orbital study of the hydration of (CH ₃) ₃ S ⁺ and (CH ₃) ₂ S ⁺ +CH ₂ CO ₂ ⁻ . Structural Chemistry, 1996, 7, 281-300.	1.0	13
1260	The site of protonation of bifunctional bases with competing basic centers. I. Aromatic nitriles. Structural Chemistry, 1996, 7, 321-327.	1.0	14
1261	Molecular orbital study of the structure and interactions of ylidene rhodanines. Structural Chemistry, 1996, 7, 37-49.	1.0	8
1262	Structures of four o-nitrobenzonitriles. Acta Crystallographica Section B: Structural Science, 1996, 52, 344-351.	1.8	3
1263	Equilibrium and non-equilibrium solvent effects in electrophilic halogenation of ethylenic compounds. Computational and Theoretical Chemistry, 1996, 371, 107-116.	1.5	17
1264	Hyperconjugation as it affects conformational analysis. Computational and Theoretical Chemistry, 1996, 370, 135-146.	1.5	51
1265	The UHF potential energy surfaces of linear polyenes in the lowest excited triplet state. Computational and Theoretical Chemistry, 1996, 369, 67-73.	1.5	3
1266	Density functional study of N-methylpyrrole transformation into N-methylisoindole through cycloaddition-elimination reactions. Computational and Theoretical Chemistry, 1996, 370, 85-91.	1.5	21
1267	Basis set influence on the ab initio description of the dihydrogen complex [Os(PH ₃) ₂ Cl(CO)H(H ₂)] ₁ . Computational and Theoretical Chemistry, 1996, 371, 59-68.	1.5	3

#	ARTICLE	IF	CITATIONS
1268	Theoretical studies of models of thermotropic liquid crystalline polymers. Computational and Theoretical Chemistry, 1996, 388, 27-33.	1.5	1
1269	Intramolecular hydrogen bonding and molecular structure of 2-iminomethyl-phenol and molecular structure of iminomethyl-benzene from ab initio MO calculations. Computational and Theoretical Chemistry, 1996, 388, 107-113.	1.5	3
1270	Geometrical consequences of resonance-assisted hydrogen bonding in 2-nitrovinyl alcohol and indication of a slight attractive Oâ€¦H interaction in 2-nitroethanol. An ab initio molecular orbital investigation. Computational and Theoretical Chemistry, 1996, 388, 315-319.	1.5	1
1271	Structural effects of spiroconjugation: crystal structures of spiro[4.4]nonatetraene and spiro[4.4]nona-1,3,7-triene. Computational and Theoretical Chemistry, 1996, 374, 299-304.	1.5	5
1272	An infrared and raman spectroscopic study of crystalline trans-crotonic acid. Computational and Theoretical Chemistry, 1996, 377, 181-192.	1.5	0
1273	Polynorbornene: synthesis, properties and simulations. Macromolecular Chemistry and Physics, 1996, 197, 3435-3453.	1.1	174
1274	Ein stabiler Lithiumamidâ€¦Methylphosphanoxidâ€¦Komplex: Strukturuntersuchungen und MOâ€¦Rechnungen zum Mechanismus der Protonenabstraktion durch Alkalimetallreagentien. Angewandte Chemie, 1996, 108, 2071-2073.	1.6	2
1275	Theoretical investigations on 1,2-ethanediol: The problem of intramolecular hydrogen bonds. Journal of Computational Chemistry, 1996, 17, 133-147.	1.5	54
1276	An ab initio study of heterodienophiles addition to 2,3-diaza-1,3-butadiene: An example of endo-lone-pair effect on the reaction energy barrier. Journal of Computational Chemistry, 1996, 17, 298-305.	1.5	8
1277	Force field parameters for carbohydrates. Journal of Computational Chemistry, 1996, 17, 450-468.	1.5	112
1278	The structure of 1-chlorosilatrane: An ab initio molecular orbital and a density functional theory study. Journal of Computational Chemistry, 1996, 17, 767-780.	1.5	21
1279	Origins of relative acidity: First and second period hydrides. Journal of Computational Chemistry, 1996, 17, 1771-1781.	1.5	9
1280	Molecular polarization potential maps of the nucleic acid bases. International Journal of Quantum Chemistry, 1996, 57, 123-135.	1.0	144
1281	An ab initio MO study on the thymine dimer and its radical cation. International Journal of Quantum Chemistry, 1996, 57, 949-957.	1.0	20
1282	Size and shape dependence of the electrostatic potential in cluster models of the MgO(100) surface. International Journal of Quantum Chemistry, 1996, 58, 241-250.	1.0	43
1283	Basis set and correlation effects on geometry of octahedral second-row transition-metal complexes. International Journal of Quantum Chemistry, 1996, 60, 1331-1343.	1.0	2
1284	UV photoelectron and ab initio quantum mechanical characterization of nucleotides: The valence electronic structure of anionic 2'-deoxyadenosine-5'-phosphate. International Journal of Quantum Chemistry, 1996, 60, 1735-1743.	1.0	5
1285	Ab initio MO study of the solvent effect on the SN2 reaction of the trimethylsulfonium cation with chloride anion. Heteroatom Chemistry, 1996, 7, 273-279.	0.4	4

#	ARTICLE	IF	CITATIONS
1286	Curvature versus nuclear relaxation contributions to the static vibrational polarizability of polyacetylene chains. <i>Chemical Physics Letters</i> , 1996, 248, 301-308.	1.2	20
1287	Ab initio study of C ₂₀ isomers: geometry and vibrational frequencies. <i>Chemical Physics Letters</i> , 1996, 248, 121-126.	1.2	66
1288	Radical hydrogen transfer reactions: benchmark calculations on the C ₂ H ₄ + H → C ₂ H ₄ transition state. <i>Chemical Physics Letters</i> , 1996, 249, 496-500.	1.2	11
1289	Study of prototypical Diels-Alder reactions by a hybrid density functional/Hartree-Fock approach. <i>Chemical Physics Letters</i> , 1996, 251, 393-399.	1.2	36
1290	Ab initio molecular orbital calculations of the static polarizabilities of xanthone analogues. <i>Chemical Physics Letters</i> , 1996, 251, 125-131.	1.2	22
1291	The diagonal born-oppenheimer correction for He ²⁺ and F+H ₂ . <i>Chemical Physics Letters</i> , 1996, 251, 52-58.	1.2	48
1292	Proton-ordered ice structures at zero pressure. A quantum-mechanical investigation. <i>Chemical Physics Letters</i> , 1996, 253, 201-208.	1.2	66
1293	Theoretical study of molecular dynamics in model base pairs. <i>Chemical Physics Letters</i> , 1996, 256, 370-376.	1.2	90
1294	Accurate small split-valence 3-21SP and 4-22SP basis sets for the first-row atoms. <i>Chemical Physics Letters</i> , 1996, 259, 151-158.	1.2	17
1295	Vibrational polarizability and hyperpolarizability of p-nitroaniline. <i>Chemical Physics Letters</i> , 1996, 261, 57-65.	1.2	79
1296	Binding properties of carbohydrate sulfamates based on ab initio G ₃₁ + G ₃ calculations on N-methyl and N-ethyl sulfamate anions. <i>Carbohydrate Research</i> , 1996, 286, 17-39.	1.1	10
1297	Conformers of Saturated Chains: Matrix Isolation, Structure, IR and UV Spectra of <i>Si₄Me₁₀</i> . <i>Chemistry - A European Journal</i> , 1996, 2, 529-538.	1.7	85
1298	Dynamic Behavior in Solution of the <i>Trans-Hydridodihydrogen Complex [OsHCl(²)(H₂)(CO)(P₃)₂]</i> : Ab Initio and NMR Studies. <i>Chemistry - A European Journal</i> , 1996, 2, 815-825.	1.7	56
1299	The Silaguanidinium Cation and the Search for a Stable Silylium Cation in Condensed Phases. <i>Chemistry - A European Journal</i> , 1996, 2, 869-876.	1.7	32
1300	Crystal Structure of a Representative Mixed Adduct of Trimethylaluminium and a Lithium Amide and a Theoretical MO Study on Model Systems. <i>Chemische Berichte</i> , 1996, 129, 1293-1300.	0.2	16
1301	A Stable Methyl Phosphane Oxide/Lithium Amide Complex: a Structural and MO Computational Investigation of the Mechanism of Proton Abstraction by Alkali Metal Reagents. <i>Angewandte Chemie International Edition in English</i> , 1996, 35, 1942-1944.	4.4	38
1302	Mono- and dianion of benzoquinone-linked [60]fullerene. <i>Tetrahedron Letters</i> , 1996, 37, 7987-7990.	0.7	36
1303	Theoretical study of the structure and vibrational spectrum of 1,3-dithiole-2-thione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 279-286.	2.0	5

#	ARTICLE	IF	CITATIONS
1304	Density functional theory study of vibrational spectra part 5. Structure, dipole moment, and vibrational assignment of azulene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1996, 52, 1211-1220.	2.0	9
1305	Density functional theory study of vibrational spectra. 4. Comparison of experimental and calculated frequencies of all-trans-1,3,5,7-octatetraene "The end of normal coordinate analysis?". <i>Vibrational Spectroscopy</i> , 1996, 12, 73-79.	1.2	15
1306	Density functional theory study of vibrational spectra. 3. Assignment of fundamental vibrational modes of quadricyclane. <i>Vibrational Spectroscopy</i> , 1996, 12, 65-71.	1.2	11
1307	Quantumchemical study of the isobutane cracking on zeolites. <i>Applied Catalysis A: General</i> , 1996, 146, 225-247.	2.2	116
1308	Prediction of relative potency of ketone protease inhibitors using molecular orbital theory. <i>Bioorganic and Medicinal Chemistry</i> , 1996, 4, 1673-1677.	1.4	9
1309	Chlorinated byproducts from the photoassisted catalytic oxidation of trichloroethylene and tetrachloroethylene in the gas phase using porous TiO ₂ pellets. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1996, 97, 175-179.	2.0	63
1310	Vibration frequencies of NCO species as an intermediate for selective reduction of nitrogen monoxide over copper ion-exchanged ZSM-5. <i>Journal of Molecular Catalysis A</i> , 1996, 109, 51-54.	4.8	9
1311	Benzyl(trimethylsilyl)amidolithium: structural studies by ab initio mo and X-RAY crystallographic methods, and comparison with the known structures of dibenzyl and bis(trimethylsilyl) analogues. <i>Polyhedron</i> , 1996, 15, 3533-3542.	1.0	18
1312	A theoretical study of a model of N-tert-butyl- β -phenylnitron (PBN) as active oxygen species scavenger. <i>Chemical Physics</i> , 1996, 204, 313-326.	0.9	3
1313	Theoretical study for the basicities of methylamines in aqueous solution: A RISM-SCF calculation of solvation thermodynamics. <i>Chemical Physics</i> , 1996, 203, 53-67.	0.9	41
1314	Structural effects of spiroconjugation: crystal structures of spiro[4.4]nonatetraene and spiro[4.4]nona-1,3,7-triene. <i>Journal of Molecular Structure</i> , 1996, 374, 299-304.	1.8	21
1315	Ab initio and semiempirical (AM1) structural studies of O-(2,2,2-trichloro-1-hydroxyethyl)-benzamidoxime and its hydrogen bonded dimer. <i>Journal of Molecular Structure</i> , 1996, 375, 267-272.	1.8	3
1316	FTIR-IR spectroscopic study of the phytohormone auxin (Indol-3-ylacetic Acid, IAA) and its n-alkylated and monohalogenated derivatives. <i>Journal of Molecular Structure</i> , 1996, 382, 177-185.	1.8	9
1317	Copper-substituted ethanes as a model for copper-acetylene interactions on the metal surface Quantum mechanical study of the structure and bonding of copper-acetylene and copper-ethylene		

#	ARTICLE	IF	CITATIONS
1322	On quantum molecular similarity measures (QMSM) and indices (QMSI). Journal of Mathematical Chemistry, 1996, 19, 47-56.	0.7	59
1323	The bonding of acetylene and ethylene in high-valent and low-valent transition metal compounds. Journal of Organometallic Chemistry, 1996, 525, 269-278.	0.8	64
1324	Theoretical and experimental studies of the structure and vibrational spectra of NTO. Journal of Molecular Structure, 1996, 384, 87-99.	1.8	46
1325	Standard procedure to obtain a convenient set of scale factors in the SQMFF method. Journal of Molecular Structure, 1996, 385, 49-54.	1.8	9
1326	Interaction of hydrogen and CF _y radicals on the diamond (100)2 Å ⁻¹ surface: an ab initio study. Applied Surface Science, 1996, 107, 122-127.	3.1	2
1327	Lithium diffusion in $\hat{1}^3$ -LiAlO ₂ , a molecular dynamics simulation. Journal of Nuclear Materials, 1996, 232, 131-137.	1.3	28
1328	Ab Initio Study of $\hat{1}^{\pm}$ -Chlorinated Ethyl Hydroperoxides CH ₃ CH ₂ OOH, CH ₃ CHClOOH, and CH ₃ CCl ₂ OOH: \hat{A} Conformational Analysis, Internal Rotation Barriers, Vibrational Frequencies, and Thermodynamic Properties. The Journal of Physical Chemistry, 1996, 100, 8240-8249.	2.9	104
1329	Density Functional Theory Study of Molecular Structures and Vibrational Spectra of 3,4- and 2,3-Pyridyne. The Journal of Physical Chemistry, 1996, 100, 3430-3434.	2.9	48
1330	An ab Initio Investigation of Lithium Ion Hydration. The Journal of Physical Chemistry, 1996, 100, 601-605.	2.9	58
1331	Fluorescence \hat{e} infrared spectroscopy of tropolone and tropolone \hat{e} OD. Journal of Chemical Physics, 1996, 105, 2595-2604.	1.2	75
1332	Exploring chromium (VI) dioxodihalides chemistry: Is density functional theory the most suitable tool?. Journal of Chemical Physics, 1996, 104, 9499-9510.	1.2	28
1333	Improved radial grids for quadrature in molecular density \hat{e} functional calculations. Journal of Chemical Physics, 1996, 104, 9848-9858.	1.2	121
1334	A test of partial third order electron propagator theory: Vertical ionization energies of azabenzenes. Journal of Chemical Physics, 1996, 105, 2762-2769.	1.2	39
1335	New operators for electronic density calculation. II. Application to hydrogen, first \hat{e} row atoms, and first \hat{e} row diatomic hydrides. Journal of Chemical Physics, 1996, 105, 1479-1491.	1.2	20
1336	The intramolecular vibrations of prototypical polythiophenes. Journal of Chemical Physics, 1996, 104, 9704-9718.	1.2	44
1337	Electron correlation effects on the static longitudinal second hyperpolarizability of polymeric chains. Moller \hat{e} Plesset perturbation theory investigation of hydrogen model chains. Journal of Chemical Physics, 1996, 105, 3592-3603.	1.2	29
1338	An investigation of the quantum chemical description of the ethylenic double bond in reactions. I. The electrophilic addition of hydrochloric acid to ethylene. Journal of Chemical Physics, 1996, 105, 6910-6920.	1.2	7
1339	The structure of alkali halide dimers: A critical test of ionic models and new ab initio results. Journal of Chemical Physics, 1996, 104, 8032-8042.	1.2	21

#	ARTICLE	IF	CITATIONS
1340	Investigation of the reliability of density functional methods: Reaction and activation energies for Si-C bond cleavage and H ₂ elimination from silanes. <i>Journal of Chemical Physics</i> , 1996, 104, 148-158.	1.2	112
1341	Energy Decomposition Analyses for Many-Body Interaction and Applications to Water Complexes. <i>The Journal of Physical Chemistry</i> , 1996, 100, 14316-14328.	2.9	256
1342	Ab initio molecular orbital study of the mechanism of photodissociation of trans-azomethane. <i>Journal of Chemical Physics</i> , 1996, 105, 2333-2345.	1.2	37
1343	CONFORMATIONAL ISOMERISM IN GLYCINE AND DITHIOGLYCINE: A COMPARATIVE MOLECULAR ORBITAL STUDY. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 1996, 116, 153-173.	0.8	3
1344	Cation-Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+(1,2-dimethoxyethane) _x , x= 1 and 2, and Li+(12-crown-4). <i>The Journal of Physical Chemistry</i> , 1996, 100, 16116-16125.	2.9	146
1345	Cation-Ether Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of Li+[O(CH ₃) ₂] _x , x= 1-4. <i>The Journal of Physical Chemistry</i> , 1996, 100, 1605-1614.	2.9	141
1346	Interfacing Electronic Structure Theory with Dynamics. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11512-11525.	2.9	72
1347	Gas Phase Ion-Molecule Reactions in Phosphine/Silane Mixtures. <i>The Journal of Physical Chemistry</i> , 1996, 100, 155-162.	2.9	26
1348	Spectroscopic and Theoretical Studies of the Complexes between Nitrous Acid and Ammonia. <i>The Journal of Physical Chemistry</i> , 1996, 100, 539-545.	2.9	75
1349	Ab Initio Calculations on the Use of Helium and Neon as Probes of the van der Waals Surfaces of Molecules. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2588-2596.	2.9	47
1350	Valence Bond Analysis of the Lone Pair Bond Weakening Effect for the X-H Bonds in the Series XHn= CH ₄ , NH ₃ , OH ₂ , FH. <i>The Journal of Physical Chemistry</i> , 1996, 100, 6463-6468.	2.9	28
1351	Ab Initio Calculations of Electric Field Gradients in Cadmium Complexes. <i>The Journal of Physical Chemistry</i> , 1996, 100, 4803-4809.	2.9	30
1352	Ab Initio Molecular Orbital Study of the Acidity of Hydrated Lithium Hydroxide. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15748-15752.	2.9	10
1353	Theoretical Study of the Structure and Vibrational Spectrum of N,N-Dimethylformamide. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16822-16827.	2.9	42
1354	Analytical Second Derivatives for Effective Core Potential. Application to Transition Structures of Cp ₂ Ru ₂ (H) ₄ and to the Mechanism of Reaction Cu + CH ₂ N ₂ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 10936-10944.	2.9	35
1355	Tetramethylene Optimized by MRCI and by CASSCF with a Multiply Polarized Basis Set. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15083-15086.	2.9	25
1356	A Comparative Study of the Gas-Phase Acidities of Aliphatic Alcohols and Carboxylic Acids from Generalized Valence Bond and Generalized Multistructural Calculations. <i>The Journal of Physical Chemistry</i> , 1996, 100, 15105-15110.	2.9	20
1357	Calculated Gas-Phase Acidities Using Density Functional Theory: Is It Reliable?. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17465-17471.	2.9	99

#	ARTICLE	IF	CITATIONS
1358	Quadratic Nonlinear Optical Susceptibilities of a New SHG Material, 3-Aminoxanthone: A Theoretical Study on Its Molecular and Crystal Susceptibilities. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19344-19349.	2.9	10
1359	Matrix Infrared Spectra and ab Initio Calculations of the Nitrous Acid Complexes with N ₂ and CO. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11610-11615.	2.9	55
1360	Energies and Geometries of Isographic Hydrogen-Bonded Networks. 1. The (8) Graph Set. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2957-2967.	2.9	32
1361	Computed Optical Absorption and Photoluminescence Spectra of Neutral Oxygen Vacancies in α -Quartz. <i>Physical Review Letters</i> , 1997, 79, 753-756.	2.9	138
1362	Vibrations and soliton dynamics of positively charged polyacetylene chains. <i>Journal of Chemical Physics</i> , 1997, 107, 5433-5444.	1.2	49
1363	The gas-phase infrared spectra of anthracene-h ₁₀ and anthracene-d ₁₀ . <i>Journal of Chemical Physics</i> , 1997, 106, 9004-9012.	1.2	37
1364	Density functional crystal orbital study on the normal vibrations of polyacetylene and polymethineimine. <i>Journal of Chemical Physics</i> , 1997, 107, 10075-10084.	1.2	66
1365	Microwave spectroscopic and ab initio studies of the hydrogen-bonded trimethylamine-hydrogen sulfide complex. <i>Journal of Chemical Physics</i> , 1997, 107, 2227-2231.	1.2	20
1366	The C ₆ H ₆ -(H ₂ O) ₂ complex: Theoretical predictions of the structure, energetics, and tunneling dynamics. <i>Journal of Chemical Physics</i> , 1997, 106, 849-863.	1.2	31
1367	Electron-positron momentum density in TTF-TCNQ. <i>Physical Review B</i> , 1997, 55, 2048-2055.	1.1	8
1368	Diels-Alder reactions: An assessment of quantum chemical procedures. <i>Journal of Chemical Physics</i> , 1997, 106, 8727-8732.	1.2	49
1369	Dielectric friction effects on rotational reorientation of three cyanine dyes in n-alcohol solutions. <i>Journal of Chemical Physics</i> , 1997, 107, 7601-7612.	1.2	19
1370	Quantum-chemical ab initio Study on the Adenine-Difluorotoluene Complex - A Mimic for the Adenine-Thymine Base Pair. <i>Journal of Biomolecular Structure and Dynamics</i> , 1997, 15, 619-624.	2.0	52
1371	Proton-ordered models of ordinary ice for quantum-mechanical studies. <i>Journal of Chemical Physics</i> , 1997, 106, 8030-8040.	1.2	67
1372	Conrotatory and disrotatory pathways in the electrocyclic isomerization of cyclobutene to cis-butadiene: The spin-coupled viewpoint. <i>Journal of Chemical Physics</i> , 1997, 107, 8917-8926.	1.2	11
1373	A least-action variational method for determining tunneling paths in multidimensional system. <i>Journal of Chemical Physics</i> , 1997, 107, 10506-10514.	1.2	17
1374	Linear and nonlinear polarizabilities of polydiacetylene and polybutatriene chains: An ab initio coupled Hartree-Fock investigation. <i>Journal of Chemical Physics</i> , 1997, 107, 2463-2480.	1.2	59
1375	Stilbenoid molecules: An experimental and theoretical study of trans-1-(2-pyridyl)-2-(4-pyridyl)-ethylene and the parent molecule. <i>Journal of Chemical Physics</i> , 1997, 107, 1073-1078.	1.2	9

#	ARTICLE	IF	CITATIONS
1376	Tetrahedral quadrangular carbon clusters. <i>Molecular Physics</i> , 1997, 92, 441-444.	0.8	9
1377	Active Site Structure in Zeolite-Supported Lean NO _x Catalysts. <i>Materials Research Society Symposia Proceedings</i> , 1997, 492, 231.	0.1	0
1378	Gas-Phase Generation and Photoelectron Spectrum of 1,1-Dimethyl-N-Dimethylsilylsilanimine. <i>Main Group Chemistry</i> , 1997, 2, 97-106.	0.4	8
1379	An ab initio study of anharmonicity and matrix effects on the hydrogen-bonded BrH:NH complex 3. <i>Molecular Physics</i> , 1997, 92, 429-440.	0.8	6
1380	Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons: Applications to Chromatography. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5374-5377.	1.1	18
1381	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Ground and Electronically Excited States of the Cyclic Conjugated Hydrocarbons: Cyclobutadiene, Benzene, and Cyclooctatetraene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5712-5718.	1.1	36
1382	IR Structural Identification of Oxocumulene-HCl Complexes Generated in Cryogenic Matrixes. The Product-like Transition State of the Corresponding Electrophilic Addition. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1093-1098.	1.1	27
1383	Conformational equilibrium and potential-energy surface of 1-chlorobutane by microwave spectroscopy and ab initio calculations. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 2131-2137.	1.7	12
1384	Transacetalization of 1,3-dioxane with acylium and sulfinyl cations in the gas phase. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 2105-2111.	0.9	17
1385	Ab initio theoretical investigation of the mechanism for lactone formation from halocarboxylates: leaving group, substituent, solvent and isotope effects. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 959-966.	0.9	18
1386	1,2-Di-tert-butyltetrafluorodisilane, ButSiF ₂ SiF ₂ But: vibrational spectra and molecular structure in the gas phase by electron diffraction and ab initio calculations. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 2475-2482.	1.1	6
1387	Structure determination from sparse data: geometries of the monohalogenophosphines. <i>Chemical Communications</i> , 1997, , 231-232.	2.2	2
1388	Experimental and theoretical study of monosubstituted guanidines by vibrational spectroscopy Part 1. Structure of cyanoguanidine. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 1357-1360.	1.7	17
1389	Markovnikov addition to alkenes. A different view from core-electron spectroscopy and theory. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 749-756.	0.9	32
1390	Field dependence of the protonation equilibrium of 2-pyridinecarboxylic acid on copper in sulfuric acid. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 1321-1324.	1.7	6
1391	C-H...C Hydrogen bonding involving ylides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 2241-2248.	0.9	28
1392	Conformations and rotational barriers of 2,2-bi-1H-imidazole Semiempirical, ab initio, and density functional theory calculations. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 2967-2971.	1.7	1
1393	Synthesis and reactivity of [OsH(C ₆ H ₄ (CH=CH)) ₂ (CO)(PPri ₃) ₂] and the formato compounds [Os{(E)-CH=CHPh}(I-2-O ₂ CH)(CO)(PPri ₃) ₂] and [OsH(I-2-O ₂ CH)(CO)(PPri ₃) ₂]*. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 181-192.	1.1	31

#	ARTICLE	IF	CITATIONS
1394	Conformational analysis of 2-(carboxycyclopropyl)glycine agonists of glutamate receptors in aqueous solution using a combination of NMR and molecular modelling experiments and charge calculations. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 2677-2690.	0.9	5
1395	Density Functional Theory Calculations of the Effects of Local Composition and Defect Structure on the Proton Affinity of $H\ddot{a}^{\sim}$ ZSM-5. <i>Journal of Physical Chemistry B</i> , 1997, 101, 10058-10064.	1.2	55
1396	Quantum Chemical Investigation of Structures, Rotational Barriers, and Vibrational Spectra of the Rotamers of Ethyl Nitrite (CH_3CH_2ONO). <i>Journal of Physical Chemistry A</i> , 1997, 101, 5580-5586.	1.1	14
1397	Molecular Structure of 1,3,5-Triazine in Gas, Solution, and Crystal Phases and by ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 1997, 101, 10029-10038.	1.1	18
1398	Examination of the Valence Tautomers Benzene Oxide and Oxepin and Two Derivative Systems by ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3371-3376.	1.1	27
1399	Gas-Phase Characterization of Unhindered Silanimines by Photoelectron Spectroscopy: An Experimental and Theoretical Study of the SiN Double Bond. <i>Inorganic Chemistry</i> , 1997, 36, 1482-1487.	1.9	28
1400	Photochemical Reactions of Silylene with Ethene and Silene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 10053-10062.	1.1	3
1401	Carbenes as Pure Donor Ligands: A Theoretical Study of Beryllium Carbene Complexes. <i>Organometallics</i> , 1997, 16, 442-448.	1.1	80
1402	Ab initio CLOPPA decomposition of the static molecular polarizability tensor. <i>Molecular Physics</i> , 1997, 91, 105-112.	0.8	15
1403	Binding of Nitric Oxide to First-Transition-Row Metal Cations: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8530-8539.	1.1	71
1404	Elongated Dihydrogen Complexes: A Combined Electronic DFT + Nuclear Dynamics Study of the $[Ru(H\ddot{A}\ddot{A}\ddot{H})(C_5H_5)(H_2PCH_2PH_2)]^+$ Complex. <i>Journal of the American Chemical Society</i> , 1997, 119, 9840-9847.	6.6	64
1405	A Density Functional Study of the Vibrations of Three Oligomers of Thiophene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7283-7291.	1.1	33
1406	A Theoretical Case Study of Substituent Effects and Microsolvation on the Binding Specificity of Crown Ethers. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7292-7298.	1.1	37
1407	Competition between Steric and Electronic Control of Structure in $Ru(CO)_2L_2L^{\sim}$ Complexes. <i>Organometallics</i> , 1997, 16, 1979-1993.	1.1	51
1408	Characterization of a Resting State Model of Peroxidases by ab Initio Methods: Optimized Geometries, Electronic Structures, and Relative Energies of the Sextet, Quartet, and Doublet Spin States. <i>Journal of the American Chemical Society</i> , 1997, 119, 9848-9851.	6.6	15
1409	Systematic Analysis of Bond Energies Calculated by the Integrated Molecular Orbital Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4641-4645.	1.1	19
1410	Cluster model calculations of oxygen vacancies in SiO_2 and MgO Formation energies, optical transitions and EPR spectra. <i>Faraday Discussions</i> , 1997, 106, 155-172.	1.6	59
1411	Theoretical Characterization of the Vibrational Properties at the Aluminum/trans-Polyacetylene Interface. <i>Journal of Physical Chemistry B</i> , 1997, 101, 4193-4202.	1.2	11

#	ARTICLE	IF	CITATIONS
1412	A Charge Density Analysis of Cationic and Anionic Hydrogen Bonds in a π -Proton Sponge-Complex. <i>Journal of the American Chemical Society</i> , 1997, 119, 11502-11509.	6.6	103
1413	Regarding the Structures and Fluxionality of Tricyclopentadienylaluminum Compounds. <i>Organometallics</i> , 1997, 16, 871-879.	1.1	39
1414	Structures, Automerizations, and Isomerizations of C ₃ H ₂ Isomers. <i>Journal of the American Chemical Society</i> , 1997, 119, 5847-5856.	6.6	141
1415	Stepwise Introduction of π -Electron Cross-Conjugation: A Possible Access to [5]Radialenes?. <i>Journal of Organic Chemistry</i> , 1997, 62, 5339-5343.	1.7	4
1416	Electronic Structure Investigation and Nuclear Quadrupole Interactions in \hat{I}^2 -HMX. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8302-8308.	1.1	10
1417	Structure and Dynamics of LR π -H ₄ (L = Cp, Tp) Systems. A Theoretical Study. <i>Organometallics</i> , 1997, 16, 3805-3814.	1.1	48
1418	Resolving Discrepancies between Theory and Experiment: IR Spectrum of the Proton-Shared HBr:Pyridine Complex. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4481-4483.	1.1	8
1419	Theoretical Calculations of Coefficients of Friction between Weakly Interacting Surfaces. <i>Journal of Physical Chemistry A</i> , 1997, 101, 10045-10052.	1.1	20
1420	Reaction of FO Radicals with CO: An ab Initio Study of the Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1172-1177.	1.1	10
1421	Hydroxide Attack on Acetylene: Theoretical Structures and Energies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1758-1762.	1.1	3
1422	Characteristics of the LinC ₆₀ Complexes for n = 1-6 and 12: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5551-5554.	1.1	15
1423	Computational Insight into the Chemistry of \hat{I}^2 -(Phosphatoxy)alkyl Radicals: [3,2]- and [1,2]-Phosphatoxy Rearrangements and a New Pathway for syn-Elimination of Phosphate. <i>Journal of the American Chemical Society</i> , 1997, 119, 2889-2893.	6.6	23
1424	Transacetalization with Acylium Ions. A Structurally Diagnostic Ion/Molecule Reaction for Cyclic Acetals and Ketals in the Gas Phase. <i>Journal of Organic Chemistry</i> , 1997, 62, 5096-5103.	1.7	58
1425	Evidence from ¹³ C and ²⁹ Si Hyperfine Structure Calculations against the $\hat{I}f^*$ -Configuration of Cyclopolysilane Radical Anions As Determined by ENDOR Spectroscopy. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7874-7878.	1.1	3
1426	Gas-Phase Conformational Analysis of 1,4,7-Trithiacyclononane. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9180-9184.	1.1	8
1427	Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb(\hat{I} -5-C ₅ H ₄ SiMe ₃) ₂ (\hat{I} -2-H ₂)(CNR)] ₂ +Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. <i>Journal of the American Chemical Society</i> , 1997, 119, 6107-6114.	6.6	57
1428	Molecular Structure of 3,4-Dimethylenehexa-1,5-diene ([4]Dendralene), C ₈ H ₁₀ , in the Gas Phase As Determined by Electron Diffraction and ab Initio Calculations. <i>Journal of Organic Chemistry</i> , 1997, 62, 2767-2773.	1.7	34
1429	Novel [3 + 2] 1,3-Cycloaddition of the Ionized Carbonyl Ylide +CH ₂ OCH ₂ with Carbonyl Compounds in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1997, 119, 3550-3557.	6.6	28

#	ARTICLE	IF	CITATIONS
1430	Site Preference Energetics, Fluxionality, and Intramolecular M ⁿ H ⁿ -N Hydrogen Bonding in a Dodecahedral Transition Metal Polyhydride. <i>Inorganic Chemistry</i> , 1997, 36, 5505-5511.	1.9	34
1431	Systematic Study of the Potential Energy Surface for the Base-Induced Elimination Reaction of Fluoride Ion with Ethyl Fluoride Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1997, 101, 208-218.	1.1	33
1432	Mechanisms of SiO ₂ Etching: Ab Initio Calculations on the Reactions of CF _m -(m = 3 ⁿ -1) and NF _n -(n = 2, 1) Ions with Local Surface Models. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5377-5381.	1.2	1
1433	Ab Initio Determination of the Force Field of Dichloromethane, Verified by Gas-Phase Infrared Frequencies and Intensities and Applied to a Combined Electron Diffraction and Microwave Investigation of Geometry. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5919-5925.	1.1	10
1434	[Cp ₂ M] Metallocene Species Promoted Reductive Coupling of Cl ₂ CPR: Synthesis, Structure, and Reactivity of the First 3,4-Dihalo-1,2-dihydro-1,2-diphosphetes. <i>Organometallics</i> , 1997, 16, 4551-4556.	1.1	12
1435	Ab Initio and Semiempirical Studies on the Transition Structure of the Baeyer and Villiger Rearrangement. The Reaction of Acetone with Performic Acid. <i>Journal of Physical Chemistry A</i> , 1997, 101, 192-200.	1.1	31
1436	Structure and Bonding of the Isoelectronic Hexacarbonyls [Hf(CO) ₆] ²⁻ , [Ta(CO) ₆] ⁻ , W(CO) ₆ , [Re(CO) ₆] ⁺ , [Os(CO) ₆] ²⁺ , and [Ir(CO) ₆] ³⁺ : A Theoretical Study. <i>Organometallics</i> , 1997, 16, 4807-4815.	1.1	128
1437	Ab Initio and Nonlocal Density Functional Study of 1,3,5-Trinitro-s-triazine (RDX) Conformers. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8720-8726.	1.1	141
1438	Structure and Stability of Y-Conjugated Silylium Cations [Si(XH) ₃] ⁺ (X = O, S, Se, and Te). <i>Journal of the American Chemical Society</i> , 1997, 119, 11078-11085.	6.6	9
1439	Quantum Chemical Reaction Path and Transition State for a Model Cope (and Reverse Cope) Elimination. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3554-3560.	1.1	32
1440	[1,2]-Acyloxy Shifts in Radicals. A Computational Investigation of Substituent and Solvent Effects. <i>Journal of the American Chemical Society</i> , 1997, 119, 1087-1093.	6.6	39
1441	Theoretical Investigation of Thiophene Oligomers: A Spin-Coupled Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4437-4443.	1.1	12
1442	Flash Vacuum Thermolysis: First Gas-Phase Generation of Unhindered Silylidenephosphanes and Characterization by Photoelectron Spectroscopy. <i>Organometallics</i> , 1997, 16, 1635-1640.	1.1	14
1443	From Peptide to Non-Peptide. 3. Atropisomeric GPIIb/IIIa Antagonists Containing the 3,4-Dihydro-1H-1,4-benzodiazepine-2,5-dione Nucleus. <i>Journal of Medicinal Chemistry</i> , 1997, 40, 717-729.	2.9	58
1444	Cation ⁿ -Ether Complexes in the Gas Phase: Bond Dissociation Energies of Na ⁺ (dimethyl ether) _x , x = 1 ⁿ -4; Na ⁺ (1,2-dimethoxyethane) _x , x = 1 and 2; and Na ⁺ (12-crown-4). <i>Journal of Physical Chemistry A</i> , 1997, 101, 831-839.	1.1	127
1445	An ab Initio MO Study on the Transformation of Acetylene to Vinylidene in the Coordination Sphere of Rhodium(I). The Intra- and Intermolecular Proton Transfer Mechanism. <i>Journal of the American Chemical Society</i> , 1997, 119, 360-366.	6.6	135
1446	Novel Aspects of the [1,3] Sigmatropic Silyl Shift in Allylsilane. <i>Journal of the American Chemical Society</i> , 1997, 119, 807-815.	6.6	28
1447	Synthesis of Volatile Cyclic Silylamines and the Molecular Structures of Two 1-Aza-2,5-disilacyclopentane Derivatives. <i>Inorganic Chemistry</i> , 1997, 36, 4360-4368.	1.9	23

#	ARTICLE	IF	CITATIONS
1448	Assessment of Procedures for Calculating Radical Hyperfine Structures. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1352-1359.	1.1	75
1449	Hydrogen Bonding between Amino Acid Backbone and Side Chain Analogues: A High-Level ab Initio Study. <i>Journal of the American Chemical Society</i> , 1997, 119, 12952-12961.	6.6	63
1450	π -Donor Bonds in SiON Units: An Inherent Structure- Determining Property Leading to (4+) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 667 <i>Journal of the American Chemical Society</i> , 1997, 119, 4143-4148.	6.6	93
1451	A Theoretical Study of the Reaction $H_2 + Fe(CO)_4 \rightarrow H_2Fe(CO)_4$. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2358-2363.	1.1	42
1452	Theoretical Characterization of an Intermediate for the [3 + 2] Cycloaddition Mechanism in the Bis(dihydroxy-quinidine)-3,6-Pyridazine-Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of Organic Chemistry</i> , 1997, 62, 7892-7894.	1.7	27
1453	Endohedral Metallofullerenes. Are the Isolated Pentagon Rule and Fullerene Structures Always Satisfied?. <i>Journal of the American Chemical Society</i> , 1997, 119, 12693-12694.	6.6	157
1454	Mechanistic Aspects of the Alternating Copolymerization of Propene with Carbon Monoxide Catalyzed by Pd(II) Complexes of Unsymmetrical Phosphine-Phosphite Ligands. <i>Journal of the American Chemical Society</i> , 1997, 119, 12779-12795.	6.6	183
1455	Effect of a Polar Environment on the Conformation of Phospholipid Head Groups Analyzed with the Onsager Continuum Solvation Model. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2996-3004.	1.1	19
1456	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of β -Lactam Antibiotics. A Theoretical Study Including Solvent Effects. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3581-3588.	1.2	56
1457	Quantum Mechanics and Molecular Mechanics Studies of the Low-Energy Conformations of 9-Crown-3. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1920-1926.	1.1	12
1458	Full-Optimized Reaction Space MCSCF+MP2 Study on Reactions of Diradical Systems: $o\text{-C}_6\text{H}_4(\text{CH})_2$, $o\text{-C}_6\text{H}_4\text{CHN}$, and $o\text{-C}_6\text{H}_4\text{N}_2$. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3377-3381.	1.1	2
1459	Cation-Ether Complexes in the Gas Phase: Bond Dissociation Energies of $K^+(\text{dimethyl ether})_x$, $x = 1$ to 4; $K^+(\text{1,2-dimethoxyethane})_x$, $x = 1$ and 2; and $K^+(\text{12-crown-4})$. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4254-4262.	1.1	98
1460	Ab Initio Study of the Mechanism of Photolytic Deazation of 2,3-Diazabicyclo[2.2.2]oct-2-ene and 2,3-Diazabicyclo[2.2.1]hept-2-ene. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2379-2383.	1.1	7
1461	Ring Opening of Silacyclobutane. <i>Journal of the American Chemical Society</i> , 1997, 119, 11966-11973.	6.6	26
1462	Cation-Ether Complexes in the Gas Phase: Bond Dissociation Energies of $M^+(\text{dimethyl ether})_x$, $x = 1$ to 3, $M^+(\text{1,2-dimethoxyethane})_x$, $x = 1$ and 2, and $M^+(\text{12-crown-4})$ Where $M = \text{Rb}$ and Cs . <i>Journal of Physical Chemistry A</i> , 1997, 101, 7007-7017.	1.1	104
1463	An ab Initio QCISD Study of the Potential Energy Surface for the Reaction $\text{HNO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{OH}$. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9430-9438.	1.1	25
1464	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of N_2O_2 . <i>Journal of Physical Chemistry A</i> , 1997, 101, 4283-4289.	1.1	21
1465	Theoretical Studies of Diels-Alder Reactions of Acetylenic Compounds. <i>Journal of Organic Chemistry</i> , 1997, 62, 6991-6996.	1.7	58

#	ARTICLE	IF	CITATIONS
1466	Ab Initio Study of M ⁺ :18-Crown-6 Microsolvation. Journal of Physical Chemistry A, 1997, 101, 2723-2731.	1.1	109
1467	Possible Nitrogen Fixation by Disilabutadiene. Organometallics, 1997, 16, 5058-5063.	1.1	12
1468	Crystal Packing and Molecular Dynamics Studies of the 5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one Crystal. Journal of Physical Chemistry B, 1997, 101, 3605-3613.	1.2	33
1469	Theoretical study of bifurcating reaction paths. Journal of Chemical Physics, 1997, 107, 1137-1146.	1.2	54
1470	Theoretical Study of Thermal Decomposition Mechanisms of Isoxazole. Journal of Physical Chemistry A, 1997, 101, 7231-7235.	1.1	14
1471	Experimental and Theoretical Studies of SiF _n (CO) ₂ ⁺ Cations with n = 2 and 3: A Search for Pentacoordinate Cationic Silicon. Journal of Physical Chemistry A, 1997, 101, 7258-7264.	1.1	7
1472	The alkali metal trifluorides M ⁺ F ₃ ⁻ : how well can theory predict experiment?. Molecular Physics, 1997, 90, 515-524.	0.8	7
1473	Theoretical Study of Cation/Ether Complexes: The Alkali Metals and Dimethyl Ether. Journal of Physical Chemistry A, 1997, 101, 6125-6131.	1.1	58
1474	Molecular Structures and Conformations of Polyphosphazenes: A Study Based on Density Functional Calculations of Oligomers. Journal of the American Chemical Society, 1997, 119, 3611-3618.	6.6	66
1475	Gaseous and crystalline phase molecular structures of 4,6-dichloropyrimidine, 2,6-dichloropyrazine and 3,6-dichloropyridazine. Journal of the Chemical Society Perkin Transactions II, 1997, , 857-868.	0.9	12
1476	Mechanism of Water Exchange for the Di- and Trivalent Metal Hexaqua Ions of the First Transition Series. Journal of the American Chemical Society, 1997, 119, 5230-5238.	6.6	165
1477	First principles implementation of solvent effects without outlying charge error. Journal of Chemical Physics, 1997, 106, 6622-6633.	1.2	213
1478	Molecular structure of S-ethylthioacrylate Combined vibrational spectroscopic and ab initio SCF-MO study. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 3619-3624.	1.7	3
1479	Theoretical Study of Potential Energy Surface and Thermal Rate Constants for the C ₆ H ₅ + H ₂ and C ₆ H ₆ + H Reactions. Journal of Physical Chemistry A, 1997, 101, 3189-3196.	1.1	116
1480	Ab Initio and DFT Potential Energy Surfaces for Cyanuric Chloride Reactions. Journal of Physical Chemistry A, 1997, 101, 3400-3407.	1.1	2
1481	Covalence and spin polarisation in tetraphenylarsonium tetrachloronitridotchnetate(VI) studied by polarised neutron diffraction. Journal of the Chemical Society Dalton Transactions, 1997, , 1447-1454.	1.1	4
1482	An Ab Initio Study of Hydrogen Abstraction from Cluster Models for the Diamond Surface. Journal of Physical Chemistry B, 1997, 101, 9574-9580.	1.2	19
1483	The π -Donor Ability of the Halogens in Cations and Neutral Molecules. A Theoretical Study of AX ₃ ⁺ , AH ₂ X ⁺ , YX ₃ , and YH ₂ X (A = C, Si, Ge, Sn, Pb; Y = B, Al, Ga, In, Tl; X = F, Cl, Br, I). Journal of the American Chemical Society, 1997, 119, 6648-6655.	6.6	146

#	ARTICLE	IF	CITATIONS
1484	Coordination Chemistry and Mechanisms of Metal-Catalyzed CC-Coupling Reactions. 10. Ligand Dissociation in Rhodium-Catalyzed Hydroformylation: A Theoretical Study. <i>Organometallics</i> , 1997, 16, 701-708.	1.1	77
1485	Towards mechanosynthesis of diamondoid structures: I. Quantum-chemical molecular dynamics simulations of sila-adamantane synthesis on hydrogenated Si(111) surface with the STM. <i>Nanotechnology</i> , 1997, 8, 132-144.	1.3	5
1486	Infrared Spectrum of a Molecular Ice Cube: The S4 and D2d Water Octamers in Benzene-(Water)8. <i>Science</i> , 1997, 276, 1678-1681.	6.0	433
1487	Interaction of DNA Base Pairs with Various Metal Cations (Mg ²⁺ , Ca ²⁺ , Sr ²⁺ , Ba ²⁺ , Cu ⁺ , Ag ⁺ , Au ⁺ , Zn ²⁺ ,) Tj ETQq1 1 0.784314 rgBT Interaction. <i>Journal of Physical Chemistry B</i> , 1997, 101, 9670-9677.	1.2	222
1488	Molecular surface structure of ice(0001): dynamical low-energy electron diffraction, total-energy calculations and molecular dynamics simulations. <i>Surface Science</i> , 1997, 381, 190-210.	0.8	160
1489	Ab initio cluster calculations of the chemisorption of hydrogen on the Si(111) surface. <i>Surface Science</i> , 1997, 394, 235-249.	0.8	16
1490	On the origin of the 5.0 and 7.6 eV absorption bands in oxygen deficient α -quartz and amorphous silica. A first principles quantum-chemical study. <i>Journal of Non-Crystalline Solids</i> , 1997, 216, 1-9.	1.5	30
1491	Quantum-Chemical Justification of the Zeolite Acid Strength Measurement by Infrared Spectroscopy. <i>Journal of Physical Chemistry B</i> , 1997, 101, 2116-2119.	1.2	26
1492	The chemical properties of 1-substituted 4-oxopyrimidinium cations. <i>Journal of Heterocyclic Chemistry</i> , 1997, 34, 161-170.	1.4	1
1493	Vibrational spectra (FT-IR, Raman and MI-IR) of α - and β -alanine. <i>Journal of Molecular Structure</i> , 1997, 410-411, 343-348.	1.8	36
1494	Analysis of the vibrational static and dynamic second hyperpolarizabilities of polyacetylene chains. <i>Synthetic Metals</i> , 1997, 85, 1047-1050.	2.1	29
1495	Theoretical, structural and NMR studies of fluxionality in thiolato-bridged platinum(II)-platinum(IV) dinuclear complexes. <i>Inorganica Chimica Acta</i> , 1997, 265, 89-102.	1.2	20
1496	Ab initio molecular orbital study on the mechanism of amide hydrolysis dependent on leaving groups. <i>Tetrahedron</i> , 1997, 53, 4317-4330.	1.0	35
1497	The determination of the equilibrium structures of oxygen, ozone, and hydrogen peroxide using the ab initio and density functional theory methods. <i>Computational and Theoretical Chemistry</i> , 1997, 389, 251-256.	1.5	33
1498	The conformational space of selected aldo-pyrano-hexoses. <i>Computational and Theoretical Chemistry</i> , 1997, 395-396, 29-40.	1.5	26
1499	The antineoplastic behaviour of nitrosoureas: an ab initio study. <i>Computational and Theoretical Chemistry</i> , 1997, 389, 191-198.	1.5	1
1500	Periodic Hartree-Fock study of (HF) ∞ chain. <i>Computational and Theoretical Chemistry</i> , 1997, 389, 147-154.	1.5	7
1501	Studies of LaAlO ₃ {100} surfaces by molecular dynamics simulations. <i>Computational and Theoretical Chemistry</i> , 1997, 390, 193-198.	1.5	24

#	ARTICLE	IF	CITATIONS
1502	Theoretical studies of thermal syn elimination reaction of organic amine oxide, sulfoxide and phosphoxide by ab initio and density functional methods. Computational and Theoretical Chemistry, 1997, 389, 257-263.	1.5	12
1503	Static electronic and vibrational polarizabilities of poly(dimethylsilane) chains. Computational and Theoretical Chemistry, 1997, 391, 67-73.	1.5	6
1504	Incorporation of solvent effects into ab initio molecular orbital calculations by the generalized Born formula. Formulation, parameterization, and applications. Computational and Theoretical Chemistry, 1997, 393, 141-150.	1.5	32
1505	Geometrical consequences of fluorination and intermolecular hydrogen bond formation in fluoroformic acid and trifluoroacetic acid dimers from ab initio MO calculations. Computational and Theoretical Chemistry, 1997, 393, 111-119.	1.5	15
1506	Molecular structure and intramolecular hydrogen bonding in 4,6-dinitroresorcinol and 2,5-dinitrohydroquinone from ab initio molecular orbital calculations. Computational and Theoretical Chemistry, 1997, 393, 121-126.	1.5	8
1507	Ab initio studies on four alkyl nitric esters. Computational and Theoretical Chemistry, 1997, 393, 207-212.	1.5	20
1508	Ab initio structural analysis of furylimidazoles. Computational and Theoretical Chemistry, 1997, 393, 97-110.	1.5	4
1509	An ab initio study of the structure and energetics of the bisulfite ion in the gas phase and in aqueous solution. Computational and Theoretical Chemistry, 1997, 394, 1-9.	1.5	15
1510	Monte Carlo simulation study on the conformation and interaction of the glycine zwitterion in aqueous solution. Computational and Theoretical Chemistry, 1997, 397, 113-119.	1.5	22
1511	Calculations of the structure and spectra of the putative transient peroxide intermediates of peroxidases. Computational and Theoretical Chemistry, 1997, 398-399, 497-505.	1.5	4
1512	The energetically preferred orientation of the hydroxyl group in cyclohexanol Ab initio and force field calculations. Computational and Theoretical Chemistry, 1997, 398-399, 395-404.	1.5	4
1513	Force field parameterization of copper(I)-olefin systems from density functional calculations. Computational and Theoretical Chemistry, 1997, 397, 39-50.	1.5	19
1514	Destabilised carbocations: A comparison of the C ₂ H ₄ NS ⁺ and C ₂ H ₄ NO ⁺ potential energy surfaces. Computational and Theoretical Chemistry, 1997, 401, 117-125.	1.5	13
1515	Intramolecular sulfur-oxygen interactions: An ab initio molecular orbital and density functional theory investigation. Computational and Theoretical Chemistry, 1997, 418, 139-154.	1.5	21
1516	Structure-stability relationships in unsaturated sulfur compounds VI. An ab initio study of the stable conformations of (E)- and (Z)-2-methylthio-, methylsulfinyl- and methylsulfonyl-2-butenes. Computational and Theoretical Chemistry, 1997, 418, 189-196.	1.5	10
1517	The ground state of ethylene. Computational and Theoretical Chemistry, 1997, 400, 169-176.	1.5	6
1518	Ab initio effective core potential calculations on lanthanide complexes: basis sets and electron correlation effects in the study of [Gd-(H ₂ O) ₉] ³⁺ . Computational and Theoretical Chemistry, 1997, 392, 75-85.	1.5	16
1519	The effects of basis set and blocking groups on the conformational energies of glycyI and alanyl dipeptides A Hartree-Fock and MP2 study. Computational and Theoretical Chemistry, 1997, 392, 101-109.	1.5	19

#	ARTICLE	IF	CITATIONS
1520	Comparison of reaction pathways calculated by different algorithms for disilane and water trimer. <i>Zeitschrift für Physik D-Atoms Molecules and Clusters</i> , 1997, 40, 229.	1.0	6
1521	A Theoretical and Experimental Study on Acid-Catalyzed Isomerization of 1-Acylaziridines to the Oxazolines. Reexamination of a Possible S _N i Mechanism by Using ab Initio Molecular Orbital Calculations. <i>Journal of Organic Chemistry</i> , 1997, 62, 3081-3088.	1.7	48
1522	Linkage isomerism, kinetics and electrochemistry of ruthenium-edta complexes of benzotriazole. <i>Transition Metal Chemistry</i> , 1997, 23, 13-16.	0.7	19
1523	Density functional theory studies of zeolite structure, acidity, and reactivity. <i>Topics in Catalysis</i> , 1997, 4, 157-171.	1.3	71
1524	Diatomic interaction energies in the topological theory of atoms in molecules. <i>Theoretica Chimica Acta</i> , 1997, 95, 1-12.	0.9	6
1525	Structures and energies of seleno derivatives of biuret. Ab Initio comparative studies of diselenobiuret, selenobiuret, and selenothiobiuret. <i>Structural Chemistry</i> , 1997, 8, 245-256.	1.0	0
1526	Hydration of the carboxylate group: An ab initio molecular orbital study of acetate-water complexes. <i>Structural Chemistry</i> , 1997, 8, 293-307.	1.0	22
1527	Quantum-mechanical vibrational spectrum and conformational analysis for the 1,5-cyclooctadiene. <i>Vibrational Spectroscopy</i> , 1997, 13, 213-219.	1.2	2
1528	Density functional theory study of vibrational spectra, 6: assignment of fundamental vibrational frequencies of benzene isomers: Dewar benzene, benzvalene, trimethylenecyclopropane, prismane, and 3,4-dimethylenecyclobutene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 259-269.	2.0	13
1529	Density functional theory study of vibrational spectra: 9. Structures and vibrational assignments of dicyanobenzenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 721-731.	2.0	21
1530	Vibrational modes in thymine molecule from an ab initio MO calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 393-407.	2.0	43
1531	Raman scattering tensors in thymine molecule from an ab initio MO calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 409-419.	2.0	19
1532	The gas-phase infrared spectra of phenanthrene-h ¹⁰ and phenanthrene-d ¹⁰ . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1997, 53, 1839-1851.	2.0	18
1533	Specific and bulk solvent nonadditive contributions to the in-solution binding energy of ammonium-water clusters. <i>Chemical Physics</i> , 1997, 214, 113-121.	0.9	14
1534	The electronic spectroscopy of 1,2,3-triazine. <i>Chemical Physics</i> , 1997, 221, 11-21.	0.9	14
1535	MD study of an infinitely dilute aqueous solution of formaldehyde using different ab initio potentials. <i>Chemical Physics</i> , 1997, 223, 251-257.	0.9	10
1536	Theory and calculation of nuclear shielding constants. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1997, 31, 317-342.	3.9	59
1537	Pyrrolo-diazines. 4. Structure and chemistry of 3,4-dihydropyrrolo[1,2-a]pyrazine. <i>Tetrahedron</i> , 1997, 53, 9341-9356.	1.0	11

#	ARTICLE	IF	CITATIONS
1538	Experimental and molecular orbital calculational study of the stereoselective Horner-Wittig reaction with phosphine oxides: Control of stereoselectivity by lithium. <i>Journal of Organometallic Chemistry</i> , 1997, 529, 29-33.	0.8	27
1539	Theoretical evidence for stereoselective lithiations of 2-alkoxy-1,1-diodo-1-alkenes An ab initio study. <i>Journal of Organometallic Chemistry</i> , 1997, 548, 185-189.	0.8	9
1540	A theoretical study of the interaction of water molecules with the Cu(100), Ag(100) and Au(100) surfaces. <i>Journal of Electroanalytical Chemistry</i> , 1997, 420, 209-218.	1.9	86
1541	The proton affinities and proton transfer in imine, amidine and guanidine series. <i>Journal of Molecular Structure</i> , 1997, 416, 21-32.	1.8	18
1542	Core ionization energies of amides as a probe of structure and bonding. <i>Journal of Molecular Structure</i> , 1997, 413-414, 477-485.	1.8	8
1543	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding. IV. The HBr-pyridine complex. <i>Journal of Molecular Structure</i> , 1997, 436-437, 367-386.	1.8	27
1544	Periodic Hartree-Fock calculation of the A _{1g} (T _z) and E _g (T _x , T _y) phonon modes in ice VIII. <i>Journal of Molecular Structure</i> , 1997, 436-437, 443-449.	1.8	5
1545	[(η -5-C ₅ Me ₅)Al(η -5-C ₅ H ₅) ₂ Fe(CO) ₄] ⁺ synthesis, Structure, and Bonding. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 70-72.	4.4	129
1546	Relative Configuration and Synthesis of a New C-4 Branched Sugar, a Component of the Lipooligosaccharide LOS-III from <i>Mycobacterium gastris</i> . <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 72-75.	4.4	20
1547	Dihydrogen Formation in a Trihydride Metallocene and Its Elimination, Both Assisted by Lewis Acids: The [Cp ₂ NbH ₃]+BH ₃ System. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 265-266.	4.4	23
1548	Ab Initio Density Functional vs Hartree Fock Predictions for the Structure of [18]Annulene: Evidence for Bond Localization and Diminished Ring Currents in Bicycloannelated [18]Annulenes. <i>Angewandte Chemie International Edition in English</i> , 1997, 36, 745-748.	4.4	45
1549	Thermodynamics of hydrogen bonding from molecular orbital theory: 1. Water. <i>AIChE Journal</i> , 1997, 43, 1589-1596.	1.8	28
1550	[(η -5-C ₅ Me ₅)Al(η -5-C ₅ H ₅) ₂ Fe(CO) ₄] ⁺ synthesis, Struktur, Bindungsverhältnisse. <i>Angewandte Chemie</i> , 1997, 109, 95-97.	1.6	84
1551	Lewis-Säuren begünstigen die Umwandlung eines Metallocentrihydrids in einen Diwasserstoffkomplex und die H ₂ -Freisetzung aus ihm: das System [Cp ₂ NbH ₃]+BH ₃ . <i>Angewandte Chemie</i> , 1997, 109, 259-261.	1.6	2
1552	Voraussagen zur Struktur von [18]Annulenen mit ab-initio-Dichtefunktional- und Hartree-Fock-Rechnungen im Vergleich: Belege für Bindungslokalisierung und verringerte Ringströme in bicycloannelierten [18]Annulenen. <i>Angewandte Chemie</i> , 1997, 109, 765-768.	1.6	3
1553	Bromine Complexes of Ethylene and Cyclopropene: Matrix Spectroscopic Identification, Photochemical Reactions, Ab Initio Studies. <i>Liebigs Annalen</i> , 1997, 1997, 317-326.	0.8	12
1554	Structural Aspects of Cyclopropyl Homoconjugation: Experimental Studies and Ab Initio Calculations. <i>Liebigs Annalen</i> , 1997, 1997, 1429-1435.	0.8	6
1555	Structural Aspects of Cyclopropyl Conjugation: Experimental Studies and Ab Initio Calculations. <i>Liebigs Annalen</i> , 1997, 1997, 2047-2053.	0.8	17

#	ARTICLE	IF	CITATIONS
1556	Density Functional Studies on Amino-Substituted Methane and Silane. <i>Chemische Berichte</i> , 1997, 130, 1745-1749.	0.2	10
1557	A Comprehensive Qualitative and Quantitative Molecular Orbital Analysis of the Factors Governing the Dichotomy in the Dinorcaradiene 1,6-Methano[10]annulene system. <i>Chemistry - A European Journal</i> , 1997, 3, 958-968.	1.7	16
1558	The Nature of the Metal-Silicon Bond in $[M(\text{SiR}_3)_3\text{H}_3(\text{PPh}_3)_3]$ (M = Ru, Os) And the Crystal Structure of $[\text{Os}\{\text{Si}(\text{N}(\text{pyrrolyl})_3)_3\text{H}_3(\text{PPh}_3)_3]$. <i>Chemistry - A European Journal</i> , 1997, 3, 1608-1616.	1.7	52
1559	A computational study of a host-guest complex. <i>Journal of Molecular Recognition</i> , 1997, 10, 159-168.	1.1	3
1560	AB INITIO MO AND MONTE CARLO SIMULATION STUDY ON THE CONFORMATION OF L-ALANINE ZWITTERION IN AQUEOUS SOLUTION. <i>Journal of Physical Organic Chemistry</i> , 1997, 10, 145-151.	0.9	32
1561	Quantum-mechanical and molecular mechanics conformational analysis of 1,5-cyclooctadiene. <i>Journal of Computational Chemistry</i> , 1997, 18, 254-259.	1.5	18
1562	Rotational barriers of disilane, hexafluorodisilane, and hexamethyldisilane: Ab initio, density functional, and molecular mechanics (MM3) studies. <i>Journal of Computational Chemistry</i> , 1997, 18, 1523-1533.	1.5	17
1563	Catalytic and bulk solvent effects on proton transfer: Formamide as a case study. <i>Journal of Computational Chemistry</i> , 1997, 18, 1993-2000.	1.5	44
1564	Toward a general protocol for the study of static and dynamic properties of hydrogen-bonded systems. <i>International Journal of Quantum Chemistry</i> , 1997, 61, 429-442.	1.0	24
1565	A study of methanetetraol dehydration to carbonic acid. <i>International Journal of Quantum Chemistry</i> , 1997, 62, 315-322.	1.0	4
1566	Partial third-order quasiparticle theory: An application to the photoelectron spectrum of S-tetrazine. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 291-299.	1.0	9
1567	The electronic structure of borabenzene: Combination of an aromatic π -sextet and a reactive π -framework. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 441-449.	1.0	26
1568	Comparison of electron propagator methods for calculating electron detachment energies of anions. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 463-469.	1.0	19
1569	Reaction path for the insertion reaction of SnCl_2 into the Pt(SINGLE BOND)Cl bond: An ab initio study. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 643-650.	1.0	25
1570	Vibrational versus electronic first hyperpolarizabilities of mono- and disubstituted benzenes: An ab initio coupled Hartree-Fock investigation. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 689-696.	1.0	20
1571	Understanding the mechanism of the addition of organomagnesium reagents to 2-hydroxypropanal: An ab initio molecular orbital analysis. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 719-728.	1.0	3
1572	A molecular orbital study of the dimerization process of vinyl monomers. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 767-785.	1.0	4
1573	Ab initio and molecular mechanics conformational analysis of neutral L-proline. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 1033-1045.	1.0	43

#	ARTICLE	IF	CITATIONS
1574	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding: evidence of a dramatic effect of the matrix on the structure and vibrational spectrum of HBr:3,5-dichloropyridine. <i>Chemical Physics Letters</i> , 1997, 264, 109-112.	1.2	6
1575	Removal of the bottleneck in local correlation methods. <i>Chemical Physics Letters</i> , 1997, 265, 660-666.	1.2	17
1576	Ab initio study of collisions between Li and C60. <i>Chemical Physics Letters</i> , 1997, 266, 427-430.	1.2	4
1577	Ab initio studies of the oxidation of methane with oxo-metal cations. <i>Chemical Physics Letters</i> , 1997, 270, 357-362.	1.2	13
1578	An Instanton approach to hindered torsions: methyl glycolate " a case study. <i>Chemical Physics Letters</i> , 1997, 271, 189-196.	1.2	8
1579	Structures of the Ca@C82 isomers: a theoretical prediction. <i>Chemical Physics Letters</i> , 1997, 274, 226-230.	1.2	75
1580	Vibrational frequencies of diatomic molecules from Car and Parrinello molecular dynamics. <i>Chemical Physics Letters</i> , 1997, 275, 506-512.	1.2	23
1581	Density functional theory studies of the quadrupole moments of benzene and naphthalene. <i>Chemical Physics Letters</i> , 1997, 277, 252-256.	1.2	15
1582	Kinetic isotope effect in hydrogen abstraction from 2-propanol by hydrogen and deuterium radicals. A pulse radiolysis Fourier transform electron spin resonance study. <i>Chemical Physics Letters</i> , 1997, 280, 353-358.	1.2	12
1583	Structural study of endohedral dimetallofullerenes Sc2 @C84 and Sc2 @C74. <i>Chemical Physics Letters</i> , 1997, 276, 55-61.	1.2	6
1584	Charge transfer, polarizability and stability of Li@C60 complexes. <i>Chemical Physics Letters</i> , 1998, 285, 221-225.	1.2	25
1585	A density functional study of the internal rotation in the quadruply bonded Mo2Cl4(PH3)4 complex. <i>Chemical Physics Letters</i> , 1998, 287, 243-249.	1.2	16
1586	Vibronic interactions in s-trans-butadiene. <i>Chemical Physics Letters</i> , 1998, 287, 275-281.	1.2	8
1587	Calculations of circular intensity differences in electric-field-induced second harmonic generation. <i>Chemical Physics Letters</i> , 1998, 288, 371-376.	1.2	4
1588	Five-coordinate platinum (II) alkyne complexes: synthesis, ab initio calculations and crystal and molecular structure of [PtI2(Me2phen)I·2PhC≡¼CPh]·CHCl3. <i>Inorganica Chimica Acta</i> , 1998, 275-276, 500-509. ^{1,2}	1.2	28
1589	PAPQMD parametrization of molecular systems with cyclopropyl rings: conformational study of homopeptides constituted by 1-aminocyclopropane-1-carboxylic acid. <i>Journal of Computer-Aided Molecular Design</i> , 1998, 12, 259-273.	1.3	18
1590	Aspects of the mechanism of catalysis of glucose oxidase: a docking, molecular mechanics and quantum chemical study. <i>Journal of Computer-Aided Molecular Design</i> , 1998, 12, 425-440.	1.3	51
1591	Tautomeric equilibria in 8-oxopurines: implications for mutagenicity. , 1998, 12, 373-373.		38

#	ARTICLE	IF	CITATIONS
1592	Theoretical Study of Rotational Isomerism in Ethyl Pseudohalides. <i>Structural Chemistry</i> , 1998, 9, 161-167.	1.0	4
1593	Thermodynamic Properties of Bromomethanes and Bromomethyl Radicals: An ab Initio Study. <i>International Journal of Thermophysics</i> , 1998, 19, 719-730.	1.0	7
1594	The spin-coupled description of phenylenedimethylidene. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998, 94, 3301-3305.	1.7	5
1595	D. Proton transfer in complex systems, liquids and biological systems: Proton transfer reactions at the surface of Ice. Heterogeneous reactions involved in stratospheric ozone depletion. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1998, 102, 518-526.	0.9	39
1596	Cis,trans,cis or All-cis Geometry in d0Octahedral Dioxo Complexes. An IMOMM Study of the Role of Steric Effects. <i>Inorganic Chemistry</i> , 1998, 37, 3321-3325.	1.9	28
1597	Structural and Geometrical Isomerizations of Cyclopropane. Quantum Chemical and RRKM Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3299-3306.	1.1	28
1598	Theoretical Study of the Molecular Properties of Cerium Trihalides and Tetrahalides CeX _n (n = 3, 4; X = F, Cl, Br, I). <i>Journal of Physical Chemistry A</i> , 1998, 102, 1118-1124.	1.1	24
1599	A perturbation theory using a local potential from Hartree-Fock orbitals. <i>Chemical Physics Letters</i> , 1998, 296, 1-7.	1.2	5
1600	Analysis of laser-induced fluorescence spectra of the (π ³) _g ←(π ³) _g transition with calculated Franck-Condon factors of CH ₂ CFO. <i>Chemical Physics Letters</i> , 1998, 298, 93-100.	1.2	6
1601	Infrared matrix isolation and theoretical studies of SO ₂ ←HNO ₃ and SO ₂ ←HONO systems. <i>Chemical Physics</i> , 1998, 228, 17-29.	0.9	23
1602	On the localization of the electronic excitation in supramolecules built up by equivalent units linked by hydrogen bonds. <i>Chemical Physics</i> , 1998, 228, 1-7.	0.9	4
1603	Electronic structure and optical spectra of MDF-2 oligoetheracrylate. <i>Materials Chemistry and Physics</i> , 1998, 56, 7-13.	2.0	16
1604	Static first hyperpolarizability of small all-trans polymethincimine oligomers. Basis set and electron correlation effects. <i>Computational and Theoretical Chemistry</i> , 1998, 425, 69-79.	1.5	20
1605	Comparison of density functional and MP2 geometry optimizations of Na(H ₂ O) _n (n = 1-3) clusters. <i>Computational and Theoretical Chemistry</i> , 1998, 425, 87-94.	1.5	6
1606	Double harmonic vibrational second hyperpolarizabilities of polyynes chains. <i>Computational and Theoretical Chemistry</i> , 1998, 425, 115-122.	1.5	19
1607	Electronic structure of chromone and its hydroxylated derivatives on positions 2 and 3. <i>Computational and Theoretical Chemistry</i> , 1998, 423, 235-243.	1.5	18
1608	Theoretical study of the properties of the radical PS, its anion and cation. <i>Computational and Theoretical Chemistry</i> , 1998, 425, 237-247.	1.5	17
1609	p-Phenylenebis(methylene): a CASSCF study of $\tilde{\nu}_2$, $\tilde{\nu}_3$ and $\tilde{\nu}_4$ electronic states. <i>Computational and Theoretical Chemistry</i> , 1998, 424, 29-35.	1.5	4

#	ARTICLE	IF	CITATIONS
1610	Ab initio investigations of the geometric conformation of glycidic methyl esters and the related complexes with a lithium cation: a contribution to the understanding of regioselective openings of these esters with lithium reagents. Computational and Theoretical Chemistry, 1998, 428, 27-34.	1.5	1
1611	The influence of basis sets in the calculations of momentum expectation values for diatomic molecules. Computational and Theoretical Chemistry, 1998, 426, 35-45.	1.5	4
1612	A theoretical study of the addition of CH ₃ MgCl to chiral $\hat{\pm}$ -alkoxy carbonyl compounds. Computational and Theoretical Chemistry, 1998, 426, 263-275.	1.5	3
1613	A CIS study of the solvent effects on the electronic absorption spectra of push-pull ethylenes. Computational and Theoretical Chemistry, 1998, 429, 131-141.	1.5	7
1614	Ab initio calculations in tricyclo[3,3,1,13,7]decane, tricyclo[3,3,1,13,7]decsilane and their silicon-carbon mixed derivatives, C ₁₀ $\hat{\sim}$ nSinH ₁₆ (n = 0, 4, 6, 10). Computational and Theoretical Chemistry, 1998, 432, 105-113.	1.5	1
1615	A computational study of imidazole, 4-nitroimidazole, 5-nitroimidazole and 4,5-dinitroimidazole. Computational and Theoretical Chemistry, 1998, 432, 41-53.	1.5	44
1616	The effect of small substituents on the properties of indole. An ab initio 6-31G* study. Computational and Theoretical Chemistry, 1998, 433, 203-216.	1.5	12
1617	On the geometry of 3-amino-sydnonones. Computational and Theoretical Chemistry, 1998, 433, 291-299.	1.5	5
1618	Theoretical study of the thermal interconversion mechanism between the norbornadiene and quadricyclane radical cations. Computational and Theoretical Chemistry, 1998, 434, 59-66.	1.5	20
1619	The binding of water to the carboxylate group in R $\hat{\sim}$ CO ₂ $\hat{\sim}$ (R=H, CH ₃ , NH ₂ , OH, and F): an ab initio molecular orbital study. Computational and Theoretical Chemistry, 1998, 455, 239-256.	1.5	6
1620	Ab Initio study of the structure, cooperativity and vibrational properties of the H ₂ O:(HCl) ₂ hydrogen bonded complex. Computational and Theoretical Chemistry, 1998, 452, 55-66.	1.5	5
1621	Theoretical study of some pyrazole derivatives and rare earth metal complexes. Computational and Theoretical Chemistry, 1998, 453, 17-28.	1.5	9
1622	Analytical second derivatives in ab initio Hartree-Fock crystal orbital theory of polymers. Computational and Theoretical Chemistry, 1998, 451, 121-134.	1.5	20
1623	Dynamic reaction path study of SiH ₄ +F $\hat{\sim}$ $\hat{\sim}$ SiH ₄ F $\hat{\sim}$ and the Berry pseudorotation with valley $\hat{\sim}$ ridge inflection. Computational and Theoretical Chemistry, 1998, 451, 163-177.	1.5	25
1624	Calculation of the structure and absorption spectra of phthalocyanines in the gas-phase and in solution. Computational and Theoretical Chemistry, 1998, 455, 33-50.	1.5	85
1625	Conformational ab initio study of ascorbic acid. Computational and Theoretical Chemistry, 1998, 454, 175-185.	1.5	23
1626	Theoretical study of the methylic reactivity of substituted alkenes. Computational and Theoretical Chemistry, 1998, 430, 1-7.	1.5	0
1627	Isoelectronic Arduengo-Type Carbene Analogues with the Group IIIa Elements Boron, Aluminum, Gallium, and Indium. , 1998, 1998, 305-310.		67

#	ARTICLE	IF	CITATIONS
1628	1,2-Diphosphetes with Unusual Structures – A Quantum Chemical Investigation of Bonding Properties†. European Journal of Inorganic Chemistry, 1998, 1998, 951-955.	1.0	7
1629	On the Electronic Nature of a Butadienyl Biradical – Experiments and ab initio MO Calculations. European Journal of Organic Chemistry, 1998, 1998, 1447-1453.	1.2	9
1630	Raman scattering tensors of tyrosine. , 1998, 4, 61-71.		48
1633	C3(SINGLE BOND)M? Bond contribution to polarizability tensor and3J(C1M?) NMR coupling constant in 1-X-3-M-bicyclo[1.1.1]pentanes. Journal of Computational Chemistry, 1998, 19, 181-188.	1.5	13
1634	Theoretical investigation of unimolecular decomposition channels of furan4. Journal of Computational Chemistry, 1998, 19, 240-249.	1.5	42
1635	Ab initio conformational analysis of cyclooctane molecule. Journal of Computational Chemistry, 1998, 19, 524-534.	1.5	33
1636	Accurate molecular electrostatic potentials based on modified PRDDO/M wave functions: III. Extension of thePESP method for calculation of electrostatic potential-derived atomic charges to compounds containing Li+, Na+, Mg2+, K+, Ca2+, Zn2+, and I. Journal of Computational Chemistry, 1998, 19, 1456-1469.	1.5	2
1637	Influence of environment on proton-transfer mechanisms in model triads from theoretical calculations. Journal of Computational Chemistry, 1998, 19, 1675-1688.	1.5	27
1638	Oxygen and proton pathways in cytochrome c oxidase. , 1998, 30, 100-107.		197
1639	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. International Journal of Quantum Chemistry, 1998, 66, 9-24.	1.0	33
1640	Structure of theT1-state wave function of linear polyenes. International Journal of Quantum Chemistry, 1998, 67, 101-106.	1.0	6
1641	Ab initio study of the reaction mechanism of water dissociation into the ionic species OH? and H3O+. International Journal of Quantum Chemistry, 1998, 68, 253-259.	1.0	12
1642	Electrostatic effect of the polar bond-polarizable bond interaction on13C chemical shifts. International Journal of Quantum Chemistry, 1998, 70, 105-112.	1.0	3
1643	Topology of electronic densities taken from parametric methods: A predictive tool?. International Journal of Quantum Chemistry, 1998, 70, 113-123.	1.0	11
1644	Electron propagator theory of conformational effects on anisole and thioanisole photoelectron spectra. International Journal of Quantum Chemistry, 1998, 70, 1037-1043.	1.0	15
1645	Nonresonant frequency dispersion of the electronic second hyperpolarizability of all-trans polysilane chains: An ab initio TDHF oligomeric approach. International Journal of Quantum Chemistry, 1998, 70, 751-761.	1.0	8
1646	Intramolecular hydrogen bonding in resonance-stabilized systems. International Journal of Quantum Chemistry, 1998, 70, 863-875.	1.0	16
1647	The interface of electronic structure and dynamics for reactions in solution. International Journal of Quantum Chemistry, 1998, 70, 887-896.	1.0	74

#	ARTICLE	IF	CITATIONS
1648	A structural and theoretical study of the monolithiation of hydroxylamines1Dedicated to Professor Ken Wade on the occasion of his 65th birthday and in recognition of his outstanding and ongoing contributions to Main Group Chemistry.1. Journal of Organometallic Chemistry, 1998, 550, 233-240.	0.8	17
1649	Formation of the lithium alkylaluminium secondary amide [Me ₂ Al{PhCH ₂ } ₂ N}ZLiA·THF] by a methane elimination/amide insertion process1Dedicated to Professor Ken Wade on the occasion of his 65th birthday in recognition of his sterling contribution to inorganic chemistry. REM adds his personal thanks in warm appreciation of two invaluable years spent working for, and learning from KW.1. Journal of Organometallic Chemistry, 1998, 550, 355-358.	0.8	6
1650	Molecular structure and vibrational spectra of methyl cyanoacetate: an FT-IR, raman and ab initio molecular orbital study. Journal of Molecular Structure, 1998, 443, 41-56.	1.8	7
1651	Conformational analysis and photolysis of matrix isolated 3-chloropropanoyl chloride monitored by FTIR spectroscopy. Journal of Molecular Structure, 1998, 443, 163-173.	1.8	6
1652	Investigation of the reactivity of thiophene compounds towards butyllithium using the molecular electrostatic potential. Journal of Molecular Structure, 1998, 445, 187-195.	1.8	4
1653	Intramolecular interactions in ortho-substituted phenols: survey of DFT-B3LYP calculated data. Journal of Molecular Structure, 1998, 448, 191-199.	1.8	39
1654	Molecular structure and conformations of tetrahydrofurfuryl alcohol from a joint gas-phase electron diffraction and ab initio molecular orbital investigation. Journal of Molecular Structure, 1998, 448, 29-41.	1.8	10
1655	On the difference between hydrogen fluoride and hydrogen chloride crystals. Journal of Molecular Structure, 1998, 450, 259-263.	1.8	4
1656	Matrix effects in the low-temperature ozonation of ethylene, tetramethylethylene and 1-hexene. Journal of Molecular Structure, 1998, 449, 177-201.	1.8	15
1657	Structural incorporation of nitrogen into zeolites, and alpos: ab initio molecular orbital calculations on stability and basicity. Journal of Molecular Catalysis A, 1998, 133, 241-250.	4.8	17
1658	Gas phase agostic bonding in pyridine SiFn+ (n = 1, 3) cluster ions investigated by the kinetic method. International Journal of Mass Spectrometry, 1998, 179-180, 195-205.	0.7	13
1659	Vibrational spectra of acid and alkaline glycine salts. Vibrational Spectroscopy, 1998, 16, 35-54.	1.2	154
1660	The importance of electron correlation for the ground state structure of porphycene and tetraoxaporphyrin-dication. Chemical Physics, 1998, 227, 331-348.	0.9	36
1661	Mass-selected "matrix isolation" infrared spectroscopy of the I~A·(H ₂ O) ₂ complex: making and breaking the inter-water hydrogen-bond. Chemical Physics, 1998, 239, 485-491.	0.9	131
1662	An ab initio time-dependent Hartree-Fock study of solvent effects on the polarizability and second hyperpolarizability of polyacetylene chains within the polarizable continuum model. Chemical Physics, 1998, 238, 153-163.	0.9	28
1663	Resonant ion-dip infrared spectroscopy of benzene"(water)"(methanol) clusters with n+m=4, 5. Chemical Physics, 1998, 239, 83-96.	0.9	24
1664	The drying of 3-glycidoxypropyltrimethoxy silane. Applied Surface Science, 1998, 134, 247-253.	3.1	26
1665	Ab initio HF/DFT studies of the chemisorption of hydrogen on the cluster simulated Si(111)-(3 3) Tj ETQq1 1 0,784314 rgBT /Overl	0.8	10

#	ARTICLE	IF	CITATIONS
1666	Exploration of the Mechanism of the Oxidation of Sulfur Dioxide and Bisulfite by Hydrogen Peroxide in Water Clusters Using Ab Initio Methods. <i>Journal of the American Chemical Society</i> , 1998, 120, 3431-3439.	6.6	26
1667	6-31G* basis set for atoms K through Zn. <i>Journal of Chemical Physics</i> , 1998, 109, 1223-1229.	1.2	1,766
1668	Assessment of conventional density functional schemes for computing the polarizabilities and hyperpolarizabilities of conjugated oligomers: An ab initio investigation of polyacetylene chains. <i>Journal of Chemical Physics</i> , 1998, 109, 10489-10498.	1.2	453
1669	Structure and Energetics of Ground-State Hypericin: Comparison of Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1647-1651.	1.1	48
1670	Density-functional crystal orbital study on the structures and energetics of polyacetylene isomers. <i>Physical Review B</i> , 1998, 57, 11994-12001.	1.1	52
1671	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. II. Application to the effective fragment potential method. <i>Journal of Chemical Physics</i> , 1998, 108, 4772-4782.	1.2	105
1672	Cavity size in reaction field theory. <i>Journal of Chemical Physics</i> , 1998, 109, 10543-10558.	1.2	105
1673	Binding of dioxygen in a picket-fence porphyrin complex of iron. A theoretical QM/MM study. <i>New Journal of Chemistry</i> , 1998, 22, 327-322.	1.4	22
1674	First structurally characterised lithium hexafluorophosphate complexes with acyclic Lewis bases: ion-separated $[\text{Li}_2(\text{hmpa})_5]^{2+}(\text{PF}_6^{2-})$ and ion-contacted $[(\text{pmdeta})\text{LiPF}_6]_2$ [hmpa = (Me ₂ N) ₃ PO; pmdeta = MeN(CH ₂ CH ₂ NMe ₂) ₂]. <i>Chemical Communications</i> , 1998, , 1011-1012.	2.2	21
1675	Alkali metal-1-azaallyl complexes: X-ray crystallographic, NMR spectroscopic and ab initio calculational studies. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 3431-3436.	1.1	19
1676	Theoretical studies of metal complexes of anhydrotetracycline: interaction with ZnII. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 2531-2536.	1.1	9
1677	Molecular structure of trimethylamine-gallane, Me ₃ N-GaH ₃ : ab initio calculations, gas-phase electron diffraction and single-crystal X-ray diffraction studies. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 3685-3692.	1.1	37
1678	On the origin of 1,5-induction in tin(IV) halide-promoted reactions of 4-alkoxyalk-2-enylstannanes with aldehydes. <i>Chemical Communications</i> , 1998, , 899-900.	2.2	19
1679	Properties of tetramethyleneethane (TME) as revealed by ion chemistry and ion photoelectron spectroscopy. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998, , 1015-1022.	0.9	55
1680	Identity-reaction proton transfers from nitrogen acids yielding localized vs. delocalized conjugate bases. An ab initio study. <i>Canadian Journal of Chemistry</i> , 1998, 76, 821-827.	0.6	6
1681	A triylide carbocycle™: cyclononane-1,4,7-triammonium triylide. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998, , 2335-2336.	0.9	0
1682	X-Ray crystal and ab initio structure of 3-ethynylcyclopropene: a curiously short carbon-carbon double bond. <i>Chemical Communications</i> , 1998, , 1137-1138.	2.2	15
1683	The molecular structure of dichloro(dimethylamino)phosphine. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 3239-3242.	1.1	8

#	ARTICLE	IF	CITATIONS
1684	Breaking an electronically preferred symmetry by steric effects in a series of [Ir(biph)X(QR3)2] compounds (X=Cl or I, Q=P or As). <i>New Journal of Chemistry</i> , 1998, 22, 1493-1498.	1.4	22
1685	O-Oximosilanes: weak $\hat{\sigma}^2$ -donor interactions as secondary bonds. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998, , 2537-2540.	1.1	9
1686	Phosphines exchange in quadruply bonded metal dimers: theoretical proposal for an alternative to the internal flip mechanism. <i>Chemical Communications</i> , 1998, , 1443-1444.	2.2	8
1687	Opposing steric and electronic contributions in OsCl2H2(PPr3i)2. A theoretical study of an unusual structure. <i>New Journal of Chemistry</i> , 1998, 22, 5-9.	1.4	34
1688	The Kubas Complex Revisited. A Theoretical Study of Dihydrogen Addition and Structure of the Dihydride Form. <i>Organometallics</i> , 1998, 17, 190-195.	1.1	38
1689	Raman Spectroscopic Measurements and ab Initio Molecular Orbital Studies of Cadmium(II) Hydration in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 1998, 102, 3564-3573.	1.2	42
1690	A Theoretical Insight into the Ability of Group 6 ML5 Metal Fragments to Break the H $\hat{\sigma}$ -H Bond. <i>Organometallics</i> , 1998, 17, 4932-4939.	1.1	34
1691	Matrix Photochemistry of Cycloheptatriene: $\hat{\sigma}$ Site Effects. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4758-4768.	1.1	15
1692	Density Functional Study on Activation of ortho-CH Bond in Aromatic Ketone by Ru Complex. Role of Unusual Five-Coordinated d6 Metallacycle Intermediate with Agostic Interaction. <i>Journal of the American Chemical Society</i> , 1998, 120, 12692-12693.	6.6	105
1693	Potential models for simulations of the solvated proton in water. <i>Journal of Chemical Physics</i> , 1998, 109, 5547-5564.	1.2	187
1694	Structure and Vibrational Properties of Sodium Disilicate Glass from ab Initio Molecular Orbital Calculations. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8372-8378.	1.2	35
1695	Experimental and Theoretical Studies of Double Minima in the Potential-Energy Surfaces for HF-Elimination Reactions of SiFx(OH)y+ with H2O (x= 1 $\hat{\sigma}$ ^3,y= 0 $\hat{\sigma}$ ^2) via Intramolecular H-Atom Transfer. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1162-1169.	1.1	15
1696	A Steeply Pyramidal Silylamine: $\hat{\sigma}$ N,O-Dimethyl-N-silylhydroxylamine. <i>Inorganic Chemistry</i> , 1998, 37, 3593-3598.	1.9	9
1697	Isomerization of Cyclopropanecarbonitrile. Quantum Chemical and Model Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 5876-5885.	1.1	13
1698	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. <i>Journal of Chemical Physics</i> , 1998, 109, 4171-4181.	1.2	228
1700	Self-Consistent Reaction Field Calculations of Nonequilibrium Solvent Effects on Proton Transfer Processes through Low-Barrier Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10728-10735.	1.1	15
1701	Ab Initio Studies on Cyanoacetylene Oligomers: $\hat{\sigma}$ Rings and Chains versus Stacked Clusters. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9286-9296.	1.1	11
1702	Reversible Photoinitiated Isomerization Reaction of BrOBr to BrBrO: $\hat{\sigma}$ A Combined Matrix Isolation and ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1083-1089.	1.1	18

#	ARTICLE	IF	CITATIONS
1703	Theoretical Study on the Urea-Hydrogen Peroxide 1:1 Complexes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 778-784.	1.1	58
1704	High Resolution Infrared Spectroscopy of the CO ₂ -Br ₂ Weakly Bound Complex. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2792-2797.	1.1	4
1705	Saturation of the Optical Band Gap and Properties of Five-Membered Heteroaromatic Oligomers. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1710-1712.	1.2	24
1706	Synthesis and Characterization of OsX{NHC(Ph)C ₆ H ₄ }H ₂ (PiPr ₃) ₂ (X = H, Cl, Br, I): Nature of the H ₂ Unit and Its Behavior in Solution. <i>Organometallics</i> , 1998, 17, 4065-4076.	1.1	81
1707	Theoretical Study of the Olefin Insertion Reaction in the Heterobimetallic Pt(H)(PH ₃) ₂ (SnCl ₃)(C ₂ H ₄) Compound. <i>Organometallics</i> , 1998, 17, 1961-1967.	1.1	42
1708	Geometry Optimization of Charged Molecules in an External Electric Field Applied to F-H ₂ O and I-H ₂ O. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1365-1370.	1.1	7
1709	Geminal Bond Participation and Reactivities of Z- vs E-1-Substituted Butadienes in the Diels-Alder Reactions. <i>Journal of Organic Chemistry</i> , 1998, 63, 7820-7824.	1.7	43
1710	Highly Electrophilic Olefin Polymerization Catalysts. Counteranion and Solvent Effects on Constrained Geometry Catalyst Ion Pair Structure and Reactivity. <i>Journal of the American Chemical Society</i> , 1998, 120, 8257-8258.	6.6	112
1711	Inertness of the Aryl-F Bond toward Oxidative Addition to Osmium and Rhodium Complexes: Thermodynamic or Kinetic Origin?. <i>Journal of the American Chemical Society</i> , 1998, 120, 12634-12640.	6.6	90
1712	Theoretical Evidence for Transannular Metal-Metal Interactions in Dinuclear Coinage Metal Complexes. <i>Inorganic Chemistry</i> , 1998, 37, 6002-6006.	1.9	86
1713	Effect of the Spinning Motion of the Dihydrogen Ligand on the Properties of an Elongated Dihydrogen Complex. A Theoretical Study of the trans-[Os(HA-H)Cl(H ₂ PCH ₂ CH ₂ PH ₂) ₂] ⁺ Complex. <i>Journal of the American Chemical Society</i> , 1998, 120, 8168-8176.	6.6	45
1714	CO Adsorption Isotherms on Ice by Fourier Transform Infrared Spectroscopy and New Insights of the Ice Surface from Quantum ab Initio Investigations. <i>Journal of Physical Chemistry B</i> , 1998, 102, 89-98.	1.2	46
1715	Valence and Dipole Binding of Electrons to Uracil. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1274-1278.	1.1	148
1716	σ -Donor Interactions of Exceptional Strength in N,N-Dimethylhydroxylaminochlorosilane, ClH ₂ SiONMe ₂ . <i>Journal of the American Chemical Society</i> , 1998, 120, 7320-7327.	6.6	66
1717	Structural Consequences of π -Donation by NR ₂ Groups: An Ab Initio Study of Tetrakis(dimethylamino)ethylene (TDAE) and Its Unsubstituted Analog. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10151-10158.	1.1	9
1718	Theoretical Study of the Reaction of Alkylolithium with Pyridylphosphines. <i>Journal of Organic Chemistry</i> , 1998, 63, 1131-1137.	1.7	7
1719	Structure of 1-Naphthol-Water Clusters Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6227-6233.	1.1	59
1720	Four-Electron Reduction of Diazo Compounds at a Single Tungsten Metal Center: A Theoretical Study of the Mechanism. <i>Journal of the American Chemical Society</i> , 1998, 120, 6598-6602.	6.6	21

#	ARTICLE	IF	CITATIONS
1721	An Ab Initio Study of the Isomerization of Mg^{2+} and Ca^{2+} Pyrophosphates. <i>Journal of the American Chemical Society</i> , 1998, 120, 6113-6120.	6.6	19
1722	Structure Determination of Methyl Nicotinate and Methyl Picolinate by Gas Electron Diffraction Combined with ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1405-1411.	1.1	14
1723	Transition Metal Coordinated $Al(X)_2$ and $Ga(X)_2$ Fragments. <i>Journal of the American Chemical Society</i> , 1998, 120, 1237-1248.	6.6	114
1724	Ab Initio Study of Nitromethane Deprotonation by $(OH)_n \cdot nH_2O$ Clusters. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3977-3984.	1.1	14
1725	Oxygen Atom Transfer to Positive Ions: A Novel Reaction of Ozone in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1998, 120, 7869-7874.	6.6	17
1726	Ab Initio Studies of Proton Sponges (V): A 1,4,7,10-Tetraaza-tricyclo[5,5,2,2,4,10]hexa-decane, a Tricyclic Proton Sponge. <i>Journal of Organic Chemistry</i> , 1998, 63, 7117-7119.	1.7	28
1727	The Simplest Azabutadienes in Their N-Protonated Forms. Generation, Stability, and Cycloaddition Reactivity in the Gas Phase. <i>Journal of Organic Chemistry</i> , 1998, 63, 4889-4897.	1.7	26
1728	Synthesis and Spectroscopic and Theoretical Characterization of the Elongated Dihydrogen Complex $OsCl_2(\eta^2-H_2)(NH_2CPh_2)(P^iPr_3)_2$. <i>Inorganic Chemistry</i> , 1998, 37, 5033-5035.	1.9	43
1729	Theoretical Study of Transition Metal Compounds with Molybdenum $^{6+}$ and Tungsten $^{6+}$ Phosphorus Triple Bonds. <i>Inorganic Chemistry</i> , 1998, 37, 1805-1811.	1.9	50
1730	Optical Absorption and Nonradiative Decay Mechanism of E^{2+} Center in Silica. <i>Physical Review Letters</i> , 1998, 81, 377-380.	2.9	113
1731	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in $Ir(H)_2(PtBu_2Ph)_2^+$. <i>Journal of the American Chemical Society</i> , 1998, 120, 361-365.	6.6	121
1732	Density Functional Studies of Weak Base Interactions with Hydroxyl Groups: Models for Adsorption Complexes of Weak Bases in Microporous Materials. <i>Journal of Physical Chemistry B</i> , 1998, 102, 4507-4515.	1.2	19
1733	A Quantum Chemical Investigation of the $C=O$ Bond Length and Stretching Mode of the Phenolate Anion. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10128-10133.	1.1	24
1734	Mechanism of the Acetylene \rightarrow Vinylidene Rearrangement in the Coordination Sphere of a Transition Metal. <i>Organometallics</i> , 1998, 17, 2089-2095.	1.1	65
1735	How Malonaldehyde Bonds Change during Proton Transfer. <i>Journal of Physical Chemistry A</i> , 1998, 102, 5065-5073.	1.1	87
1736	Hydrogen Migration and Lithium Iodide β -Elimination in 1-Iodo-1-lithioethene. Concerted vs Stepwise Mechanism. <i>Organometallics</i> , 1998, 17, 5390-5396.	1.1	15
1737	Fluorescence Spectroscopic Studies of Anthracene Adsorbed into Zeolites: From the Detection of Cation π Interaction to the Observation of Dimers and Crystals. <i>Langmuir</i> , 1998, 14, 4284-4291.	1.6	79
1738	Three-Bond $C=O\rightarrow C=C$ Spin-Coupling Constants in Carbohydrates: Development of a Karplus Relationship. <i>Journal of the American Chemical Society</i> , 1998, 120, 11158-11173.	6.6	132

#	ARTICLE	IF	CITATIONS
1739	Ab Initio MCSCF Study on Electronically Excited Singlet States of Fulvalene Systems: Energy Component Analysis of the Pseudo-Jahn-Teller Effect. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6668-6675.	1.1	9
1740	Density Functional Theory Calculations of the Structures, Binding Energies, and Infrared Spectra of Methanol Clusters. <i>Journal of Physical Chemistry A</i> , 1998, 102, 82-94.	1.1	183
1741	Ab Initio Study of Aziridines and Diaziridines: Nitrogen Inversion, Ring Opening, and Thermochemistry. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3193-3201.	1.1	43
1742	EPR and IR spectral properties of hydrogen-associated bulk and surface defects in SiO ₂ : Ab initio calculations. <i>Physical Review B</i> , 1998, 58, 7745-7752.	1.1	54
1743	Dual-Level Direct Dynamics Calculations of the Reaction Rates for a Jahn-Teller Reaction: Hydrogen Abstraction from CH ₄ or CD ₄ by O(3P). <i>Journal of Physical Chemistry A</i> , 1998, 102, 4899-4910.	1.1	109
1744	Synthesis, Properties, and Structure of Poly(silyl)pyridines. The Phantom of Intramolecular Si-N Bonding. <i>Organometallics</i> , 1998, 17, 4444-4453.	1.1	19
1745	Theoretical Studies of the Structure, Tautomerism, and Vibrational Spectra of 3-Amino-5-nitro-1,2,4-triazole. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10348-10357.	1.1	33
1746	On the Topology of the Electron Charge Density at the Bond Critical Point of the Electron-Pair Bond. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9244-9254.	1.1	20
1747	Theoretical Study of Cation/Ether Complexes: Alkali Metal Cations with 1,2-Dimethoxyethane and 12-Crown-4. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3813-3819.	1.1	90
1748	Energy Component Analysis of the Pseudo-Jahn-Teller Effect in the Ground State of the Trifulvalene Anion, Pentafulvalene Cation, and Heptafulvalene Anion Radicals. <i>Journal of Physical Chemistry A</i> , 1998, 102, 490-495.	1.1	7
1749	Quantum Chemical Characterization of Cycloaddition Reactions between the Hydroxyallyl Cation and Dienes of Varying Nucleophilicity. <i>Journal of Organic Chemistry</i> , 1998, 63, 5523-5532.	1.7	56
1750	CO ₂ -Fluorocarbon and CO ₂ -Hydrocarbon Interactions from First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2231-2236.	1.1	107
1751	Effect of Hydrogen Bonding on the Vibrations of p-Benzoquinone Radical Anion. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1230-1235.	1.1	19
1752	Transition states for chemical reactions I. Geometry and classical barrier height. <i>Journal of Chemical Physics</i> , 1998, 108, 5704-5713.	1.2	173
1753	Molecular structures of tetraborane(10) derivatives: ab initio calculations for H ₂ MB ₃ H ₈ (M = B, Al, Ga). <i>Transactions</i> , 1998, , 2147-2154.	1.1	10
1754	Ab Initio Investigation of the Methylimidazole-Indole Complexes as Models of the Histidine-Tryptophan Pair. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6152-6160.	1.1	26
1755	N-Heterocyclic Carbene, Silylene, and Germylene Complexes of MCl (M = Cu, Ag, Au). A Theoretical Study. <i>Organometallics</i> , 1998, 17, 5801-5809.	1.1	316
1756	Fitting basis sets for the RI-MP2 approximate second-order many-body perturbation theory method. <i>Journal of Chemical Physics</i> , 1998, 109, 1593-1600.	1.2	51

#	ARTICLE	IF	CITATIONS
1757	Calculating the logarithmic mean excitation energy from the Shannon information entropy of the electronic charge density. <i>Physical Review A</i> , 1998, 57, 4512-4517.	1.0	29
1758	Electric and magnetic properties of fullerenes. <i>Journal of Chemical Physics</i> , 1998, 109, 572-577.	1.2	70
1759	Ab Initio Study of the Regiochemistry of 1,3-Dipolar Cycloadditions. Reactions of Diazomethane and Formonitrile Oxide with Ethene, Propene, Acrylonitrile, and Methyl Vinyl Ether. <i>Journal of Organic Chemistry</i> , 1998, 63, 7425-7436.	1.7	51
1760	Density Functional Study of the Vibrational Spectra of Octahedral Transition-Metal Hexacarbonyls: Neutral Molecules (M = Cr, Mo, W) and Isoelectronic Ions (M = V, Nb, Ta; Mn, Re; Fe, Ru, Os; Co, Rh, Ir; Tj ETQq1 1 0178431478 BT / Over		
1761	Molecular Orbital and IMOMM Studies of the Chain Transfer Mechanisms of the Diimine \sim M(II)-Catalyzed (M = Ni, Pd) Ethylene Polymerization Reaction. <i>Organometallics</i> , 1998, 17, 1850-1860.	1.1	105
1762	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 1. Hydrolysis and Initial Condensation. <i>Journal of the American Chemical Society</i> , 1998, 120, 11432-11438.	6.6	83
1763	Diminishing π -Stabilization of an Unsaturated Metal Center: Hydrogen Bonding to OsHCl(CO)(PtBu ₂ Me) ₂ . <i>Journal of the American Chemical Society</i> , 1998, 120, 12553-12563.	6.6	36
1764	Structure, Bonding, and Stability of Small Boron \sim Lithium Clusters. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1608-1614.	1.1	29
1765	To Bend or Not To Bend: A Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d ⁸ Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998, 37, 804-813.	1.9	126
1766	Interpretation of Activation Volumes for Water Exchange Reactions Revisited: Ab Initio Calculations for Al ³⁺ , Ga ³⁺ , and In ³⁺ , and New Experimental Data. <i>Journal of the American Chemical Society</i> , 1998, 120, 6569-6577.	6.6	95
1767	Comparison of AM1 and PM3 in MOPAC6 with Literature for the Thermodynamic Parameters of C1 and C2 Chlorocarbons. <i>Industrial & Engineering Chemistry Research</i> , 1998, 37, 3497-3507.	1.8	7
1768	Model molecular dynamics simulation of hydrochloric acid ionization at the surface of stratospheric ice. <i>Faraday Discussions</i> , 1998, 110, 301-322.	1.6	102
1769	Ab initio study of HCl and HF interaction with crystalline ice. I. Physical adsorption. <i>Journal of Chemical Physics</i> , 1998, 108, 9516-9528.	1.2	72
1770	Structure and magnetic properties of benzyl, anilino, and phenoxyl radicals by density functional computations. <i>Journal of Chemical Physics</i> , 1998, 109, 10244-10254.	1.2	57
1771	The hydrogen-bonding topologies of indole \cdots (water) _n clusters from resonant ion-dip infrared spectroscopy. <i>Journal of Chemical Physics</i> , 1998, 108, 3379-3382.	1.2	113
1772	Ab initio studies on the electronic excited states and photodissociation of O ₃ anion. <i>Journal of Chemical Physics</i> , 1998, 108, 7684-7694.	1.2	9
1773	Analytical energy gradients in second-order Møller \cdots Plesset perturbation theory for extended systems. <i>Journal of Chemical Physics</i> , 1998, 109, 4147-4155.	1.2	48
1774	Vibrational dynamics of defect modes in vitreous silica. <i>Physical Review B</i> , 1998, 58, 5322-5328.	1.1	53

#	ARTICLE	IF	CITATIONS
1775	Ab initio theory of optical transitions of point defects in SiO ₂ . Physical Review B, 1998, 57, 818-832.	1.1	189
1776	Optical transitions and EPR properties of two-coordinated Si, Ge, Sn and related H(I), H(II), and H(III) centers in pure and doped silica from ab initio calculations. Physical Review B, 1998, 58, 6090-6096.	1.1	91
1777	Calculation of electronic affinity and vertical detachment energy of the water dimer complex using the density functional theory. Journal of Chemical Physics, 1998, 108, 7967-7972.	1.2	22
1778	Resonant ion-dip infrared spectroscopy of the S ₄ and D _{2d} water octamers in benzene-(water) ₈ and benzene ₂ -(water) ₈ . Journal of Chemical Physics, 1998, 109, 6601-6614.	1.2	123
1779	Vibrational and electronic second hyperpolarizabilities of all-trans polysilane chains. Journal of Chemical Physics, 1998, 109, 4624-4637.	1.2	22
1780	Localized low-frequency dynamics in SiO ₂ glass. Journal of Chemical Physics, 1998, 108, 8130-8138.	1.2	37
1781	Density functional solvation model based on CM2 atomic charges. Journal of Chemical Physics, 1998, 109, 9117-9133.	1.2	120
1782	C ₂₄ : Ring or fullerene?. Journal of Chemical Physics, 1998, 108, 3213-3217.	1.2	31
1783	Chemisorption of deuterium on an ultrathin Ge film deposited over Si(100) α -2 \times 1: Existence of a dideuteride phase. Physical Review B, 1998, 58, 9949-9954.	1.1	6
1784	Ab initio potential energy surface by modified Shepard interpolation: Application to the CH ₃ +H ₂ \rightarrow CH ₄ +H reaction. Journal of Chemical Physics, 1998, 109, 4281-4289.	1.2	47
1785	A comparative study of anharmonicity and matrix effects on the complexes XH:NH ₃ , X=F, Cl, and Br. Journal of Chemical Physics, 1998, 108, 3205-3212.	1.2	65
1786	A combined molecular dynamics α ab initio study of H ₂ adsorption on ideal, relaxed, and temperature-reconstructed MgO(111) surfaces. Journal of Chemical Physics, 1998, 109, 7515-7521.	1.2	31
1787	STABILIZATION OF OXIDIZED SULFUR AND SELENIUM CENTERS IN ORGANIC CHALCOGENS BY THREE-ELECTRON SULFUR-SULFUR, SELENIUM-SELENIUM, AND SULFUR-SELENIUM BONDS. A THEORETICAL STUDY USING THE SEMIEMPIRICAL PARAMETRIC METHOD 3 (PM3). Phosphorus, Sulfur and Silicon and the Related Elements, 1998, 141, 111-134.	0.8	7
1788	Density functional crystal orbital study on the normal vibrations and phonon dispersion curves of all-trans polyethylene. Journal of Chemical Physics, 1998, 108, 7901-7908.	1.2	34
1789	Structure, bonding, and energetics of C ₇₂ α isomers. Journal of Chemical Physics, 1998, 109, 87-93.	1.2	15
1790	On the effects of basis set truncation and electron correlation in conformers of 2-hydroxyacetamide. Advances in Quantum Chemistry, 1998, 32, 93-107.	0.4	2
1791	Systematic Sequences of Even-Tempered Gaussian Primitives for Diatomic Molecules in Solution: A Preliminary Study using Continuum Solvation Models. Advances in Quantum Chemistry, 1998, , 285-313.	0.4	1
1792	The Nuclear-Chemical Method of Carbenium and Silylenium Cation Generation. α Ab Initio Calculations in Radiochemistry. Main Group Chemistry, 1998, 2, 203-206.	0.4	6

#	ARTICLE	IF	CITATIONS
1793	Theoretical Study of the Effect of a Lewis Acid on Hydrogen Exchange Coupling in a Trihydride Metallocene: The Cp ₂ NbH ₃ -AlH ₃ System. <i>Inorganic Chemistry</i> , 1998, 37, 2334-2339.	1.9	12
1794	Electron momentum density of TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) studied by Compton scattering. <i>Journal of Physics Condensed Matter</i> , 1999, 11, 9025-9032.	0.7	2
1795	Effects of the nuclear transformation ¹¹¹ Ag(I) to ¹¹¹ Cd(II) in a single crystal of Ag[¹¹¹ Ag](imidazole) ₂ NO ₃ . <i>Physical Review B</i> , 1999, 59, 14182-14190.	1.1	9
1796	Molecular simulation of static hyper-Rayleigh scattering: A calculation of the depolarization ratio and the local fields for liquid nitrobenzene. <i>Journal of Chemical Physics</i> , 1999, 111, 9711-9719.	1.2	32
1797	Measurement and simulation of nuclear inelastic-scattering spectra of molecular crystals. <i>Physical Review B</i> , 1999, 59, 975-984.	1.1	103
1798	On the electronic structure of SiO ₂ and its anion. <i>Molecular Physics</i> , 1999, 96, 549-553.	0.8	5
1799	Dissociation of water on the surface of galena (PbS): A comparison of periodic and cluster models. <i>Journal of Chemical Physics</i> , 1999, 111, 6942-6946.	1.2	25
1800	Direct formation of solid ammonium chloride particles from HCl and NH ₃ vapors. <i>Journal of Chemical Physics</i> , 1999, 110, 11121-11124.	1.2	45
1801	Long-range effects in optimizing the geometry of stereoregular polymers. II. Hydrogen fluoride chains as a working example. <i>Journal of Chemical Physics</i> , 1999, 111, 5324-5330.	1.2	20
1802	The accurate calculation and prediction of the bond dissociation energies in a series of hydrocarbons using the IMOMO (integrated molecular orbital+molecular orbital) methods. <i>Journal of Chemical Physics</i> , 1999, 111, 8799-8803.	1.2	67
1803	Infrared spectroscopy of negatively charged water clusters: Evidence for a linear network. <i>Journal of Chemical Physics</i> , 1999, 110, 6268-6277.	1.2	116
1804	Energetic and structural features of the CH ₄ +O(3P) → CH ₃ +OH abstraction reaction: Does perturbation theory from a multiconfiguration reference state (finally) provide a balanced treatment of transition states?. <i>Journal of Chemical Physics</i> , 1999, 111, 10046-10052.	1.2	29
1805	Fast computation of analytical second derivatives with effective core potentials: Application to Si ₈ C ₁₂ , Ge ₈ C ₁₂ , and Sn ₈ C ₁₂ . <i>Journal of Chemical Physics</i> , 1999, 111, 8778-8784.	1.2	16
1806	Large two-photon absorption cross sections in two-dimensional, charge-transfer, cumulene-containing aromatic molecules. <i>Journal of Chemical Physics</i> , 1999, 111, 7758-7765.	1.2	98
1807	Electronic structure and spectral properties of paramagnetic point defects in Si ₃ N ₄ . <i>Physical Review B</i> , 1999, 60, 12617-12625.	1.1	37
1808	Mechanism of C ₄ F ₈ dissociation in parallel-plate-type plasma. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1999, 17, 2557-2571.	0.9	49
1809	Monte Carlo simulation of F [•] (H ₂ O) ₄ using an ab initio potential. <i>Journal of Chemical Physics</i> , 1999, 110, 4338-4346.	1.2	54
1810	Fully relativistic ab initio calculations of the energies of chiral molecules including parity-violating weak interactions. <i>Physical Review A</i> , 1999, 60, 4439-4453.	1.0	152

#	ARTICLE	IF	CITATIONS
1811	Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins. <i>Journal of Chemical Physics</i> , 1999, 110, 9135-9144.	1.2	68
1812	Reaction field effects on nitrogen shielding. <i>Journal of Chemical Physics</i> , 1999, 110, 1611-1622.	1.2	86
1813	Ab initio calculations for N-methyl-1-(N ^ε -acetylaminio)- <i>t</i> -2-phenylcyclohexane- <i>r</i> -1-carboxamide: a $\hat{\Gamma}^3$ -turn mimetic. <i>Tetrahedron</i> , 1999, 55, 1399-1406.	1.0	6
1814	Squaric acid difluoride. <i>Journal of Fluorine Chemistry</i> , 1999, 99, 99-104.	0.9	5
1815	Structure elucidation and photochemistry of substituted carboxylic compounds by low temperature matrix-isolation and solid state vibrational spectroscopy. <i>Journal of Molecular Structure</i> , 1999, 480-481, 83-99.	1.8	9
1816	A concerted SCF-MO ab initio and vibrational spectroscopic study of the conformational isomerism in 2-aminoethanol. <i>Journal of Molecular Structure</i> , 1999, 482-483, 591-599.	1.8	61
1817	Cis / trans -isomerizations in 1,2-bis(2-thienyl)ethene derivatives: a joint experimental and computational approach. <i>Journal of Molecular Structure</i> , 1999, 485-486, 87-96.	1.8	8
1818	Molecular structure and vibrational spectra of methyl glycolate and methyl $\hat{\Gamma}^3$ -hydroxy isobutyrate. <i>Journal of Molecular Structure</i> , 1999, 509, 183-199.	1.8	15
1819	Color and substitution pattern in anthocyanidins. A combined quantum chemical $\hat{\Gamma}^3$ chemometrical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 761-771.	2.0	15
1820	A comparative study of vibrational anharmonicity in the bihalide anions XHX $\hat{\Gamma}^3$: X=F, Cl, Br. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 719-729.	2.0	30
1821	Raman spectrum of [5 $\hat{\Gamma}^3$ - ¹³ C]thymidine: vibrations of its 5 $\hat{\Gamma}^3$ -end atomic group. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 1999, 55, 1887-1896.	2.0	10
1822	Experimental and theoretical studies of gas-phase reactions of SiF _x ⁺ (x = 1 $\hat{\Gamma}^3$ 3) with ammonia: intramolecular H-atom transfer reactions with SiF ₃ ⁺ and F ₂ Si(NH ₂). <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 381-392.	0.7	8
1823	A model for predicting the solubility of 1,3,5-trinitro-1,3,5-s-triazine (RDX) in supercritical CO ₂ : isothermal $\hat{\Gamma}^3$ isobaric Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 1999, 155, 177-191.	1.4	13
1824	A DVR analysis of some vibrational modes in the elongated dihydrogen complex [Ru($\hat{\Gamma}^3$ -2-H ₂)(C ₅ H ₅)(H ₂ PCH ₂ PH ₂)] ⁺ . <i>Chemical Physics</i> , 1999, 241, 155-166.	0.9	17
1825	The thyl peroxyl radical: formation and UV spectrum. A multiconfigurational ab initio study. <i>Chemical Physics</i> , 1999, 244, 175-183.	0.9	7
1826	A theoretical study of the isomerization pathways for HBrO ₂ isomers. <i>Chemical Physics</i> , 1999, 247, 387-394.	0.9	11
1827	1.8 and 1.9 $\hat{\Gamma}^3$... resolution structures of the <i>Penicillium amagasakiense</i> and <i>Aspergillus niger</i> glucose oxidases as a basis for modelling substrate complexes. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 969-977.	2.5	264
1828	Two-photon absorption in five-membered heteroaromatic oligomers. <i>Optics Communications</i> , 1999, 168, 297-303.	1.0	27

#	ARTICLE	IF	CITATIONS
1829	Colchicine red-ox chemistry revisited: Cathodic behavior and EPR observation of an intermediate radical anion. <i>Tetrahedron</i> , 1999, 55, 11601-11608.	1.0	7
1830	Ab initio study of the amino group twisting and wagging reaction paths in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. <i>Chemical Physics</i> , 1999, 240, 9-18.	0.9	54
1831	Effect of solvent fluctuations on proton transfer dynamics: a hybrid AM1/MM molecular dynamics simulation on the $[H_3N^+H^+NH_3]^+$ system. <i>Chemical Physics</i> , 1999, 240, 93-99.	0.9	9
1832	Energy gradient method for the ground, excited, ionized, and electron-attached states calculated by the SAC (symmetry-adapted cluster)/SAC+CI (configuration interaction) method. <i>Chemical Physics</i> , 1999, 242, 177-193.	0.9	57
1833	Vibrational versus electronic first hyperpolarizabilities of π -conjugated organic molecules: an ab initio Hartree-Fock investigation upon the effects of the nature of the linker. <i>Chemical Physics</i> , 1999, 245, 213-226.	0.9	72
1834	Cluster models of the dissociation of water on the surface of galena (PbS). <i>Chemical Physics Letters</i> , 1999, 299, 527-531.	1.2	38
1835	On the performance of density functional theory for symmetry-breaking problems. <i>Chemical Physics Letters</i> , 1999, 302, 425-430.	1.2	128
1836	Structure and internal rotation in quadruply bonded $\hat{\text{I}}_{\pm}\text{-Mo}_2\text{Cl}_4(\text{P}^{\hat{=}}\text{P})_2$ complexes: a density functional theory study of the cis-Mo ₂ Cl ₄ (PH ₃) ₄ complex. <i>Chemical Physics Letters</i> , 1999, 303, 621-628.	1.2	11
1837	Gradients in valence bond theory. <i>Chemical Physics Letters</i> , 1999, 310, 553-556.	1.2	10
1838	Ab initio molecular orbital study of the isomerization reaction surfaces of C ₃ and C ₃ ⁺ . <i>Chemical Physics Letters</i> , 1999, 312, 65-70.	1.2	21
1839	Ab initio localisation of adsorption sites in guest/host systems: application to the system thionine in zeoliteNaY. <i>Chemical Physics Letters</i> , 1999, 311, 485-490.	1.2	2
1840	Theoretical study of structures and dynamic properties of Sc ₃ @C ₈₂ . <i>Chemical Physics Letters</i> , 1999, 313, 45-51.	1.2	23
1841	A density functional study on the formation of stereoerrors in the stereoselective propene polymerization with zirconocene catalysts. <i>Journal of Organometallic Chemistry</i> , 1999, 592, 11-21.	0.8	23
1842	Quantum and simulation studies of $X^{\sim}(H_2O)_n$ systems. <i>Electrochimica Acta</i> , 1999, 45, 659-673.	2.6	39
1843	An ab initio study on the structure of the ground state of the C ₃ O ₂ molecule. <i>Chemical Physics Letters</i> , 1999, 303, 50-56.	1.2	6
1844	Computational confirmation of C ₅ N ₂ observed in rare-gas matrices. <i>Chemical Physics Letters</i> , 1999, 305, 451-457.	1.2	15
1845	Vibrational effects on the polarizability and second hyperpolarizability of ethylene. <i>Chemical Physics Letters</i> , 1999, 307, 484-492.	1.2	40
1846	The geometrical effect on the chemical reactivity of nucleophilic carbenes. A theoretical study. <i>Chemical Physics Letters</i> , 1999, 308, 283-288.	1.2	17

#	ARTICLE	IF	CITATIONS
1847	Vibrations of the cubane molecule: inelastic neutron scattering study and theory. <i>Chemical Physics Letters</i> , 1999, 309, 234-240.	1.2	15
1848	Negative ion resonances and vibrational mode selectivity in inelastic electron scattering studies of hydrogen and diethylsilane adsorbed on Si(100). <i>Chemical Physics Letters</i> , 1999, 313, 805-811.	1.2	2
1849	Evaluation of the charge penetration energy between non-orthogonal molecular orbitals using the Spherical Gaussian Overlap approximation. <i>Chemical Physics Letters</i> , 1999, 315, 140-144.	1.2	61
1850	The Dimer of Cyanodiacetylene: Stacking vs. Hydrogen Bonding. <i>Monatshefte für Chemie</i> , 1999, 130, 1017-1030.	0.9	0
1851	Theoretical modeling of constrained geometry catalysts beyond the naked cation approach. <i>Topics in Catalysis</i> , 1999, 7, 45-60.	1.3	25
1852	Title is missing!. <i>Structural Chemistry</i> , 1999, 10, 263-276.	1.0	1
1853	Title is missing!. <i>Journal of Solution Chemistry</i> , 1999, 28, 1045-1070.	0.6	28
1854	A natural orbital diagnostic for multiconfigurational character in correlated wave functions. <i>Journal of Chemical Physics</i> , 1999, 110, 4199-4207.	1.2	90
1855	Theoretical Studies on the Continuum Solvation of Some N,N-Dimethyl- and N-Methyl, N-acetyl-Guanidine and Guanidinium Conformers. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1857-1867.	1.1	13
1856	Study on the Isomerization of 1-Acylazetidone. A Comparative Study with the Case of 1-Acylaziridine. <i>Journal of Organic Chemistry</i> , 1999, 64, 5686-5690.	1.7	2
1857	Atomic and molecular forms of oxygen on Ag(331). Theoretical analysis using the DFT method. <i>Journal of Structural Chemistry</i> , 1999, 40, 343-349.	0.3	3
1858	Modelling of Aniline-Vermiculite and Tetramethylammonium-Vermiculite; Test of Force Fields. <i>Journal of Molecular Modeling</i> , 1999, 5, 8-16.	0.8	16
1859	Intramolecular non-bonded interactions between oxygen and group VIA elements. An ab initio molecular orbital and density functional theory investigation of the structures of $HX-CH_2-CHO$ ($X=S, Se$ and Te). <i>Computational and Theoretical Chemistry</i> , 1999, 459, 187-199.	1.5	5
1860	Theoretical studies of the NTO unimolecular decomposition. <i>Computational and Theoretical Chemistry</i> , 1999, 460, 79-102.	1.5	39
1861	Properties of phosphorothioate DNA analogs. An ab initio study of prototype model linkages derived from dimethyl-phosphate anion. <i>Computational and Theoretical Chemistry</i> , 1999, 460, 103-116.	1.5	6
1862	A theoretical study on reaction mechanism of oxidative coupling reaction of p-phenylenediamine with phenol: a proposal of the route via a [5,5]-sigmatropic rearrangement. <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 429-438.	1.5	5
1863	Unconventional cage structures of endohedral metallofullerenes. <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 97-104.	1.5	66
1864	A density functional theory study of the pyrolysis mechanisms of indole. <i>Computational and Theoretical Chemistry</i> , 1999, 461-462, 569-579.	1.5	13

#	ARTICLE	IF	CITATIONS
1865	A theoretical study on the conformations, energetics, and solvation effects on the cation- π interaction between monovalent ions Li ⁺ , Na ⁺ , and K ⁺ and naphthalene molecules. Computational and Theoretical Chemistry, 1999, 468, 85-94.	1.5	22
1866	Ab initio GB study of solvent effect on the cis- \leftrightarrow -trans isomerization of 4-dimethylamino-4-nitroazobenzene. Computational and Theoretical Chemistry, 1999, 468, 95-104.	1.5	18
1867	Ab initio studies on the conformations, thermodynamic properties and rotational isomerization of diphenylamine (DPA). Computational and Theoretical Chemistry, 1999, 489, 151-157.	1.5	12
1868	Experimental and computational studies of the structure and vibrational spectra of azetidine derivatives. Computational and Theoretical Chemistry, 1999, 491, 67-80.	1.5	4
1869	DTMM and COSMIC molecular mechanics parameters for alkylsilanes. Computational and Theoretical Chemistry, 1999, 490, 219-232.	1.5	4
1870	A theoretical investigation of indole tautomers. Computational and Theoretical Chemistry, 1999, 491, 211-222.	1.5	24
1871	Ab initio effective core potential study of equatorially coordinated uranyl species: effect of hydration to the calculated properties. Computational and Theoretical Chemistry, 1999, 487, 33-38.	1.5	21
1872	Preference in formation of three-, five-, and six-membered rings in cyclization of the primary unsaturated radical studied with the hybrid density functional theory method. Computational and Theoretical Chemistry, 1999, 492, 285-291.	1.5	9
1873	Ab initio and density functional studies on bonding nature of the N-N bonds in 1,2,5-trinitroimidazole and 1,2,4,5-tetranitroimidazole. International Journal of Quantum Chemistry, 1999, 72, 145-154.	1.0	18
1874	A new partitioning scheme for molecular interacting systems within a multiconfigurational or monoconfigurational Hartree-Fock formalism. International Journal of Quantum Chemistry, 1999, 72, 157-176.	1.0	7
1875	The polarizability and the second hyperpolarizability of tetrakis(phenylethynyl)ethene and several of its lithiated derivatives. International Journal of Quantum Chemistry, 1999, 72, 177-187.	1.0	9
1876	Serine peptidase catalytic machinery: Cooperative one-step mechanism. International Journal of Quantum Chemistry, 1999, 73, 161-174.	1.0	21
1877	Ab initio study of preferential interactions between aromatic side chains. International Journal of Quantum Chemistry, 1999, 73, 175-186.	1.0	8
1878	Aromaticity of bent benzene rings: A VBSCF study. International Journal of Quantum Chemistry, 1999, 74, 213-221.	1.0	39
1879	Pseudospectral calculation of the gas-phase acidities of aliphatic alcohols. International Journal of Quantum Chemistry, 1999, 74, 417-422.	1.0	3
1880	Monte Carlo simulations of water clusters on a parallel computer using an ab initio potential. International Journal of Quantum Chemistry, 1999, 74, 709-719.	1.0	6
1881	Bond length alternation effects on the static electronic polarizability and second hyperpolarizability of polyacetylene chains. International Journal of Quantum Chemistry, 1999, 75, 441-447.	1.0	40
1882	Theoretical study of the peroxy radicals RO ₂ self-reaction: Structures and stabilization energies of the intermediate RO ₄ R for various R. International Journal of Quantum Chemistry, 1999, 75, 671-682.	1.0	13

#	ARTICLE	IF	CITATIONS
1883	Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 683-692.	1.0	20
1884	Comprehensive ab initio quantum mechanical and molecular orbital (MO) analysis of cisplatin: Structure, bonding, charge density, and vibrational frequencies. <i>Journal of Computational Chemistry</i> , 1999, 20, 365-382.	1.5	88
1885	An Experimental and Theoretical Study of Gaseous Products in the Radiolysis of Germane/Ethylene Mixtures. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 323-332.	1.0	11
1886	Intermediates and Products of the Hexachlorosilane Cleavage of Group 14 Element Phosphanes and Amines – Molecular Structure of Di-tert-butyl(trichlorosilyl)phosphane in the Gas Phase Determined by Electron Diffraction and ab Initio Calculations. <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 1381-1392.	1.0	19
1887	The Lewis Basicity of Diaminocarbene – A Theoretical Study of Donor–Acceptor Complexes of C(NH ₂) ₂ , NH ₃ and CO with the Lewis Acids EF ₃ , ECl ₃ (E = B, Al, Ga, In), TiF ₄ and TiCl ₄ . <i>European Journal of Inorganic Chemistry</i> , 1999, 1999, 2037-2045.	1.0	46
1888	Sulfonyl-Stabilized Allylic Norbornenyl and Norbornyl Carbanions: Structure and Stereoselectivity of Reaction with Electrophiles. <i>European Journal of Organic Chemistry</i> , 1999, 1999, 1627-1651.	1.2	30
1890	The electronic structure of transition metal compounds. <i>Theoretical and Computational Chemistry</i> , 1999, , 555-570.	0.2	1
1891	A Modified Version of the Cornell et al. Force Field with Improved Sugar Pucker Phases and Helical Repeat. <i>Journal of Biomolecular Structure and Dynamics</i> , 1999, 16, 845-862.	2.0	882
1892	Stability of Hyperlithiated Borides. <i>Journal of Physical Chemistry A</i> , 1999, 103, 710-715.	1.1	15
1893	Structure, Chemical Bonding, and Nuclear Quadrupole Interactions of ¹¹² Cd(OH) ₂ : Experiment and First Principles Calculations. <i>Inorganic Chemistry</i> , 1999, 38, 2860-2867.	1.9	28
1894	Steric Course and Mechanism of the Water Exchange of the Ruthenium(III) Aqua Pentaammine Ion. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9345-9348.	1.1	26
1895	IMOMO-G2MS Approaches to Accurate Calculations of Bond Dissociation Energies of Large Molecules. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4580-4586.	1.1	40
1896	Experimental and ab initio spectra of the persistent carbocation generated upon adsorption of vinylanisole in acid zeolites. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3689-3695.	1.3	15
1897	Highly active ethylene polymerisation catalysts based on iron: an ab initio study. <i>Chemical Communications</i> , 1999, , 1333-1334.	2.2	71
1898	Structural and electronic changes accompanying reduction of Cr(CO) ₄ (bpy) to its radical anion: a quantum chemical interpretation of spectroelectrochemical experiments. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 3081-3086.	1.1	14
1899	The synthesis of C[Si(CH ₃) ₂ X] ₃ SiX ₃ compounds (X = H, Cl, Br and OH) and the molecular structure of C[Si(CH ₃) ₂ H] ₃ SiH ₃ in the gas phase; a study by electron diffraction and ab initio molecular orbital calculations. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 2293-2302.	1.1	10
1900	Multidimensional tunneling dynamics on HSiOH cis-trans isomerization with interpolated potential energy surface. <i>Journal of Chemical Physics</i> , 1999, 111, 3410-3419.	1.2	19
1901	Tetrachloropyrimidine: molecular structure by electron diffraction, vibrational analysis by infrared, Raman and inelastic neutron scattering spectroscopies, and quantum mechanical calculations. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3453-3460.	1.3	2

#	ARTICLE	IF	CITATIONS
1902	Structure and low-frequency vibrational properties of (H ₂ O) ₁₀ composed of a ring form of (H ₂ O) ₄ and a cage form of (H ₂ O) ₆ . <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 3473-3479.	1.3	2
1903	Pyramidal inversion energies and conformational analysis of chalcogen-onium imides based on ab initio MO calculations. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1469-1474.	0.9	18
1904	Synthesis and molecular structures of N,N-dimethylhydroxylamino-trichlorosilane and -germane. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 4291-4297.	1.1	27
1905	1,1,2-Tri-tert-butyldisilane, But ₂ HSiH ₂ But: vibrational spectra and molecular structure in the gas phase by electron diffraction and ab initio calculations. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 2303-2310.	1.1	15
1906	Theoretical evidence of a feasible concerted antara-antara cycloaddition. <i>Chemical Communications</i> , 1999, , 903-904.	2.2	1
1907	Mg clusters on MgO surfaces: study of the nucleation mechanism with MIES and ab initio calculations. <i>Faraday Discussions</i> , 1999, 114, 173-194.	1.6	77
1908	Structural studies of the chiral lithium amides [PhC(H)Me] ₂ NLi and [PhCH ₂ {PhC(H)Me}NLi·THF] derived from \pm -methylbenzylamine. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 4063-4068.	1.1	34
1909	Zinc(II) hydration in aqueous solution. A Raman spectroscopic investigation and an ab-initio molecular orbital study. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 4583-4593.	1.3	95
1910	Heterolytic dihydrogen activation in an iridium complex with a pendant basic group. <i>Chemical Communications</i> , 1999, , 297-298.	2.2	68
1911	Orbital Interactions and Solvent Effects Determining the Stability of Condensed Cyclopentadienides in Solution. <i>Journal of Organic Chemistry</i> , 1999, 64, 2821-2829.	1.7	10
1912	Studies of Silylfurans, Furylsilanes, and Silylthiophenes: Structure of 2,5-Disilylthiophene. <i>Organometallics</i> , 1999, 18, 2760-2765.	1.1	9
1913	Resonant Ion-Dip Infrared Spectroscopy of Ternary Benzene ⁿ (Water) _n (Methanol) _m Hydrogen-Bonded Clusters. <i>Journal of Physical Chemistry A</i> , 1999, 103, 503-513.	1.1	28
1914	Theoretical study on linear dicyanide and dicarbonyl complexes of the metals Au, Hg, and Tl. On the possible existence of a [Tl(CO) ₂] ₃ ⁺ cation. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 3783-3790.	1.1	7
1915	Superacid protonation of dihydrocyclobuta[e]pyrene and its C ₆₀ -o-quinodimethane adduct. An NMR, ab initio/GIAO and AM1/PM3 study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2129-2132.	0.9	6
1916	UV-vis and IR spectroscopic characterization of diphenyl disulfide radical cation in acid zeolites and its rearrangement to thianthrenium radical cation. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 145-152.	0.9	6
1917	Hexameric chiral \pm -amino lithium alkoxides: a solid-state and theoretical structural investigation. <i>New Journal of Chemistry</i> , 1999, 23, 499-507.	1.4	19
1918	The reaction of acetone and ammonia on acid zeolites. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 2613-2620.	1.3	8
1919	The molecular structures of 2-, 3- and 4-chloropyridine and chloropyrazine in the gas phase by electron diffraction and ab initio calculations. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 745-754.	0.9	9

#	ARTICLE	IF	CITATIONS
1920	Identity-reaction proton transfers from oxygen acids yielding localized vs. delocalized conjugate bases. An ab initio study. Canadian Journal of Chemistry, 1999, 77, 810-816.	0.6	9
1921	Sodium hydrotris(methimazolyl)borate, a novel soft, tridentate ligand: preparation, structure and comparisons with sodium hydrotris(pyrazolyl)borate. Journal of the Chemical Society Dalton Transactions, 1999, , 2119-2126.	1.1	127
1922	Ab Initio Methods for the Calculation of NMR Shielding and Indirect Spin-Spin Coupling Constants. Chemical Reviews, 1999, 99, 293-352.	23.0	1,318
1923	Hydrogen Bond Types, Binding Energies, and ¹ H NMR Chemical Shifts. Journal of Physical Chemistry A, 1999, 103, 8121-8124.	1.1	96
1924	Infra-red, electron paramagnetic resonance and X-ray photoemission spectral properties of point defects in silica from first-principle calculations. Journal of Non-Crystalline Solids, 1999, 245, 175-182.	1.5	12
1925	Bonding features in endohedral metallofullerenes. Topological analysis of the electron density distribution. Chemical Physics Letters, 1999, 302, 312-316.	1.2	50
1926	Synthesis and Structure of [Ni{Ga-C(SiMe ₃) ₃ }] ₄ and Quantum-Chemical Verification of Strong π Back-Bonding in the Model Compounds [Ni(EMe) ₄] (E = B, Al, Ga, In, Tl). Organometallics, 1999, 18, 3778-3780.	1.1	99
1927	The Nature of Electronic Contact in Self-Assembled Monolayers for Molecular Electronics: Evidence for Strong Coupling. Journal of Physical Chemistry B, 1999, 103, 8915-8919.	1.2	59
1928	Structures and binding enthalpies of M+(H ₂ O) _n clusters, M=Cu, Ag, Au. Journal of Chemical Physics, 1999, 110, 1475-1491.	1.2	110
1929	The molecular and crystal structures of the tris(dimethylamino)phosphoranes (Me ₂ N) ₃ P-X (X=...=...BH ₃). J. Phys. Chem. 1999, 103, 7843-7848.	1.1	8
1930	Reactions of Laser-Ablated Y and La Atoms, Cations and Electrons with O ₂ . Infrared Spectra and Density Functional Calculations of the MO, MO ⁺ , MO ₂ , MO ₂ ⁺ , and MO ₂ ⁻ Species in Solid Argon. Journal of Physical Chemistry A, 1999, 103, 6525-6532.	1.1	53
1931	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	1.1	79
1932	Pyrrlodiazines. 5. Synthesis, Structure, and Chemistry of Pyrrolo[1,2-c]pyrimidine. Dipolar Cycloaddition of Pyrrolo[1,2-c]pyrimidinium Ylides. Journal of Organic Chemistry, 1999, 64, 7788-7801.	1.7	33
1933	Are There Structurally Relevant Attractive Interactions between Nitrogen Atoms and Group 14 Elements in Their Aminomethyl Compounds?. Organometallics, 1999, 18, 3437-3444.	1.1	24
1934	Intramolecular C-H Insertion Reactions of Boroxo Fischer Carbene Complexes. Regio- and Diastereoselective Modification of Terpenes. Journal of the American Chemical Society, 1999, 121, 8776-8782.	6.6	18
1935	Solvation of Sodium Chloride: An Effective Fragment Study of NaCl(H ₂ O) _n . Journal of Physical Chemistry A, 1999, 103, 4162-4166.	1.1	88
1936	Nature of the Metal-Alkene Bond in Platinum Complexes of Strained Olefins. Organometallics, 1999, 18, 457-465.	1.1	59
1937	Benzannulation Effect on Ene-diyne Cycloaromatization: An ab Initio Molecular Orbital Study. Journal of Physical Chemistry A, 1999, 103, 7672-7675.	1.1	53

#	ARTICLE	IF	CITATIONS
1938	Structure and Bonding of Chlorine Oxides and Peroxides: ClO_x , ClO_x ($x=1-4$), and Cl_2O_x ($x=1-8$). <i>Journal of Physical Chemistry A</i> , 1999, 103, 3078-3088.	1.1	74
1939	Synthesis and Molecular Structures in the Gas Phase of <i>N,N</i> -Dimethylaminoxy-trimethylsilane and -trimethylgermane. <i>Inorganic Chemistry</i> , 1999, 38, 5323-5328.	1.9	21
1940	DFT Study of the Role of Bridging Diphosphine Ligands in the Structure and the Internal Rotation in Quadruply Bonded Metal Dimers of the $\text{Mo}_2\text{Cl}_4(\text{P}^{\wedge}\text{P})_2$ Type. <i>Inorganic Chemistry</i> , 1999, 38, 5443-5448.	1.9	14
1941	Intramolecular <i>N</i> -Donor-Stabilized Silenes: An <i>ab Initio</i> MO Study of 1-Methylene-5-methyl-5-aza-2,8-dioxo-1-silacyclooctane. <i>Organometallics</i> , 1999, 18, 4692-4699.	1.1	11
1942	Density Functional Studies of the Formation of Nitrous Acid from the Reaction of Nitrogen Dioxide and Water Vapor. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7848-7855.	1.1	48
1943	Modeling the Spectroscopy of the Lowest Excited Singlet State of <i>cis,trans</i> -1,3,5,7-Octatetraene: The Role of Symmetry Breaking and Vibronic Interactions. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2220-2226.	1.1	15
1944	Structural Effects of C_6 Substitution in 6-(4-(Dimethylamino)phenyl)fulvenes. <i>Journal of Organic Chemistry</i> , 1999, 64, 9067-9076.	1.7	18
1945	Ground and Triplet Excited Structures and Spectroscopic Properties of Halogenated Zinc-meso-Tetraphenylporphyrin. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9378-9382.	1.1	37
1946	Aquation of the Chloro Pentaammine Complexes of Cobalt(III) and Chromium(III): Do the Almost Equal Activation Parameters Arise from a Common Mechanism?. <i>Inorganic Chemistry</i> , 1999, 38, 5730-5733.	1.9	17
1947	Direct Dynamics for Free Radical Kinetics in Solution: Solvent Effect on the Rate Constant for the Reaction of Methanol with Atomic Hydrogen. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4893-4909.	1.1	103
1948	Reaction of Carbodiphosphorane $\text{Ph}_3\text{PCPPH}_3$ with $\text{Ni}(\text{CO})_4$. Experimental and Theoretical Study of the Structures and Properties of $(\text{CO})_3\text{NiC}(\text{PPh}_3)_2$ and $(\text{CO})_2\text{NiC}(\text{PPh}_3)_2$. <i>Organometallics</i> , 1999, 18, 619-626.	1.1	93
1949	<i>Ab Initio</i> Monte Carlo Simulated Annealing Study of $\text{HCl}(\text{H}_2\text{O})_n$ ($n=3, 4$) Clusters. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4631-4640.	1.1	79
1950	Experimental and Theoretical Study of the Kinetic and Thermodynamic Sites of Protonation in $(\text{CO})\text{Pt}(\text{P}^{\wedge}\text{P})_2\text{Pt}(\text{P}^{\wedge}\text{P})_2$. <i>Inorganic Chemistry</i> , 1999, 38, 5257-5265.	1.9	14
1951	Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1140-1149.	1.1	254
1952	Molecular Structure of 3,4-Difluorofuran-2,5-dione (Difluoromaleic Anhydride) As Determined by Electron Diffraction and Microwave Spectroscopy in the Gas Phase and by Theoretical Computations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1758-1767.	1.1	10
1953	Quantum Chemical Study of Ion-Molecule Reactions in $\text{N}_2^{++} \text{O}_2$ System. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5749-5757.	1.1	5
1954	Dissociation Pathways of Peroxyacetyl Nitrate (PAN). <i>Journal of Physical Chemistry A</i> , 1999, 103, 11451-11459.	1.1	38
1955	Density Functional Calculations on Disaccharide Mimics: Studies of Molecular Geometries and <i>Trans-O</i> -glycosidic $^3\text{JCOCH}$ and $^3\text{JCOCC}$ Spin-Couplings. <i>Journal of the American Chemical Society</i> , 1999, 121, 9843-9851.	6.6	90

#	ARTICLE	IF	CITATIONS
1956	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine-Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of the American Chemical Society</i> , 1999, 121, 1317-1323.	6.6	94
1957	XPS Study of Stilbazolium Chromophores and Their Intercalation Compounds in the MnPS ₃ Layered Phase. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3545-3551.	1.2	11
1958	Proton Transfer in Aminocyclopentadienyl Ruthenium Hydride Complexes. <i>Organometallics</i> , 1999, 18, 3981-3990.	1.1	88
1959	Intrinsic Affinities of Alkali Cations for 15-Crown-5 and 18-Crown-6: Bond Dissociation Energies of Gas-Phase M ⁺ -Crown Ether Complexes. <i>Journal of the American Chemical Society</i> , 1999, 121, 417-423.	6.6	191
1960	Local Geometry Trends and Torsional Sensitivity in N-Formyl-L-alanyl-L-alanine Amide and the Limitations of the Dipeptide Approximation. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8337-8345.	1.1	15
1961	A Theoretical Investigation of the Torsional Potential in 3,3'-Dimethyl-2,2'-bithiophene and 3,4'-Dimethyl-2,2'-bithiophene: A Comparison between HF, MP2, and DFT Theory. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6800-6804.	1.1	27
1962	A Cluster Study of Anionic Hydration: Spectroscopic Characterization of the I ⁻ ·Wn, 1 ≤ n ≤ 3, Supramolecular Complexes at the Primary Steps of Solvation. <i>Journal of Physical Chemistry A</i> , 1999, 103, 443-447.	1.1	61
1963	Symmetry Force Fields for Neutral and Ionic Transition Metal Carbonyl Complexes from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1381-1393.	1.1	27
1964	The Mechanism of Methoxy Radical Oxidation by O ₂ in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent O···O Bonding Interaction. <i>Journal of the American Chemical Society</i> , 1999, 121, 1337-1347.	6.6	77
1965	Structures and Reaction Pathways in Rhodium(I)-Catalyzed Hydrogenation of Enamides: A Model DFT Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 8741-8754.	6.6	108
1966	C-H Stretch Modes as a Probe of H-Bonding in Methanol-Containing Clusters. <i>Journal of Physical Chemistry A</i> , 1999, 103, 496-502.	1.1	61
1967	The Fragmentation of Melamine: A Study via Electron-Impact Ionization, Laser-Desorption Ionization, Collision-Induced Dissociation, and Density Functional Calculations of Potential Energy Surface. <i>Journal of Physical Chemistry B</i> , 1999, 103, 582-596.	1.2	25
1968	1,3-Dipolar Addition of Phenylazide to the Carbon-Carbon Double Bond: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1276-1282.	1.1	23
1969	A Theoretical Study of Pyrolysis Mechanisms of Pyrrole. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3917-3922.	1.1	40
1970	Phosphine Dissociation Mediates C-H Cleavage of Fluoroarenes by OsH(C ₆ H ₅)(CO)(PtBu ₂ Me) ₂ . <i>Journal of the American Chemical Society</i> , 1999, 121, 10895-10907.	6.6	26
1971	Theoretical Study of Gas-Phase Reactions of Fe(CO) ₅ with OH ⁻ and Their Relevance for the Water Gas Shift Reaction. <i>Organometallics</i> , 1999, 18, 2801-2812.	1.1	55
1972	The Hammond Postulate and the Principle of Maximum Hardness in Some Intramolecular Rearrangement Reactions. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8847-8852.	1.1	62
1973	Structure and Properties of p-Aminophenoxyl Radical. <i>Journal of Physical Chemistry A</i> , 1999, 103, 11181-11187.	1.1	17

#	ARTICLE	IF	CITATIONS
1974	Electrophilic and Nucleophilic Reactivities of the Azomethine Carbon of SAMP-Hydrazones: \hat{A} Stereoselective Synthesis of \hat{I}^3 -Amino Ketone Derivatives. <i>Journal of Organic Chemistry</i> , 1999, 64, 6329-6336.	1.7	39
1975	Electronic Structures of Polymers Containing Carbon Multiple Bond and Disilane Units in Their Backbone \hat{E} . <i>Macromolecules</i> , 1999, 32, 7045-7050.	2.2	4
1976	Torsional Potentials of Perfluoro-1,3-butadiene and Perfluoro-1,3,5-hexatriene: $\hat{A}\%$ A Comparison of ab Initio and Density Functional Results. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2821-2827.	1.1	16
1977	Density functional calculation of structure and vibrational spectra of polyenes. <i>Journal of Chemical Physics</i> , 1999, 110, 3241-3250.	1.2	35
1978	Theoretical Studies of $B2Lin(n=1\hat{a}^{\wedge}4)$. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9931-9937.	1.1	8
1979	Transition Moment Directions in Amide Crystals. <i>Journal of Physical Chemistry B</i> , 1999, 103, 8984-8991.	1.2	10
1980	Synthesis and Characterization of $OsH2Cl[\hat{I}^nN,\hat{I}^nO-(ONCR2)](PiPr3)2(CR2=C(CH2)4CH2, R=CH3)$: \hat{A} Influence of the L2Ligand on the Nature of the H2Unit in $OsH2ClL2(PiPr3)2(L2=ONCR2, NHC(Ph)C6H4)$ Complexes. <i>Organometallics</i> , 1999, 18, 4296-4303.	1.1	17
1981	Synthesis of B- and P-Heterocycles by Reaction of Cyclic Acetals and Ketals with Borinium and Phosphonium Ions. <i>Journal of Organic Chemistry</i> , 1999, 64, 3213-3223.	1.7	29
1982	Mechanisms of the Nucleophilic Substitution of the Allyl Carbons of (\hat{I}^E -Allyl)platinum and (\hat{I}^E -Allyl)palladium Complexes. <i>Inorganic Chemistry</i> , 1999, 38, 370-382.	1.9	21
1983	Does Reaction of Three-Coordinate Molybdenum(III) with $N2O$ Proceed via the Same Mechanism as with $N2$? A Theoretical Study. <i>Organometallics</i> , 1999, 18, 5653-5660.	1.1	39
1984	Theoretical Studies of the Additions of Germylenes to Ethylene. <i>Journal of the American Chemical Society</i> , 1999, 121, 11478-11485.	6.6	43
1985	Bonding Interactions of a Molecular Pair of Tweezers with Transition Metals. Theoretical Study of Bis(\hat{I}^2 -alkyne) Complexes of Copper(I), Silver(I), and Gold(I)1. <i>Organometallics</i> , 1999, 18, 887-894.	1.1	37
1986	A Non-Empirical Intermolecular Potential for Oxalic Acid Crystal Structures. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6448-6457.	1.1	38
1987	Lithiation Selectivity in Monoalkylamine/Dialkylamine Mixtures: \hat{A} A Synthetic and ab Initio Molecular Orbital Study. <i>Organometallics</i> , 1999, 18, 3589-3596.	1.1	17
1988	Formation of Phenolate Anion \hat{A} Counterion Complexes Can Explain the Vibrational Properties of the Phenolate Anion in Solution. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7867-7871.	1.1	9
1989	Photolysis of Matrix-Isolated Allenylketene: \hat{A} An Experimental and Theoretical Study of the Allenylcarbene Reactivity. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9013-9021.	1.1	14
1990	Solution and Solid-State Structure of $Ru(CO)2(Bu2PtC2H4PtBu2)$: \hat{A} Square Planar and Monomeric?. <i>Journal of the American Chemical Society</i> , 1999, 121, 3242-3243.	6.6	20
1991	Are There Metal Oxides That Prefer a $[2+2]$ Addition over a $[3\hat{A}+\hat{A}2]$ Addition to Olefins? Theoretical Study of the Reaction Mechanism of $LReO3$ Addition ($L=O-, Cl, Cp$) to Ethylene1. <i>Journal of the American Chemical Society</i> , 1999, 121, 2021-2031.	6.6	69

#	ARTICLE	IF	CITATIONS
1992	Infrared Spectrum of an Acidic Zeolite OH with Adsorbed Acetonitrile. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2553-2560.	1.1	14
1993	Gas-Phase Generation and Photoelectron Spectra of Dimethyl- and Diisopropylsilanethiones ¹ . <i>Organometallics</i> , 1999, 18, 4795-4799.	1.1	6
1994	Molecular Structure of 3,3-Diethylpentane (Tetraethylmethane) in the Gas Phase As Determined by Electron Diffraction and ab Initio Calculations. <i>Journal of Organic Chemistry</i> , 1999, 64, 4226-4232.	1.7	24
1995	Preparation, Structure, and ⁷³ Ge NMR Spectroscopy of Arylgermanes ArGeH ₃ , Ar ₂ GeH ₂ , and Ar ₃ GeH. <i>Organometallics</i> , 1999, 18, 4317-4324.	1.1	41
1996	Negative Ion Hyperconjugation in Fluorocarbanions and the Nature of the Borderline between E1cB and E2 Mechanisms. An ab Initio Study. <i>Journal of Organic Chemistry</i> , 1999, 64, 861-865.	1.7	43
1997	Cycloadditions of 16-Electron 1,3-Dipoles with Ethylene. A Density Functional and CCSD(T) Study. <i>Journal of Organic Chemistry</i> , 1999, 64, 6710-6716.	1.7	76
1998	Anionic and Neutral Complexes of Uracil and Water. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7912-7917.	1.1	81
1999	Basis Set, Level, and Continuum Solvation Effects on the Stability of a Synthetic Dipeptide: \hat{A} PIDOTIMOD. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5823-5832.	1.1	8
2000	Sodium and Lithium Environments in Single- and Mixed-Alkali Silicate Glasses. An ab Initio Molecular Orbital Study. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1854-1858.	1.2	30
2001	Thermally Activated Site Exchange and Quantum Exchange Coupling Processes in Unsymmetrical Trihydride Osmium Compounds. <i>Inorganic Chemistry</i> , 1999, 38, 1814-1824.	1.9	38
2002	Absolute Metal-Ligand σ Bond Enthalpies in Group 4 Metallocenes. A Thermochemical, Structural, Photoelectron Spectroscopic, and ab Initio Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 1999, 121, 355-366.	6.6	47
2003	Theoretical and Synthetic Studies on Dihaptoacyl and η^2 -Agostic Acyl Complexes of Molybdenum. <i>Organometallics</i> , 1999, 18, 3294-3305.	1.1	24
2004	Density Functional Theory Studies on Vibrational Spectra of Si ₂ H ₅ X (X = F, Cl, Br) and Their Isotopomers. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7437-7444.	1.1	1
2005	Thermal Addition of Disilacyclobutenes and Acetylene: \hat{A} A Theoretical Study on Diels-Alder Type Reactions. <i>Organometallics</i> , 1999, 18, 4637-4645.	1.1	13
2006	Computational and Experimental Test of Steric Influence on Agostic Interactions: \hat{A} A Homologous Series for Ir(III). <i>Journal of the American Chemical Society</i> , 1999, 121, 97-106.	6.6	105
2007	Perfluorocarbenes Produced by Thermal Cracking. Barriers to Generation and Rearrangement. <i>Journal of Organic Chemistry</i> , 1999, 64, 4850-4859.	1.7	19
2008	Kinetics of Bond Shift and Charge Transfer in Dialkynylphenylene-Bridged Dicyclooctatetraenes and Their Dianions. <i>Journal of the American Chemical Society</i> , 1999, 121, 1558-1564.	6.6	20
2009	Molecular Mechanics (MM3) Calculations on Oxygen-Containing Phosphorus (Coordination IV) Compounds. <i>Journal of Organic Chemistry</i> , 1999, 64, 5350-5360.	1.7	18

#	ARTICLE	IF	CITATIONS
2010	Density Functional Theory Studies of Hexamethylene Triperoxide Diamine. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8890-8894.	1.1	22
2011	Ultrafast Infrared Studies of the Reaction Mechanism of Silicon ^{IV} -Hydrogen Bond Activation by δ -5-CpV(CO) ₄ . <i>Journal of Physical Chemistry A</i> , 1999, 103, 10426-10432.	1.1	34
2012	The B1 and B2 Vibrational Modes Causing a D _{6h} to D _{3h} Transition in Benzene and in [18]- and [30]Annulenes. <i>Bulletin of the Chemical Society of Japan</i> , 1999, 72, 697-700.	2.0	13
2013	Radiation-Induced DNA Damage and Repair: An Approach from <i>ab initio</i> MO Method. <i>Theoretical and Computational Chemistry</i> , 1999, , 211-243.	0.2	3
2014	<title>Nonlinear optical properties of lithium-containing derivatives</title>. , 1999, ,		0
2015	A Study Towards the Design of Materials for Nonlinear Optical Applications Using First Principle Calculations. <i>Materials Research Society Symposia Proceedings</i> , 1999, 597, 325.	0.1	1
2016	Acid Ionization of HBr in a Small Water Cluster. <i>Israel Journal of Chemistry</i> , 1999, 39, 273-281.	1.0	37
2017	$\frac{1}{2}Z_{\alpha} - \frac{1}{4} \dots$ $f_{\alpha} e_{\alpha} \dots$ $\odot \frac{1}{4} \alpha^{\circ} Z_{\frac{1}{2}} \dots$ $\ddot{\alpha} \ddot{\epsilon} \dots$ $\alpha \epsilon \epsilon$: $\acute{\epsilon} \approx \zeta^{2/4} \alpha^{\circ} \alpha^{\circ} \ddot{\epsilon} \dots$ $\alpha \zeta - \frac{1}{4} \epsilon \ddot{\alpha} \ddot{\epsilon} \zeta \dagger \ddot{\epsilon} \dots$ $\zeta^{\circ} - \ddot{\alpha} \alpha \dots$ $\ddot{\epsilon} \frac{1}{4} f$. <i>Materia Japonica</i> , 2000, 30, 824-831.		
2018	Formation of an Iron-Oxo Species upon Decomposition of Dinitrogen Oxide on a Model of Fe-ZSM-5 Zeolite. <i>Bulletin of the Chemical Society of Japan</i> , 2000, 73, 29-36.	2.0	56
2019	$\hat{M}^{*} \ddot{\epsilon} L$ Odd Electron Delocalization onto Aromatic Bridging Ligands in a Paramagnetic Dirhodium Complex and Intermolecular $\ddot{\epsilon}$ -Stack Interaction in Crystal. <i>Bulletin of the Chemical Society of Japan</i> , 2000, 73, 657-668.	2.0	12
2020	Ultrafast Charge Transfer Studied by Femtosecond IR $\ddot{\epsilon}$ Spectroscopy and <i>ab initio</i> Calculations. <i>Journal of the Chinese Chemical Society</i> , 2000, 47, 721-728.	0.8	20
2021	Unraveling Environmental Effects on Hydrogen-Bonded Complexes: \hat{A} Matrix Effects on the Structures and Proton-Stretching Frequencies of Hydrogen ^{IV} -Halide Complexes with Ammonia and Trimethylamine. <i>Journal of the American Chemical Society</i> , 2000, 122, 2101-2115.	6.6	96
2022	<i>Ab initio</i> simulation of chemical shift effects from metal ion binding in Bacitracin A. <i>Journal of Computational Chemistry</i> , 2000, 21, 1-7.	1.5	12
2023	Density functional studies of cation-water complexes. <i>Journal of Computational Chemistry</i> , 2000, 21, 63-68.	1.5	8
2024	Theoretical modeling of the heme group with a hybrid QM/MM method. <i>Journal of Computational Chemistry</i> , 2000, 21, 282-294.	1.5	39
2025	A radial probability density function for analysis of canonical molecular orbitals. <i>Journal of Computational Chemistry</i> , 2000, 21, 310-321.	1.5	1
2026	Determination of substitutional sites in heterocycles from the topological analysis of the electron localization function (ELF). <i>Journal of Computational Chemistry</i> , 2000, 21, 509-514.	1.5	33
2027	Carbonyl insertion reaction into the Pt π C bond in heterobimetallic Pt(SnCl ₃)(PH ₃) ₂ (CO)(CH ₃) compound: Theoretical study. <i>Journal of Computational Chemistry</i> , 2000, 21, 668-674.	1.5	17

#	ARTICLE	IF	CITATIONS
2028	Double transacetalization of diacylium ions. , 2000, 35, 189-198.		17
2029	An ab initio investigation of lithium ion hydration. II. Tetra- versus hexacoordination and halide complexes. International Journal of Quantum Chemistry, 2000, 76, 62-76.	1.0	36
2030	Cubic fuels?. International Journal of Quantum Chemistry, 2000, 76, 434-446.	1.0	71
2031	Ab initio study of organic mixed valency. International Journal of Quantum Chemistry, 2000, 76, 552-573.	1.0	21
2032	Ab initio study of flavonoids. International Journal of Quantum Chemistry, 2000, 76, 724-732.	1.0	38
2033	Benzene chromium tricarbonyl revisited: Theoretical study of the structure and dynamics of (?6-C6H6)Cr(CO)3. International Journal of Quantum Chemistry, 2000, 77, 152-160.	1.0	31
2034	Proton transfer reactions in solution. International Journal of Quantum Chemistry, 2000, 77, 221-239.	1.0	0
2035	Density functional calculations on CO attached to PtnRu(10?n) (n = 6-10) clusters. International Journal of Quantum Chemistry, 2000, 77, 589-598.	1.0	12
2036	Insertion reaction of propene into Rh?H bond in HRh(CO)(PH3)2(C3H6) compound: A density functional study. International Journal of Quantum Chemistry, 2000, 78, 42-51.	1.0	32
2037	Electronic structure and conformation of aniline and meta-chloroaniline dimers. International Journal of Quantum Chemistry, 2000, 78, 99-111.	1.0	6
2038	Molecular surfaces from the promolecule: A comparison with Hartree-Fockab initio electron density surfaces. Journal of Computational Chemistry, 2000, 21, 933-942.	1.5	58
2039	On the Electronic Properties of Substituted Phosphanylcarbenes. European Journal of Inorganic Chemistry, 2000, 2000, 369-374.	1.0	38
2040	Pentacoordination at Fluoro-Substituted Silanes by Weak Lewis Donor Addition. European Journal of Inorganic Chemistry, 2000, 2000, 375-381.	1.0	20
2041	Photoaddition of Aliphatic Ethers to 4-Methyl-1,2,4-triazoline-3,5-dione: Application to the Synthesis of Functionalized Crown Ethers and Mechanism. European Journal of Organic Chemistry, 2000, 2000, 617-626.	1.2	15
2042	Quantum chemical characterization of cycloaddition reactions between 1,3-butadiene and oxyallyl cations of varying electrophilicity. Journal of Physical Organic Chemistry, 2000, 13, 176-186.	0.9	46
2043	On the use of supermolecule model for calculation of Young's modulus of crystalline polymers. International Journal of Quantum Chemistry, 2000, 80, 425-431.	1.0	8
2044	Calculation of static zero-point vibrational averaging corrections and other vibrational curvature contributions to polarizabilities and hyperpolarizabilities using field-induced coordinates. International Journal of Quantum Chemistry, 2000, 80, 471-479.	1.0	37
2045	Quantum mechanical investigation of the tautomerism in the azo dye Sudan III. International Journal of Quantum Chemistry, 2000, 80, 1076-1086.	1.0	23

#	ARTICLE	IF	CITATIONS
2046	Deuterium Nuclear Spin Lattice Relaxation Times and Quadrupolar Coupling Constants in Isotopically Labeled Saccharides. <i>Journal of Magnetic Resonance</i> , 2000, 144, 207-216.	1.2	11
2047	R3N+N?: a substituent with extreme electronic effects. <i>Journal of Physical Organic Chemistry</i> , 2000, 13, 293-299.	0.9	8
2048	New bonding mode of CO on stepped MgO surfaces from density functional cluster model calculations. <i>Chemical Physics Letters</i> , 2000, 320, 345-351.	1.2	49
2049	Theoretical study of geometrical effect on the deoxygenation of epoxide by singlet carbenes. <i>Chemical Physics Letters</i> , 2000, 320, 475-480.	1.2	7
2050	Torsional barriers in biphenyl, 2,2'-bipyridine and 2-phenylpyridine. <i>Chemical Physics Letters</i> , 2000, 321, 399-405.	1.2	122
2051	Vibronic structure fingerprints in NEXAFS: a theoretical study of 2-mercaptobenzoxazole. <i>Chemical Physics Letters</i> , 2000, 327, 7-12.	1.2	11
2052	Evaluation and comparison of transition states with the HCTH98 and FT97 functionals. <i>Chemical Physics Letters</i> , 2000, 326, 537-543.	1.2	4
2053	Calculated and measured vibrational frequencies in an alkanolic acid-alkylamine complex. <i>Chemical Physics Letters</i> , 2000, 327, 420-424.	1.2	7
2054	Linear scaling exchange gradients for Hartree-Fock and hybrid density functional theory. <i>Chemical Physics Letters</i> , 2000, 327, 216-223.	1.2	77
2055	A theoretical study of B2Li6. <i>Chemical Physics Letters</i> , 2000, 329, 239-247.	1.2	1
2056	The intermolecular interaction in the charge-transfer complex between NH3 and F2. A subtle case. <i>Chemical Physics Letters</i> , 2000, 316, 483-488.	1.2	11
2057	Complexation of Li+, Na+, and K+ by water and ammonia. <i>Coordination Chemistry Reviews</i> , 2000, 197, 125-139.	9.5	22
2058	Quantum chemical modelling of the heterogeneous electron transfer: from qualitative analysis to a polarization curve. <i>Electrochimica Acta</i> , 2000, 45, 3521-3536.	2.6	55
2059	Structural preferences of quadruply bonded bimetallic complexes. A DFT study of the chelated ($\hat{1}\pm$) and bridged ($\hat{1}^2$) isomers in Mo2Cl4(H2P(CH2)nPH2)2 (n=1, 2). <i>Inorganica Chimica Acta</i> , 2000, 300-302, 837-845.	1.2	5
2060	Nature of the $\hat{1}^-$ current pit TM in concentrated solutions. <i>Journal of Electroanalytical Chemistry</i> , 2000, 491, 126-138.	1.9	23
2061	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. <i>Acta Crystallographica Section B: Structural Science</i> , 2000, 56, 1018-1028.	1.8	93
2062	Vibrational analysis and structural implications of H-bonding in isolated and aggregated 2-amino-1-propanol: a study by MI-IR and Raman spectroscopy and molecular orbital calculations. <i>Journal of Molecular Structure</i> , 2000, 550-551, 365-388.	1.8	34
2063	Conformations of oligosilanes with ethyl and methyl substituents. <i>Journal of Molecular Structure</i> , 2000, 556, 105-121.	1.8	20

#	ARTICLE	IF	CITATIONS
2064	A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide. <i>Journal of Molecular Structure</i> , 2000, 556, 131-141.	1.8	21
2065	A theoretical and experimental study of weak silane- π electron donor interactions. <i>Journal of Molecular Structure</i> , 2000, 554, 163-172.	1.8	14
2066	The low frequency vibrations of hydrogen bonded adipic acid crystals. <i>Journal of Molecular Structure</i> , 2000, 520, 125-130.	1.8	4
2067	Experimental infrared spectra of matrix isolated complexes of HCl with 4-substituted pyridines. Evaluation of anharmonicity and matrix effects using data from ab initio calculations. <i>Journal of Molecular Structure</i> , 2000, 520, 1-18.	1.8	15
2068	Influence of hydrogen bonding on the conformation of ortho -aminomethylphenol. <i>Journal of Molecular Structure</i> , 2000, 523, 223-239.	1.8	15
2069	Ab initio quantum chemical and experimental study of structure, harmonic vibrational frequencies and internal Φ -SO 3 torsion of benzenesulfonate anion. <i>Journal of Molecular Structure</i> , 2000, 524, 179-188.	1.8	16
2070	Asymmetric aldol reaction of 2-cyanopropionates catalyzed by a trans-chelating chiral diphosphine- ρ -rhodium(I) complex: highly enantioselective construction of quaternary chiral carbon centers at α -positions of nitriles. <i>Journal of Organometallic Chemistry</i> , 2000, 603, 18-29.	0.8	38
2071	An ab initio study on the structure and reactivity of 1,4-disilabenzene. <i>Journal of Organometallic Chemistry</i> , 2000, 611, 280-287.	0.8	9
2072	Theoretical Study on the Reactivity of Phenyl Cation with a Propyl Group at Ortho-Position. <i>Tetrahedron</i> , 2000, 56, 1429-1436.	1.0	30
2073	A theoretical study on reaction pathways to carbanions. <i>Computers & Chemistry</i> , 2000, 24, 311-324.	1.2	6
2074	Ab initio molecular orbital studies of the positive muon and muonium in 4-arylmethyleneamino-TEMPO derivatives. <i>Physica B: Condensed Matter</i> , 2000, 289-290, 128-131.	1.3	6
2075	Structures and vibrational frequencies of pyruvic acid: density functional theory study. <i>Vibrational Spectroscopy</i> , 2000, 23, 181-186.	1.2	54
2076	Molecular structures and vibrations of m-methylaniline in the S0 and S1 states studied by laser induced fluorescence spectroscopy and ab initio calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 1905-1915.	2.0	33
2077	UV-laser photoisomerization of fumaryl chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 157-165.	2.0	18
2078	Heteronuclear diatomic force constants clarified through perturbation theory II. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 629-636.	2.0	4
2079	Structural and vibrational characterisation of 3-amino-1-propanol a concerted SCF-MO ab initio, Raman and infrared (matrix isolation and liquid phase) spectroscopy study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2000, 56, 1051-1064.	2.0	29
2080	Theoretical study of cation/ether complexes: 15-crown-5 and its alkali metal complexes. <i>International Journal of Mass Spectrometry</i> , 2000, 201, 41-58.	0.7	52
2081	Structural and electronic characterisation of the organometallic distonic ion (C6H6)Fe+(p-C6H4)A \cdot . <i>International Journal of Mass Spectrometry</i> , 2000, 201, 297-305.	0.7	7

#	ARTICLE	IF	CITATIONS
2082	Formation and structural discrimination of stable halophenylum ions in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2000, 195-196, 21-31.	0.7	3
2083	Olefin epoxidation by mono and bisperoxo complexes of Mo(VI): a density functional model study. <i>Journal of Molecular Catalysis A</i> , 2000, 158, 189-197.	4.8	51
2084	Structure-activity relationships on adrenoceptors and imidazoline-preferring binding sites (I 1,2) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 imidazoline analogue, trans 1-(4,5-dihydro-1H-imidazol-2-yl)methyl-2-hydroxyindane (PMS 952). <i>Bioorganic and Medicinal Chemistry</i> , 2000, 8, 1861-1869.	1.4	2
2085	Solvent effect on conformational equilibrium: a Monte Carlo study of 1,3-dichloropropane in carbon tetrachloride. <i>Chemical Physics</i> , 2000, 255, 123-136.	0.9	9
2086	Thermodynamic, structural, and dynamic study of the N-H...C hydrogen bond association in aqueous solution. <i>Chemical Physics</i> , 2000, 255, 73-84.	0.9	12
2087	About the vacuum UV photoabsorption spectrum of methyl fluoride (CH ₃ F): the fine structure and its vibrational analysis. <i>Chemical Physics</i> , 2000, 257, 283-299.	0.9	37
2088	Determination of protonation sites in bases from topological rules. <i>Chemical Physics</i> , 2000, 252, 279-287.	0.9	67
2089	The isomerization of HOBr to HOBrO. <i>Chemical Physics Letters</i> , 2000, 319, 650-654.	1.2	9
2090	Density functional theory study of the geometric structure and energetics of triphenylamine-based hole-transporting molecules. <i>Chemical Physics Letters</i> , 2000, 327, 13-17.	1.2	428
2091	The electronic structure of some acyl azides: cyclic-open tautomerism. <i>Chemical Physics Letters</i> , 2000, 318, 276-288.	1.2	17
2092	Dimethylaluminium enolates and alkoxides derived from trimethylaluminium and aromatic ketones: a synthetic, structural and theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 2000, 602, 15-23.	0.8	20
2093	Density functional theory study on the structure and vibrational spectra for 4-methyl-3-pentene-2-one. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 149-154.	1.5	9
2094	Structural, energetic, and vibrational features of azacubanes as energetic materials studied with density functional theory methods. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 21-30.	1.5	16
2095	A theoretical study on the conformations and energetics on the cation-π interaction between monovalent ions (M ⁺ =Li ⁺ , Na ⁺ , and K ⁺) and anthracene and phenanthrene molecules. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 201-207.	1.5	25
2096	Basis set dependence of the vibrational wavenumbers of the out-of-plane modes of conjugated π-electron ring systems. <i>Computational and Theoretical Chemistry</i> , 2000, 500, 311-321.	1.5	11
2097	Theoretical studies of biological nitrogen fixation. Part II. Hydrogen bonded networks as possible reactant and product channels. <i>Computational and Theoretical Chemistry</i> , 2000, 506, 131-146.	1.5	29
2098	The platinum-ethylene binding energy in Pt(PL ₃) ₂ (C ₂ H ₄). <i>Computational and Theoretical Chemistry</i> , 2000, 506, 223-232.	1.5	21
2099	Linearly dependent subspaces and the eigenvalue spectrum of the one-particle reduced density matrix. <i>Computational and Theoretical Chemistry</i> , 2000, 527, 181-191.	1.5	4

#	ARTICLE	IF	CITATIONS
2100	Ab initio electronic density-adjusted pseudopotentials. Computational and Theoretical Chemistry, 2000, 529, 173-182.	1.5	2
2101	Solvent effects on the relative stability of 4-nitro-1 H-imidazole and 5-nitro-1 H-imidazole. Ab initio and density functional theory calculations. Computational and Theoretical Chemistry, 2000, 532, 279-286.	1.5	11
2102	Ab initio GB study of conformational space of d-glyceraldehyde in aqueous solution. Computational and Theoretical Chemistry, 2000, 496, 145-152.	1.5	4
2103	A B3LYP hybrid density functional theory study of structural properties, energies, and heats of formation for silicon-hydrogen compounds. Computational and Theoretical Chemistry, 2000, 497, 65-73.	1.5	15
2104	Computing the heat of formation for cubane and tetrahedrane with density functional theory and complete basis set ab initio methods. Computational and Theoretical Chemistry, 2000, 499, 137-140.	1.5	73
2105	Theoretical study on the thermal isomerization reaction between meso and dl cyclomers of 4a,6a,10a,10b-tetrahydropyrido[2,1-c]pyrido[1,2-a]piperazine and its lower homologue. Computational and Theoretical Chemistry, 2000, 499, 161-173.	1.5	4
2106	DFT studies of structures and vibrational spectra of silicon-sulfur clusters (SiS ₂) _n + (n=1-5). Computational and Theoretical Chemistry, 2000, 499, 241-255.	1.5	8
2107	Ab initio GB study of prebiotic synthesis of purine precursors from aqueous hydrogen cyanide: dimerization reaction of HCN in aqueous solution. Computational and Theoretical Chemistry, 2000, 507, 53-62.	1.5	19
2108	On the wetting of saturated hydrocarbon surfaces. An exploratory molecular investigation. Computational and Theoretical Chemistry, 2000, 501-502, 535-538.	1.5	1
2109	Density functional theory and complete basis set ab initio computational study of the molecular interaction between the magnesium atom and nitrogen oxide cation: is the nitrogen oxide cation responsible for higher magnesium cation/atom ratio in the Earth's upper atmosphere?. Computational and Theoretical Chemistry, 2000, 528, 75-83.	1.5	4
2110	Elementary Jacobi rotation method for generalized valence bond perfect-pairing calculations combined with simple procedure for generating reliable initial orbitals. Computational and Theoretical Chemistry, 2000, 528, 177-191.	1.5	11
2111	An ab initio molecular orbital study of nitrosophenol/quinone monooxime equilibria. Computational and Theoretical Chemistry, 2000, 528, 237-244.	1.5	19
2112	Title is missing!. Journal of Solution Chemistry, 2000, 29, 955-986.	0.6	18
2113	Title is missing!. Structural Chemistry, 2000, 11, 121-140.	1.0	16
2114	Density functional theory predictions for small radicals containing boron and aluminium: broken symmetry problems and solutions. Molecular Physics, 2000, 98, 961-966.	0.8	6
2115	Topological Analysis of the Electron Localization Function (ELF) Applied to the Electrophilic Aromatic Substitution. Journal of Physical Chemistry A, 2000, 104, 852-858.	1.1	171
2116	Electronic structure and polarizability of ortho-benzoquinonediimine and its singly and doubly charged anions. Journal of Structural Chemistry, 2000, 41, 28-34.	0.3	0
2117	An effective scheme for selecting basis sets for ab initio calculations. Science in China Series B: Chemistry, 2000, 43, 375-388.	0.8	22

#	ARTICLE	IF	CITATIONS
2118	The interactions of square platinum(II) complexes with guanine and adenine: a quantum-chemical ab initio study of metalated tautomeric forms. <i>Journal of Biological Inorganic Chemistry</i> , 2000, 5, 178-188.	1.1	64
2119	High-Resolution Spectroscopy of the A_1g Band System of MoN. <i>Physica Scripta</i> , 2000, 62, 417-424.	1.2	2
2120	Vibrational second hyperpolarizability of symmetrically substituted 'quadrupolar' π -conjugated systems. <i>Journal of Optics</i> , 2000, 2, 247-254.	1.5	10
2121	Relative energies of the $C_2H_2S_2$ isomers 1,2-dithiete and dithioglyoxal: Peculiar basis set dependencies of density functional theory and ab initio methods. <i>Journal of Chemical Physics</i> , 2000, 113, 8430-8433.	1.2	28
2122	The structure and properties of $H_3+Ar_n^+(n=1-9)$ cations. <i>Journal of Chemical Physics</i> , 2000, 113, 3615-3620.	1.2	17
2123	Gradients in valence bond theory. <i>Journal of Chemical Physics</i> , 2000, 113, 2100-2108.	1.2	38
2124	Valence electron momentum spectroscopy of n-butane. <i>Journal of Chemical Physics</i> , 2000, 112, 8043-8052.	1.2	22
2125	Charge transfer to solvent (CTTS) energies of small $X_n^+(H_2O)_n=1-4$ ($X=F, Cl, Br, I$) clusters: Ab initio study. <i>Journal of Chemical Physics</i> , 2000, 112, 101-105.	1.2	130
2126	Resonant ion-dip infrared spectroscopy of benzene \cdot (water) $_9$: Expanding the cube. <i>Journal of Chemical Physics</i> , 2000, 113, 2290-2303.	1.2	81
2127	Collision-induced dissociation and density functional study of the structures and energies of cyclic $C_2nN_5^+$ clusters. <i>Journal of Chemical Physics</i> , 2000, 112, 9276-9281.	1.2	12
2128	Solvation of magnesium and singly ionized magnesium atoms in NH_3 clusters: Theory and experiment. <i>Journal of Chemical Physics</i> , 2000, 112, 10912-10925.	1.2	29
2129	The analytic gradient for the equation-of-motion coupled-cluster energy with a reduced molecular orbital space: An application for the first excited state of formaldehyde. <i>Journal of Chemical Physics</i> , 2000, 112, 1-4.	1.2	43
2130	Direct vibrational self-consistent field method: Applications to H_2O and H_2CO . <i>Journal of Chemical Physics</i> , 2000, 113, 1005-1017.	1.2	150
2131	The polarized infrared and Raman spectra of $\hat{I}_{\pm}T_6$ single crystal: An experimental and theoretical study. <i>Journal of Chemical Physics</i> , 2000, 112, 5957-5969.	1.2	33
2132	Isotope effect on bifurcating reaction path: Valley \cdot ridge inflection point in totally symmetric coordinate. <i>Journal of Chemical Physics</i> , 2000, 113, 477-484.	1.2	32
2133	Structure, energies, and vibrational properties of silica rings in SiO_2 glass. <i>Physical Review B</i> , 2000, 61, 234-240.	1.1	47
2134	Small clusters of II-VI materials: $ZnSi_i, i=1-9$. <i>Physical Review A</i> , 2000, 61, .	1.0	85
2135	A method to improve the agreement between calculated and observed vibrational frequencies after scaling of a quantum mechanical force field. <i>Journal of Chemical Physics</i> , 2000, 113, 8472-8477.	1.2	14

#	ARTICLE	IF	CITATIONS
2136	Coupled-cluster studies of the hyperfine splitting constants of the thioformyl radical. <i>Journal of Chemical Physics</i> , 2000, 112, 6245-6254.	1.2	13
2137	New energy partitioning scheme based on the self-consistent charge and configuration method for subsystems: Application to water dimer system. <i>Journal of Chemical Physics</i> , 2000, 112, 1623-1633.	1.2	60
2138	Modeling proton mobility in acidic zeolite clusters. I. Convergence of transition state parameters from quantum chemistry. <i>Journal of Chemical Physics</i> , 2000, 112, 6779-6786.	1.2	33
2139	An assessment of theoretical methods for the study of transition metal carbonyl complexes: [Cl ₂ Rh(CO) ₂] ⁺ and [Cl ₂ Rh(CO)] ⁺ as case studies. <i>Journal of Chemical Physics</i> , 2000, 113, 9393-9401.	1.2	23
2140	Charge transfer and charge conversion of K and N defect centers in Si ₃ N ₄ . <i>Physical Review B</i> , 2000, 61, 15005-15010.	1.1	20
2141	Spin-contamination of coupled-cluster wave functions. <i>Journal of Chemical Physics</i> , 2000, 113, 6052-6062.	1.2	87
2142	Importance of discriminator base stacking interactions: molecular dynamics analysis of A73 microhelix Ala variants. <i>Nucleic Acids Research</i> , 2000, 28, 2527-2534.	6.5	28
2143	Paramagnetic centers in Ge-doped silica: a first-principles study. <i>Physical Review B</i> , 2000, 62, 5452-5460.	1.1	39
2144	Structure and energy calculations for imide and methide anions containing perfluoroalkanesulfonyl groups. <i>Solid State Sciences</i> , 2000, 2, 115-122.	0.8	8
2145	A theoretical study of aluminium chemical vapour deposition using dimethylaluminium hydride: a surface reaction mechanism on Al(111). <i>Surface Science</i> , 2000, 444, 99-112.	0.8	10
2146	The prediction of metastable impact electronic spectra (MIES): perfect and defective MgO(001) surfaces by state-of-the-art methods. <i>Surface Science</i> , 2000, 444, 31-51.	0.8	27
2147	Triplet Excited States of Free-Base Porphin and Its β -Octahalogenated Derivatives. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4748-4754.	1.1	51
2148	2-(Hydroxyimino)propanohydroxamic acid, a new effective ligand for aluminium. <i>Dalton Transactions RSC</i> , 2000, , 4201-4208.	2.3	31
2149	Theoretical Study of the Low-Lying Electronically Excited States of Diacetylene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9009-9016.	1.1	15
2150	DNA Photoionization and Alkylation Patterns in the Interior of Guanine Runs. <i>Journal of the American Chemical Society</i> , 2000, 122, 12824-12834.	6.6	44
2151	Metal-assisted coupling of oximes and nitriles: a synthetic, structural and theoretical study. <i>Dalton Transactions RSC</i> , 2000, , 4683-4693.	2.3	51
2152	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Push-Pull π -Conjugated Systems. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4755-4763.	1.1	501
2153	Direct Methane to Methanol and Benzene to Phenol Conversions on Fe-ZSM-5 Zeolite: Theoretical Predictions on the Reaction Pathways and Energetics. <i>Journal of Physical Chemistry B</i> , 2000, 104, 734-740.	1.2	139

#	ARTICLE	IF	CITATIONS
2154	Regioselectivity and Diastereoselectivity in the 1,3-Dipolar Cycloadditions of Nitrones with Acrylonitrile and Maleonitrile. The Origin of ENDO/EXO Selectivity###Dedicated to professor G.Del Re. <i>Advances in Quantum Chemistry</i> , 2000, 36, 151-167.	0.4	16
2155	Computational Studies of the Mechanism for Proton and Hydride Transfer in Liver Alcohol Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2000, 122, 4803-4812.	6.6	168
2156	Experimental and Theoretical Analysis of the Vibrational Spectra and Theoretical Study of the Structures of 3,6-Dichloropyridazine and 3,4,5-Trichloropyridazine. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2599-2612.	1.1	13
2157	Ab initio cluster study of the structure of the Si(001) surface. <i>Journal of Chemical Physics</i> , 2000, 112, 2994-3005.	1.2	85
2158	Continuum solvent effects on various isomers of bilirubin. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4884-4890.	1.3	12
2159	Ab Initio Computational Study of Environmentally Harmful Gasoline Additives: Methyltert-Butyl Ether and Analogues. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11106-11110.	1.1	12
2160	Ground state gas and solution phase conformational dynamics of polar processes: Furfural systems. <i>Journal of Chemical Physics</i> , 2000, 113, 7519-7529.	1.2	33
2161	An unexpected electronic preference for transfer of a δ^2 -hydrogen trans to a metal-hydride bond. <i>New Journal of Chemistry</i> , 2000, 24, 855-858.	1.4	3
2162	X-Ray structures and ab initio study of the conformational properties of novel oxazole and thiazole containing di- and tripeptide mimetics. <i>Perkin Transactions II RSC</i> , 2000, , 1081-1085.	1.1	10
2163	Modeling of the adsorption on Cr ₂ O ₃ clusters of small molecules and ions present in seawater. A preliminary non-empirical study. <i>New Journal of Chemistry</i> , 2000, 24, 993-998.	1.4	8
2164	The peculiar role of cytosine in nucleoside conformational behaviour: Hydrogen bond donor capacity of nucleic bases. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5351-5353.	1.3	44
2165	A comparison of ab initio cluster and periodic calculations of the electric field gradient at sodium in NaNO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1325-1331.	1.3	13
2166	Lithiated δ^2 -cyanophosphonates: self-assembly of two-dimensional molecular sheets composed of interconnected twenty-four membered rings. <i>Dalton Transactions RSC</i> , 2000, , 4348-4353.	2.3	26
2167	Ab Initio Study of Coupled Electron Transfer/Proton Transfer in Cytochrome c Oxidase. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2367-2374.	1.1	24
2168	Synthesis, Characterization, and Theoretical Study of Stable Hydride-Azavinylidene Osmium(IV) Complexes. <i>Organometallics</i> , 2000, 19, 3100-3108.	1.1	31
2169	Structure and Bonding of Transition Metal-Boryl Compounds. Theoretical Study of [(PH ₃) ₂ (CO)ClOs-BR ₂] and [(PH ₃) ₂ (CO) ₂ ClOs-BR ₂] (BR ₂ = BH ₂ , BF ₂ , B(OH) ₂ , B(OCHCHO), Bcat). <i>Inorganic Chemistry</i> , 2000, 39, 4776-4785.	1.9	39
2170	A Remarkable Isostructural Homologous Series of Mixed Lithium-Heavier Alkali Metal tert-Butoxides [(t-BuO) ₈ Li ₄ M ₄] (M = Na, K, Rb or Cs). <i>Journal of the American Chemical Society</i> , 2000, 122, 11117-11124.	6.6	47
2171	Charge-Transfer Complexes between NH ₃ and the Halogens F ₂ , ClF, and Cl ₂ : An ab Initio Study on the Intermolecular Interaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6871-6879.	1.1	85

#	ARTICLE	IF	CITATIONS
2172	Theoretical Studies of Molybdenum Peroxo Complexes [MoOn(O2)3-n(OPH3)] as Catalysts for Olefin Epoxidation. Inorganic Chemistry, 2000, 39, 2314-2320.	1.9	55
2173	Density Functional Study on Highly Ortho-Selective Addition of an Aromatic CH Bond to Olefins Catalyzed by a Ru(H)2(CO)(PR3)3Complex. Organometallics, 2000, 19, 2318-2329.	1.1	90
2174	Theoretical Investigation of Reaction Mechanisms for Carboxylic Acid Formation in the Atmosphere. Journal of the American Chemical Society, 2000, 122, 8990-8997.	6.6	79
2175	Selective oxygen capture by lithium aluminates: a solid state and theoretical structural study. Dalton Transactions RSC, 2000, , 4304-4311.	2.3	10
2176	Tricarbonylrhenium(I) halide complexes of 2-[(4R,6R)-4,6-dimethyl-1,3-dioxan-2-yl]pyridine (L1) and 2,6-bis[(4R,6R)-4,6-dimethyl-1,3-dioxan-2-yl]pyridine (L2): structure and solution stereodynamics. Dalton Transactions RSC, 2000, , 1769-1776.	2.3	11
2177	Molecular-dynamics simulations of solvent effects in the intramolecular charge transfer of 4-(N,N-dimethylamino)benzonitrile. Physical Chemistry Chemical Physics, 2000, 2, 4341-4353.	1.3	39
2178	Ab initio study of the PtC molecule. A new assignment of the red bands to the $1\tilde{A}, \tilde{A}3\tilde{Z}\tilde{A}\tilde{Z}\tilde{A} \otimes (\tilde{A}\tilde{Z}\tilde{A} \otimes 1,0+) \tilde{A} \tilde{c}_a, \tilde{a}_e \tilde{c}_e \tilde{X}\tilde{A}, \tilde{A}1\tilde{A}\tilde{Z}\tilde{A} \tilde{+}$ transitions. Physical Chemistry Chemical Physics, 2000, 2, 2851-2856.	1.3	15
2179	Equilibria of simple thioenol/thiocarbonyl pairs. Comparison with the oxygen analogs and with the parent selenium and tellurium systems. A theoretical study. Perkin Transactions II RSC, 2000, , 2269-2279.	1.1	17
2180	Aluminium(III) hydration in aqueous solution. A Raman spectroscopic investigation and an ab initio molecular orbital study of aluminium(III) water clusters. Physical Chemistry Chemical Physics, 2000, 2, 5030-5040.	1.3	116
2181	Trihydrogermyl-substituted thiophenes. Dalton Transactions RSC, 2000, , 4117-4121.	2.3	6
2182	Molecular structure of N-trimethylsilylaziridine in the gas phase. Dalton Transactions RSC, 2000, , 1491-1497.	2.3	2
2183	Stable ion study of protonated cyclopenta[a]phenanthrenes. Structure-reactivity relationships and charge delocalization in the carbocations. Perkin Transactions II RSC, 2000, , 211-220.	1.1	10
2184	Syntheses, Molecular Structures, and Vibrational Spectra of Chloropentacarbonylrhodium(III) and -iridium(III) Undecafluorodiantimonate(V), [Rh(CO)5Cl][Sb2F11]2 and [Ir(CO)5Cl][Sb2F11]2: An Experimental and Density Functional Study. Inorganic Chemistry, 2000, 39, 1933-1942.	1.9	19
2185	Ab Initio Studies of Benzocyclopropanone, Benzocyclopropanone-Containing [2.2]paracyclophane, Its Benzyne Derivative, and the Bridged Benzobarrelene Formed by Intramolecular [4 + 2]Cycloaddition. Journal of Organic Chemistry, 2000, 65, 6620-6626.	1.7	3
2186	The Pressure Dependence of the OH Radical Yield from Ozone-Alkene Reactions. Journal of Physical Chemistry A, 2000, 104, 7821-7833.	1.1	89
2187	Structural Distortions in mer-M(H)3(NO)L2 (M = Ru, Os) and Their Influence on Intramolecular Fluxionality and Quantum Exchange Coupling. Inorganic Chemistry, 2000, 39, 1919-1932.	1.9	23
2188	Ab Initio and Density Functional Evaluations of the Molecular Conformations of \hat{I}^2 -Caryophyllene and 6-Hydroxycaryophyllene. Journal of Organic Chemistry, 2000, 65, 6910-6916.	1.7	16
2189	Polarizabilities of Carbon Dioxide and Carbodiimide. Assessment of Theoretical Model Dependencies on Dipole Polarizabilities and Dipole Polarizability Anisotropies. Journal of Physical Chemistry A, 2000, 104, 11355-11361.	1.1	17

#	ARTICLE	IF	CITATIONS
2190	Mechanism and Stereochemistry of the Water Exchange Reactions on Aqua Amine Complexes of Chromium(III): The Role of the "Spectator" Ligands. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8787-8795.	1.1	17
2191	Haptotropic Shifts in Cyclopentadienyl Organometallic Complexes: Ring Folding vs Ring Slippage. <i>Organometallics</i> , 2000, 19, 5549-5558.	1.1	50
2192	Double-Rydberg Anions: Predictions on NH ₃ AH _n - and OH ₂ AH _n -Structures. <i>Journal of the American Chemical Society</i> , 2000, 122, 12813-12818.	6.6	18
2193	Theoretical Study of the Mechanism of Carbonyl Insertion Reactions Catalyzed by Nickel Complexes. <i>Organometallics</i> , 2000, 19, 2170-2178.	1.1	18
2194	Characterization of the Rydberg Bonding in (NH ₄) ₂ -. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10855-10858.	1.1	10
2195	The computation of Karplus equation coefficients and their components using self-consistent field and second-order polarization propagator methods. <i>Molecular Physics</i> , 2000, 98, 1981-1990.	0.8	28
2197	Electrostatically Driven Geometry Changes Accompanying Charge Separation in Supposedly Rigid Bichromophoric Systems. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11628-11635.	1.1	19
2198	Theoretical Studies of the Mechanism for the Synthesis of Silsesquioxanes. 2. Cyclosiloxanes (D ₃ and) Tj ETQq1 1 0,784314 rgBT /Over 1.1 32	1.1	32
2199	Anharmonicity contributions to the vibrational second hyperpolarizability of conjugated oligomers. <i>Journal of Chemical Physics</i> , 2000, 112, 1011-1019.	1.2	54
2200	New Radical-Molecule Association Compounds. <i>Journal of the American Chemical Society</i> , 2000, 122, 9196-9200.	6.6	25
2201	An ab Initio Study of the Photochemical Decomposition of 3,3-Dimethyldiazirine. <i>Journal of Organic Chemistry</i> , 2000, 65, 7847-7857.	1.7	28
2202	Solvation of the Hydroxide Anion: A Combined DFT and Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2384-2395.	1.1	54
2203	SiONB Unit as Reference for Blocked Si-A-N Interactions in SiON Compounds. <i>Inorganic Chemistry</i> , 2000, 39, 1998-2000.	1.9	10
2204	Ab Initio Calculations on the 5-exo versus 6-endo Cyclization of 1,3-Hexadiene-5-yn-1-yl Radical: Formation of the First Aromatic Ring in Hydrocarbon Combustion. <i>Journal of the American Chemical Society</i> , 2000, 122, 11416-11422.	6.6	20
2205	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 16. Oxidative Promotion of the Migratory Insertion of Carbon Monoxide in Cyclopentadienylmethylidicarbonyliron (II). <i>Journal of Physical Chemistry A</i> , 2000, 104, 7324-7332.	1.1	11
2206	Ligand Substituent, Anion, and Solvation Effects on Ion Pair Structure, Thermodynamic Stability, and Structural Mobility in "Constrained Geometry" Olefin Polymerization Catalysts: An Ab Initio Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 2000, 122, 12764-12777.	6.6	140
2207	Theoretical Conformational Analysis of Thiacyclic Macrocycles. <i>Journal of Physical Chemistry A</i> , 2000, 104, 652-660.	1.1	71
2208	Reaction Path Hamiltonian Analysis of Dynamical Solvent Effects for a Claisen Rearrangement and a Diels-Alder Reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8058-8066.	1.1	37

#	ARTICLE	IF	CITATIONS
2209	Will an \hat{I} -3-Si3H3 Ligand Form Sandwich Compounds with Main Group Elements?. <i>Journal of the American Chemical Society</i> , 2000, 122, 1725-1728.	6.6	26
2210	Density Functional Calculation of the Electric Field Gradient in Cadmium Complexes: Comparison with Hartree-Fock, Second-Order Møller-Plesset, and Experimental Results. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6047-6055.	1.1	17
2211	Mechanism and Stereochemistry of the Water-Exchange Reaction on Aqua Pentaammine and Aqua Pentakis-Methylamine Rhodium(III) Ions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6439-6446.	1.1	12
2212	Molecular Properties from Combined QM/MM Methods. 2. Chemical Shifts in Large Molecules. <i>Journal of Physical Chemistry B</i> , 2000, 104, 3721-3743.	1.2	144
2213	Is It Possible to Synthesize a Low-Valent Transition Metal Complex with a Neutral Carbon Atom as Terminal Ligand? A Theoretical Study of $(CO)_4FeC\hat{\epsilon}$. <i>Organometallics</i> , 2000, 19, 2698-2706.	1.1	38
2214	On the Distribution of Local Molecular Symmetry in Crystals. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11439-11442.	1.1	9
2215	Ligand Macrocycle Structural Effects on Copper Dioxygen Reactivity. <i>Inorganic Chemistry</i> , 2000, 39, 4059-4072.	1.9	116
2216	Structure and Dynamics of $[Nb(\hat{I}-5-C_5H_4SiMe_3)_2(\hat{I}-2-H_2BR_2)]$ ($R_2 = O_2C_6H_4, C_8H_{14}, H_2$) Complexes. A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2000, 19, 3654-3663.	1.1	26
2217	QM/MM Boundaries Across Covalent Bonds: A Frozen Localized Molecular Orbital-Based Approach for the Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6656-6665.	1.1	136
2218	Ab Initio MCSCF Study on the Pseudo-Jahn-Teller Distortion from Planarity in Cycloheptatriene, Heptalene, and Heptafulvalene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5343-5350.	1.1	11
2219	Mechanism of the S $\hat{\alpha}$ ' N Isomerization and Aquation of the Thiocyanato Pentaammine Cobalt(III) Ion. <i>Inorganic Chemistry</i> , 2000, 39, 944-952.	1.9	11
2220	Dissociation of Ozonide in Water. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4629-4635.	1.1	14
2221	Matrix Isolation and ab Initio Study of the Hydrogen-Bonded Complex between H ₂ O ₂ and (CH ₃) ₂ O. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2033-2037.	1.1	41
2222	Ab Initio Investigation of Strain in Group 14 Polyhedrane Clusters ($MnHn: \hat{A}n = 4, 6, 8, 10, 12, 16, 20, 24$). <i>Journal of Physical Chemistry A</i> , 2000, 104, 6622-6627.	1.1	72
2223	Infrared-Induced Rotamerization of Oxalic Acid Monomer in Argon Matrix. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6956-6961.	1.1	61
2224	Photoinduced Hydrogen Atom Transfer of Free-Base Porphin. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4549-4552.	1.1	18
2225	N $\hat{\alpha}$ ' N Spin Spin Coupling Constants [$2h(15N \hat{\alpha}' 15N)$] Across N $\hat{H} \hat{A} \hat{A} \hat{N}$ Hydrogen Bonds in Neutral Complexes: To What Extent Does the Bonding at the Nitrogens Influence $2hJN-N$?. <i>Journal of the American Chemical Society</i> , 2000, 122, 10480-10481.	6.6	67
2226	$4h(31P \hat{\alpha}' 31P)$ Coupling Constants through N $\hat{H} \hat{A} \hat{A} \hat{N}$ Hydrogen Bonds: A Comparison of Computed ab Initio and Experimental Data. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7165-7166.	1.1	40

#	ARTICLE	IF	CITATIONS
2227	Unsaturated Ru(0) Species with a Constrained Bis-Phosphine Ligand: [Ru(CO) ₂ (tBu ₂ PCH ₂ CH ₂ PtBu ₂)] ₂ . Comparison to [Ru(CO) ₂ (PtBu ₂ Me) ₂]. <i>Inorganic Chemistry</i> , 2000, 39, 3957-3962.	1.9	17
2228	Theoretical Study of the Mechanism of Oxidative Addition of Allyl ⁺ Ammonium and ⁺ Iminium Salts to Low-Valent Metal Complexes. Rationalization of Selective C ⁺ N and N ⁺ H Bond Activation. <i>Organometallics</i> , 2000, 19, 4402-4415.	1.1	20
2229	Theoretical Study of the Mechanisms of Palladation of Methylene-cyclopropane and [3 + 2] Cycloadditions. <i>Inorganic Chemistry</i> , 2000, 39, 1113-1119.	1.9	40
2230	Nuclear Dynamics Discrete Variable Representation Study of the Equilibrium Isotope Effect on H ₂ Binding in M(¹⁻² H ₂)Ln Complexes: An Effective Theoretical Way To Account for Anharmonicity. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7898-7905.	1.1	19
2231	Electrostatic Protein ⁺ Chromophore Interactions Promote the all-trans ⁺ 13-cis Isomerization of the Protonated Retinal Schiff Base in Bacteriorhodopsin: An ab Initio CASSCF/MRCI Study. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11379-11388.	1.2	26
2232	Pyrrolo-Annulated Tetrathiafulvalenes: The Parent Systems. <i>Journal of Organic Chemistry</i> , 2000, 65, 5794-5805.	1.7	129
2233	Hartree-Fock and Density Functional Theory ab Initio Calculation of Optical Rotation Using GIAOs: Basis Set Dependence. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1039-1046.	1.1	264
2234	Conformational Analysis and Near-Infrared-Induced Rotamerization of Malonic Acid in an Argon Matrix. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11725-11732.	1.1	46
2235	Nature of the Chemical Bond between a Transition Metal and a Group-13 Element: Structure and Bonding of Transition Metal Complexes with Terminal Group-13 Diyl Ligands ER (E = B to Tl; R = Cp,) Tj ETQq0 0 0 rgBT /Overlook 10 Tf 5		
2236	On the Structure and Vibrational Spectrum of Tetrabromothiophene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8983-8988.	1.1	3
2237	Efficient Incorporation of Unsaturated Methionine Analogues into Proteins in Vivo. <i>Journal of the American Chemical Society</i> , 2000, 122, 1282-1288.	6.6	265
2238	Facile Synthesis of Alkynyl ⁺ and Vinylidene ⁺ Niobocene Complexes. Unexpected ¹ -Vinylidene ⁺ ² -Alkyne Isomerization. <i>Organometallics</i> , 2000, 19, 1749-1765.	1.1	32
2239	Relationship between Basicity, Strain, and Intramolecular Hydrogen-Bond Energy in Proton Sponges. <i>Journal of the American Chemical Society</i> , 2000, 122, 8238-8244.	6.6	111
2240	Ab Initio Investigation of Electron Detachment in Dicarboxylate Dianions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11786-11795.	1.1	39
2241	Hydrogen-Bonding Effects on Free-Radical Properties. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11816-11821.	1.1	31
2242	Novel Binding Modes in Tetramethoxycalix[4]arene: Implications for Ligand Design. <i>Journal of the American Chemical Society</i> , 2000, 122, 10083-10089.	6.6	54
2243	Computational electrochemistry: aqueous one-electron oxidation potentials for substituted anilines. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1231-1239.	1.3	194
2244	On the possible formation of Si=O, Si=S, and Si=Se double bonds via the reaction of silylenes with oxirane, thirane, and selenirane, respectively. An ab initio theoretical study. <i>Canadian Journal of Chemistry</i> , 2000, 78, 1496-1510.	0.6	18

#	ARTICLE	IF	CITATIONS
2245	Predicted NMR Coupling Constants Across Hydrogen Bonds: A Fingerprint for Specifying Hydrogen Bond Type?. <i>Journal of the American Chemical Society</i> , 2000, 122, 3560-3561.	6.6	100
2246	Basis set choice and basis set superposition error (BSSE) in periodic Hartree-Fock calculations on molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 1518-1523.	1.3	59
2247	Molecular Orbital Study of the First Excited State of the OLED Material Tris(8-hydroxyquinoline)aluminum(III). <i>Chemistry of Materials</i> , 2001, 13, 2632-2640.	3.2	221
2248	Corannulene as a Lewis Base: Computational Modeling of Protonation and Lithium Cation Binding. <i>Journal of the American Chemical Society</i> , 2001, 123, 6687-6695.	6.6	67
2249	The Effective Fragment Potential Method: A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. <i>Journal of Physical Chemistry A</i> , 2001, 105, 293-307.	1.1	570
2250	Can Proton-Shared or Ion-Pair N-H...N Hydrogen Bonds Be Produced in Uncharged Complexes? A Systematic ab Initio Study of the Structures and Selected NMR and IR Properties of Complexes with N-H...N Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10906-10914.	1.1	21
2251	Ionic Liquids Based on FeCl ₃ and FeCl ₂ . Raman Scattering and ab Initio Calculations. <i>Inorganic Chemistry</i> , 2001, 40, 2298-2304.	1.9	314
2252	Synthesis and crystal structure of the new heteroleptic magnesium bis(amide) [Mg(¹ / ₄ -N(H)Ph)[N(SiMe ₃) ₂] ₂ ·THF·CS ₂], and density functional MO calculations on model systems. <i>Dalton's Transactions RSC</i> , 2001, , 409-413.		18
2253	Concerted Use of Slab and Cluster Models in an ab Initio Study of Hydrogen Desorption from the Si(100) Surface. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4031-4038.	1.2	42
2254	Ab Initio MCSCF Study on Eight π -Electron Heterocyclic Conjugated Systems: Energy Component Analysis of the Pseudo-Jahn-Teller Distortion from Planarity. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1334-1342.	1.1	7
2255	A theoretical study of the nitrogen clusters formed from the ions N ₃ ⁻ , N ₅ ⁺ , and N ₅ ⁻ . <i>Journal of Chemical Physics</i> , 2001, 114, 10733-10737.	1.2	67
2256	Gas-Phase Conformations of 3-Buten-2-ol from Density-Functional Theoretical Results Together with Electron-Diffraction and Vibrational Spectroscopic Data. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1039-1049.	1.1	5
2257	Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3887-3893.	1.1	70
2258	Hydrogen bond cooperativity and electron delocalization in hydrogen fluoride clusters. <i>Journal of Chemical Physics</i> , 2001, 114, 5552-5561.	1.2	90
2259	Calculation of Optical Rotation Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5356-5371.	1.1	351
2260	First-principles electronic structure studies for the cluster modeled Si/Si(111) chemisorption system. <i>Journal of Chemical Physics</i> , 2001, 114, 436.	1.2	7
2261	Electronic Structure of Defect Centers P1, P2, and P4 in P-Doped SiO ₂ . <i>Journal of Physical Chemistry B</i> , 2001, 105, 6097-6102.	1.2	23
2262	Theory of emission state of tris(8-quinolinolato)aluminum and its related compounds. <i>Journal of Applied Physics</i> , 2001, 90, 6092-6097.	1.1	44

#	ARTICLE	IF	CITATIONS
2263	Relationship between Molecular Structure, Polarization, and Crystal Packing in 6-Arylfulvenes. ACS Symposium Series, 2001, , 112-126.	0.5	4
2264	Density Functional Theory and X-ray Investigations of P- and M-Hexamethylene Triperoxide Diamine and Its Dialdehyde Derivative. Journal of Physical Chemistry A, 2001, 105, 8763-8768.	1.1	30
2265	Ground state electronic structures and spectra of zinc complexes of porphyrin, tetraazaporphyrin, tetrabenzoporphyrin, and phthalocyanine: A density functional theory study. Journal of Chemical Physics, 2001, 114, 10757-10767.	1.2	212
2266	The Theoretical Prediction of Molecular Radical Species: a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2001, 105, 9736-9747.	1.1	142
2267	Equilibria between $\hat{\iota}^{\pm}$ - and $\hat{\iota}^2$ -Agostic Stabilized Rotamers of Secondary Alkyl Niobium Complexes. Journal of the American Chemical Society, 2001, 123, 6000-6013.	6.6	59
2268	The dispersion of the polarizability of C60: A confirmation of recent experimental results through theoretical calculations. Journal of Chemical Physics, 2001, 114, 4331-4332.	1.2	35
2269	Protonated nitrous acid (H2ONO+): Molecular structure, vibrational frequencies, and proton affinity. Journal of Chemical Physics, 2001, 115, 2117-2122.	1.2	21
2270	An ab initio electronic structure study of methyl adsorption and reaction on cluster models for the diamond surface. Diamond and Related Materials, 2001, 10, 39-47.	1.8	2
2271	Metal and Ancillary Ligand Structural Effects on Ethylene Insertion Processes at Cationic Group 4 Centers. A Systematic, Comparative Quantum Chemical Investigation at Various ab Initio Levels. Organometallics, 2001, 20, 4006-4017.	1.1	55
2272	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in Hypericin. Photochemistry and Photobiology, 2001, 74, 157.	1.3	10
2273	Simple Scheme To Evaluate Crystal Nonlinear Susceptibilities: Semiempirical AM1 Model Investigation of 3-Methyl-4-nitroaniline Crystal. Journal of Physical Chemistry A, 2001, 105, 1366-1370.	1.1	62
2274	The reaction of the unsaturated rhenium fragment {Re($\hat{\iota}$ -5-C5Me5)(CO)2} with 1,4-difluorobenzene. Thermal intramolecular conversion of a rhenium (difluorophenyl)(hydride) to Re($\hat{\iota}$ -2-C6H4F2) and a [1,4]-metallotropic shift. Dalton Transactions RSC, 2001, , 1452-1461.	2.3	42
2275	Participation of ($\hat{\iota}$ -3-Allyl)ruthenium(II) Complexes in C $\hat{\iota}$ -C Bond Formation and C $\hat{\iota}$ -C Bond Cleavage. A Theoretical Study. Organometallics, 2001, 20, 3145-3158.	1.1	16
2276	Amidolithium-mediated enolization: does proton transfer occur via a dimer intermediate with bridging carbonyls?. New Journal of Chemistry, 2001, 25, 262-267.	1.4	10
2277	Halogenation of pyrazoloquinolines and pyrazoloisoquinolines. Theoretical analysis of the regioselectivity and cross-coupling of 3-halogen derivatives. Journal of the Chemical Society, Perkin Transactions 1, 2001, , 861-866.	1.3	7
2278	Alkali metal and magnesium enamides from metallation of the alkyl ligands [(2-Pyr)(SiMe3)CH2] and [6-Me-(2-Pyr)(SiMe3)CH2]: a solid state and ab initio study. Dalton Transactions RSC, 2001, , 996-1006.	2.3	25
2279	Intramolecular hydrogen bonding in 2-deoxyribonucleosides: an AIM topological study of the electronic density. Physical Chemistry Chemical Physics, 2001, 3, 3192-3199.	1.3	69
2280	Solvation of alkane and alcohol molecules. Energy contributions. Physical Chemistry Chemical Physics, 2001, 3, 4001-4009.	1.3	25

#	ARTICLE	IF	CITATIONS
2281	A comparative study of olefin or acetylene insertion into Ru η^5 -Cp*H or Os η^5 -Cp*H of MHCl(CO)(phosphine) ₂ . New Journal of Chemistry, 2001, 25, 1382-1388.	1.4	35
2282	EVALUATION OF SEVERAL ECONOMICAL COMPUTATIONAL METHODS FOR GEOMETRY OPTIMISATION OF PHOSPHORUS ACID DERIVATIVES. Nucleosides, Nucleotides and Nucleic Acids, 2001, 20, 1381-1384.	0.4	4
2283	Calculations of dynamic hyperpolarizabilities for small and medium-sized molecules. , 2001, , 1-62.		31
2284	The improved virtual orbital-complete active space configuration interaction method, a ϵ -packageable efficient many-body method for describing electronically excited states. Journal of Chemical Physics, 2001, 114, 2592-2600.	1.2	95
2285	Pyrrrolizin-3-one and its 1,2-dihydro derivative: structures of the free molecules determined by electron diffraction and ab initio calculations and in the crystal by X-ray diffraction Electronic supplementary information (ESI) available: further experimental data. See http://www.rsc.org/suppdata/p2/b1/b102475m/ . Perkin Transactions II RSC, 2001, , 2195-2201.	1.1	5
2286	Structure and infrared (IR) assignments for the OLED material: N,N'-diphenyl-N,N'-bis(1-naphthyl)-1,1'-biphenyl-4,4'-diamine (NPB). Physical Chemistry Chemical Physics, 2001, 3, 2131-2136.	1.3	60
2287	The structure and dynamics of cationic zirconocene complexes with phenyl coordination η^5 . Dalton Transactions RSC, 2001, , 79-84.	2.3	15
2288	The crystallographic observation of molecular lithium oxide: synthesis and solid-state structure of [Me ₂ AlN(2-C ₅ H ₄ N)Ph] ₂ (O)Li ₂ ·2THF. Dalton Transactions RSC, 2001, , 2838-2843.	2.3	20
2289	Molecular structure of ButCl ₂ Si ₂ Cl ₂ But in the gas phase by electron diffraction and ab initio calculations. Molecular structures of the compounds ButX ₂ Si ₂ X ₂ But (X = Cl, Br or I) by vibrational spectroscopy, X-ray crystallography and ab initio calculations. Dalton Transactions RSC, 2001, , 2916-2925.	2.3	9
2290	The influence of square planar platinum complexes on DNA base pairing. An ab initio DFT study. Physical Chemistry Chemical Physics, 2001, 3, 4404-4411.	1.3	48
2291	Conformational isomerism in methyl cyanoacetate: A combined matrix-isolation infrared spectroscopy and molecular orbital study. Physical Chemistry Chemical Physics, 2001, 3, 4235-4241.	1.3	42
2292	Bond shift and charge transfer dynamics in methylene- and dimethylsilyl-bridged dicyclooctatetraene dianions. Perkin Transactions II RSC, 2001, , 1130-1138.	1.1	7
2293	Band Electronic Structures of Polyphenanthrene and Polyacene Doped with Lithium. Journal of Physical Chemistry B, 2001, 105, 2534-2538.	1.2	17
2294	Theoretical study of initial decomposition process of NTO dimer. Physical Chemistry Chemical Physics, 2001, 3, 2742-2746.	1.3	19
2295	Ring size effects in the C ₂ -C ₆ biradical cyclisation of enyne allenes and the relevance for neocarcinostatin. Perkin Transactions II RSC, 2001, , 1331-1339.	1.1	35
2296	DFT study of the structural and redox properties of [Cp ₂ Fe ₂ S ₄] _q complexes (q = 0, +2, +1 and -2). New Journal of Chemistry, 2001, 25, 611-617.	1.4	13
2297	What Parameters Determine N \sim N and O \sim O Coupling Constants (2h _J X-X) Across X \sim H \sim X Hydrogen Bonds?. Journal of Physical Chemistry A, 2001, 105, 930-934.	1.1	53
2298	Stability and Bonding Situation of Electron-Deficient Transition-Metal Complexes. Theoretical Study of the CO-Labilizing Effect of Ligands L in [W(CO)5L] (L = C ₂ H ₂ , NCH, N ₂ , C ₂ H ₄ , OH ₂ , SH ₂ , NH ₃ , F-, Cl-) Tj ETQq1_1.1.0.784314 rgBT Complexes [W(CO)4L] and [W(CO)3L] ₂ . Organometallics, 2001, 20, 2510-2524.	1.1	34

#	ARTICLE	IF	CITATIONS
2299	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. <i>Journal of Physical Chemistry B</i> , 2001, 105, 8445-8451.	1.2	15
2300	Dynamics of Photosubstitution Reactions of Fe(CO) ₅ : An Ultrafast Infrared Study of High Spin Reactivity. <i>Journal of the American Chemical Society</i> , 2001, 123, 6909-6915.	6.6	66
2301	Theoretical Studies on A ₃ H ₃ ⁺ (A = C, Si, Ge) as π Ligands in Organometallic Chemistry. <i>Organometallics</i> , 2001, 20, 5200-5204.	1.1	10
2302	Diffuse-Bound and Valence-Bound Anions of Cytosine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8782-8786.	1.1	44
2303	Structure and Bonding in Magnesium Difluoride Clusters: The MgF ₂ Molecule. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4126-4135.	1.1	11
2304	Energy Transfer to the Low-Energy Triplet States of 1,3-Dicarbonylazomethine Dyes: The Role of Unique Geometries and Nonadiabatic Behavior. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1214-1222.	1.1	10
2305	[2+2] versus [3+2] Addition of Metal Oxides Across CC Double Bonds: Toward an Understanding of the Surprising Chemo- and Periselectivity of Transition-Metal-Oxide Additions to Ketene. <i>Journal of the American Chemical Society</i> , 2001, 123, 10085-10094.	6.6	49
2306	A Matrix Isolation Spectroscopic and Quantum Chemical Study of Fumaric and Maleic Acid. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3922-3933.	1.1	64
2307	Bond Energies and Bonding Interactions in Fe(CO) ₅ -n(N ₂) _n (n = 0-5) and Cr(CO) ₆ -n(N ₂) _n (n = 0-6) Complexes: A Density Functional Theory Calculations and Comparisons to Experimental Data. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3773-3787.	1.1	28
2308	A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7564-7571.	1.2	74
2309	Synthesis and Stereochemistry of cis- and trans-3,4-Benzo-1,2-di(tert-butyl)-1,2-dimethyl-1,2-disilacyclobutene. <i>Organometallics</i> , 2001, 20, 1059-1061.	1.1	21
2310	Are Guanine Tetrads Stabilized by Bifurcated Hydrogen Bonds?. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8223-8225.	1.1	51
2311	Symmetry Breaking and the Molecular Structure of NO ₃ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 1662-1668.	1.1	8
2312	Mechanism of Protonation of [Pt ₃ (μ -PBut ₂) ₃ (H)(CO) ₂], Yielding the Hydride-Bridged [Pt ₃ (μ -PBut ₂) ₂ (μ -H)(PBut ₂ H)(CO) ₂]OTf (Tf = CF ₃ SO ₂), and the Spectroscopic and Theoretical Characterization of a Kinetic Intermediate. <i>Inorganic Chemistry</i> , 2001, 40, 3055-3060.	1.9	17
2313	Charge-Transfer Complexes between the Amines (CH ₃) _n NH ₃ -n (n = 0-3) and the ClF Molecule: An ab Initio and Density Functional Study on the Intermolecular Interaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2064-2072.	1.1	19
2314	Unraveling the Origin of Regioselectivity in Rhodium Diphosphine Catalyzed Hydroformylation. A DFT QM/MM Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 7630-7637.	6.6	141
2315	An ab Initio Study of Anharmonicity and Field Effects in Hydrogen-Bonded Complexes of the Deuterated Analogues of HCl and HBr with NH ₃ and N(CH ₃) ₃ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 3371-3378.	1.1	34
2316	The Importance of the Ene Reaction for the C ₂ -C ₆ Cyclization of Enyne Allenes. <i>Journal of the American Chemical Society</i> , 2001, 123, 5557-5562.	6.6	61

#	ARTICLE	IF	CITATIONS
2317	Ethylene Epoxidation with Tungsten Diperoxo Complexes: Is Relativity the Origin of Reactivity?. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4765-4772.	1.1	30
2318	Intramolecular Rearrangements on Ultrafast Timescales: Femtosecond Infrared Studies of Ring Slip in (1-C5Cl5)Mn(CO)5. <i>Journal of the American Chemical Society</i> , 2001, 123, 7425-7426.	6.6	6
2319	Reactions of a Hexahydride Osmium Complex with Aromatic Ketones: C-H Activation versus C-F Activation. <i>Organometallics</i> , 2001, 20, 442-452.	1.1	88
2320	In Search of Catalytically Active Species in the Surfactant-Mediated Biphasic Alkene Epoxidation with Mimoun-Type Complexes. <i>Organic Letters</i> , 2001, 3, 329-332.	2.4	37
2321	Conformational Analysis and Kinetics of Ring Inversion for Methylene- and Dimethylsilyl-Bridged Dicyclooctatetraene. <i>Journal of Organic Chemistry</i> , 2001, 66, 3871-3877.	1.7	3
2322	Olefin Insertion into the Rhodium-Hydrogen Bond as the Step Determining the Regioselectivity of Rhodium-Catalyzed Hydroformylation of Vinyl Substrates: A Comparison between Theoretical and Experimental Results. <i>Organometallics</i> , 2001, 20, 5394-5404.	1.1	67
2323	Spontaneous Generation of Stable Pnictinyl Radicals from "Jack-in-the-Box" Dipnictines: A Solid-State, Gas-Phase, and Theoretical Investigation of the Origins of Steric Stabilization. <i>Journal of the American Chemical Society</i> , 2001, 123, 9045-9053.	6.6	124
2324	Assessment of Density Functional Theory for Model SN2 Reactions: CH3X + F-(X = F, Cl, CN, OH, SH, NH2). <i>J. Phys. Chem. B</i> , 2001, 105, 11111-11122.	1.1	44
2325	A Computational Study of Aluminum Hydroxide Solvation. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10111-10122.	1.1	44
2326	Synthesis and Characterization of Mixed-Phosphine Osmium Polyhydrides: Hydrogen Delocalization in [OsH5P3]+ Systems. <i>Organometallics</i> , 2001, 20, 5297-5309.	1.1	20
2327	Reaction of Ni2Cp2(1/4-CO)2 with the Alkylgallium(I) and Alkylindium(I) Compounds E4[C(SiMe3)3]4 (E = Tl, Pb, Sn, Bi, Po, At, Rg). <i>Inorganic Chemistry</i> , 2001, 40, 750-755.	1.9	47
2328	Triplet Organometallic Reactivity under Ambient Conditions: An Ultrafast UV Pump/IR Probe Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 2255-2264.	6.6	82
2329	Proton Affinity of Peroxyacetyl Nitrate (PAN). <i>Journal of Physical Chemistry A</i> , 2001, 105, 750-754.	1.1	7
2330	Accurate Intraprotein Electrostatics Derived from First Principles: An Effective Fragment Potential Method Study of the Proton Affinities of Lysine 55 and Tyrosine 20 in Turkey Ovomucoid Third Domain. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3829-3837.	1.1	45
2331	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H2O2 with NH3 and N(CH3)3. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6430-6435.	1.1	24
2332	Matrix Photochemistry of Methyltrioxorhenium(VII), CH3ReO3: Formation of the Methylidene Tautomer H2CRe(O)2OH and Its Potential Relevance to Olefin Metathesis. <i>Organometallics</i> , 2001, 20, 2344-2352.	1.1	47
2333	Vibrational Properties and Structure of Pentaerythritol Tetranitrate. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6197-6202.	1.1	101
2334	Raman and Fluorescence Spectra of Size-Selected, Matrix-Isolated C14 and C18 Neutral Carbon Clusters. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3029-3033.	1.1	26

#	ARTICLE	IF	CITATIONS
2335	Equilibrium Isotope Effect for the $W(CO)_3(PCy_3)_2(H)_2/W(Co)_3(PCy_3)_2(\hat{I}\cdot 2-H_2)$ Tautomeric Equilibrium: A Nuclear Dynamics Variable Representation Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4676-4681.	1.1	11
2336	Nucleophilic Substitution by a Hydroxide Ion at a Vinylic Carbon: Ab Initio and Density Functional Theory Studies on Methoxyethene, 3-Methoxypropenal, 2,3-Dihydro-4H-pyran-4-one, and 4H-Pyran-4-one. <i>Journal of Organic Chemistry</i> , 2001, 66, 4998-5007.	1.7	13
2337	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H_2O_2 with Phosphorus and Sulfur Bases. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11365-11370.	1.1	26
2338	Superelectrophilic Tetrakis(carbonyl)palladium(II)- and -platinum(II) Undecafluorodiantimonate(V), $[Pd(CO)_4][Sb_2F_{11}]_2$ and $[Pt(CO)_4][Sb_2F_{11}]_2$: Syntheses, Physical and Spectroscopic Properties, Their Crystal, Molecular, and Extended Structures, and Density Functional Calculations: An Experimental, Computational, and Comparative Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 588-602.	6.6	74
2339	Femtosecond Infrared Study of the Dynamics of Solvation and Solvent Caging. <i>Journal of the American Chemical Society</i> , 2001, 123, 4204-4210.	6.6	36
2340	Possible Dissociative Adsorption of CH_3OH and CH_3NH_2 on $Si(100)-2 \times 1$ Surface. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10340-10347.	1.2	78
2341	Bonding Interactions in Olefin (C_2X_4 , $X = H, F, Cl, Br, I, CN$) Iron Tetracarbonyl Complexes: A Role of the Deformation Energy in Bonding and Reactivity. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8077-8085.	1.1	38
2342	Highly Energetic Tetraazidoborate Anion and Boron Triazide Adducts. <i>Inorganic Chemistry</i> , 2001, 40, 1334-1340.	1.9	101
2343	Resonant Tunneling and the Substituent Effect on Negative Differential Resistance in a Molecular Junction. <i>Materials Research Society Symposia Proceedings</i> , 2001, 708, 371.	0.1	0
2344	Can $Cp_2Zr(C_2H_4)$ Easily React with Hydrosilane? Theoretical Study. <i>Chemistry Letters</i> , 2001, 30, 1222-1223.	0.7	8
2345	Theoretical Study of a Conformational Change Occurring with Lithium Complexation to a Tetra-aza Macrocycle Containing 2,2'-Bipyridines. <i>Bulletin of the Chemical Society of Japan</i> , 2001, 74, 1241-1249.	2.0	7
2346	A multi-component model for radiation damage to DNA from its constituents. <i>Theoretical and Computational Chemistry</i> , 2001, 9, 409-466.	0.2	5
2347	Ab initio and density functional theory studies for the explanation of the antioxidant activity of certain phenolic acids. <i>Lipids</i> , 2001, 36, 181-191.	0.7	84
2348	An optimization method for large van der Waals system. <i>Science Bulletin</i> , 2001, 46, 1514-1516.	1.7	0
2349	Study of the $N\hat{H}^+H\hat{a}^-O\hat{r}^- \dots C$ proton transfer reaction in aqueous solution using classical free energy curves. <i>Chemical Physics</i> , 2001, 265, 207-215.	0.9	4
2350	The vacuum UV photoabsorption spectrum of methyl chloride (CH_3Cl) and its perdeuterated isotopomer CD_3Cl . <i>Chemical Physics</i> , 2001, 272, 277-292.	0.9	23
2351	About the photoionization of methyl chloride. <i>Chemical Physics</i> , 2001, 272, 293-313.	0.9	29
2352	Synthesis and structure of, and bonding in some derivatives of 2,6,9,10-tetraoxatricyclo[3.3.1.1.3,8]decane. <i>Acta Crystallographica Section B: Structural Science</i> , 2001, 57, 63-71.	1.8	3

#	ARTICLE	IF	CITATIONS
2353	Comparison of monolayer films of stearic acid and methyl stearate on an Al ₂ O ₃ surface. <i>Thin Solid Films</i> , 2001, 397, 102-108.	0.8	34
2354	Conformational preferences of non-nucleoside HIV-1 reverse transcriptase inhibitors. <i>Tetrahedron</i> , 2001, 57, 3243-3253.	1.0	79
2356	Experimental and theoretical identifications of the C ₃ O ₂ π -thiazole complex: a stable pre-reactive intermediate. <i>Journal of Molecular Structure</i> , 2001, 560, 197-203.	1.8	6
2357	Spectroscopic characterization of $\hat{1}\pm$ - and $\hat{1}^3$ -pyrones and their substituted 4-hydroxy and 4-methoxy derivatives: an integrated infrared, photophysical and theoretical study. <i>Journal of Molecular Structure</i> , 2001, 565-566, 59-67.	1.8	23
2358	Obtaining scaled-refined quantum mechanical force fields for large molecules: naphthalene and anthracene. <i>Journal of Molecular Structure</i> , 2001, 565-566, 373-376.	1.8	1
2359	Mean vibrational amplitudes of 1,3-butadiene, acrolein and glyoxal. <i>Journal of Molecular Structure</i> , 2001, 567-568, 211-216.	1.8	3
2360	Amide N-oxides: an ab initio molecular orbital study. <i>Journal of Molecular Structure</i> , 2001, 567-568, 303-317.	1.8	9
2361	Trifluoromethoxy benzene in the gas phase studied by electron diffraction and spectroscopy supplemented with ab initio calculations. <i>Journal of Molecular Structure</i> , 2001, 567-568, 339-360.	1.8	40
2362	Vibrational spectroscopy and ab initio MO study of the molecular structure and vibrational spectra of $\hat{1}\pm$ - and $\hat{1}^3$ -pyrones. <i>Journal of Molecular Structure</i> , 2001, 598, 287-303.	1.8	17
2363	Two possible reaction pathways for the formation of a ruthenium carbene complex by addition of acetylene to [RuH ₂ Cl ₂ (PH ₃) ₂]: a quantum chemical study. <i>Journal of Organometallic Chemistry</i> , 2001, 617-618, 225-232.	0.8	12
2364	Mechanism of the electrochemical reduction of [Fe($\hat{1}^5$ -C ₆ H ₇)(CO) ₃][PF ₆] ⁻ a theoretical approach to the intermediates. <i>Journal of Organometallic Chemistry</i> , 2001, 632, 49-57.	0.8	4
2365	Thiophene versus aryl coordination in tricarbonylmanganese complexes with interesting non-linear optical properties. <i>Journal of Organometallic Chemistry</i> , 2001, 632, 3-10.	0.8	12
2366	A novel dimanganese complex linked by an unusually strong hydrogen bond. X-ray structure of the hydrogen-bonded complex and ab initio calculations. <i>Journal of Organometallic Chemistry</i> , 2001, 629, 165-170.	0.8	11
2367	Olefin strain energies and platinum complexes of highly pyramidalised alkenes. <i>Journal of Organometallic Chemistry</i> , 2001, 635, 142-152.	0.8	10
2368	Bis(indenyl) complexes of Fe, Co, and Ni: electronic structure and preferences. <i>Journal of Organometallic Chemistry</i> , 2001, 635, 197-203.	0.8	24
2369	An ab initio quantum chemical study of reactions of hexano-6-lactam peroxy radicals with phenoxy or diphenyl radicals. <i>Polymer Degradation and Stability</i> , 2001, 74, 569-577.	2.7	3
2370	Vibrational frequencies of CO adsorbed on silica supported Mo atoms from density functional calculations. <i>Journal of Molecular Catalysis A</i> , 2001, 170, 175-186.	4.8	5
2371	Spin effects in activation of hydrocarbons. <i>Journal of Molecular Catalysis A</i> , 2001, 171, 53-72.	4.8	24

#	ARTICLE	IF	CITATIONS
2372	A combined matrix-isolation infrared spectroscopy and MO study of 1-amino-2-propanol. <i>Vibrational Spectroscopy</i> , 2001, 26, 113-131.	1.2	27
2373	Experimental and theoretical vibrational study of isatin, its 5-(NO ₂ , F, Cl, Br, I, CH ₃) analogues and the isatinato anion. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 469-481.	2.0	34
2374	Raman and FTIR spectroscopies of fluorescein in solutions. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2001, 57, 1781-1791.	2.0	130
2375	Catalyzed keto-enol tautomerism of ionized acetone: a Fourier transform ion cyclotron resonance mass spectrometry study of proton transport isomerization. <i>International Journal of Mass Spectrometry</i> , 2001, 210-211, 429-446.	0.7	35
2376	Qualitative comparison between the quantum calculations and electrospray mass spectra of complexes of polyammonium macrotricyclic ligands with dicarboxylic acids. <i>Journal of the American Society for Mass Spectrometry</i> , 2001, 12, 304-316.	1.2	8
2377	Theoretical studies on heats of formation for polynitrocubanes using the density functional theory B3LYP method and semiempirical MO methods. <i>Journal of Physical Organic Chemistry</i> , 2001, 14, 583-588.	0.9	55
2378	Intramolecular basis set superposition errors. <i>International Journal of Quantum Chemistry</i> , 2001, 82, 282-292.	1.0	31
2379	Density functional study of the relative reactivity in the concerted 1,3-dipolar cycloaddition of nitrile ylide to disubstituted ethylenes. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 318-323.	1.0	9
2380	Ab initio modeling of competitive drug-drug interactions: 5-fluorouracil dimers in the gas phase and in solution. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 128-142.	1.0	11
2381	Model systems for rod-like polyheteroarylethylenes. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 86-98.	1.0	9
2382	Nitrenes as intermediates in the thermal decomposition of aliphatic azides. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 241-248.	1.0	27
2383	Reaction mechanisms between methylamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO). <i>International Journal of Quantum Chemistry</i> , 2001, 84, 740-749.	1.0	1
2384	Sum-frequency generation first hyperpolarizability from time-dependent Hartree-Fock method. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 463-468.	1.0	11
2385	Structural elucidation of bipyridine helicate complexes and their precursors by NMR spectroscopy. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 341-354.	1.1	5
2386	¹⁵ N, ¹⁵ N spin-spin coupling constants across N-H...N and N-H...N hydrogen bonds: can coupling constants provide reliable estimates of N...N distances in biomolecules?. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, S109-S114.	1.1	49
2387	Theoretical study of silicon-sulfur clusters (SiS ₂) _n (n=1-6). <i>International Journal of Quantum Chemistry</i> , 2001, 81, 280-290.	1.0	7
2388	Density functional study of guanine and uracil quartets and of guanine quartet/metal ion complexes. <i>Journal of Computational Chemistry</i> , 2001, 22, 109-124.	1.5	117
2389	The Effect of Solvent and Fiber Treatment on the Deposition of Organic Silane Solutions Using THF and Acetone. <i>Journal of Colloid and Interface Science</i> , 2001, 241, 32-44.	5.0	8

#	ARTICLE	IF	CITATIONS
2390	MM3 parameterization for the Bi&N dative bond. Journal of Computational Chemistry, 2001, 22, 913-922.	1.5	7
2391	Quantum chemical characterization of the cytosine: 2-Aminopurine base pair. Journal of Computational Chemistry, 2001, 22, 1167-1179.	1.5	16
2392	Parallelization of multireference perturbation calculations with GAMESS. Journal of Computational Chemistry, 2001, 22, 1243-1251.	1.5	16
2393	Theoretical study of endohedral metallofullerenes: Sc ₃ ?nLanN@C80 (n=0-3). Journal of Computational Chemistry, 2001, 22, 1353-1358.	1.5	87
2394	Choice of Spin-Orbit Correction Terms in Gaussian Model Chemistries. Journal of Computational Chemistry, 2001, 22, 1552-1556.	1.5	3
2395	Conformational analysis of the HIV-1 virus reverse transcriptase nonnucleoside inhibitors: TIBO and nevirapine. Journal of Computational Chemistry, 2001, 22, 1817-1829.	1.5	14
2396	Analytical TDHF second derivatives of dynamic electronic polarizability with respect to nuclear coordinates. Application to the dynamic ZPVA correction. Journal of Computational Chemistry, 2001, 22, 1920-1932.	1.5	29
2397	Olefin Epoxidation with Transition Metal \hat{I} -2-Peroxo Complexes: The Control of Reactivity. European Journal of Inorganic Chemistry, 2001, 2001, 1819-1827.	1.0	42
2398	On the Mechanism and Stereoselectivity of the Copper(I)-Catalyzed Cyclopropanation of Olefins \hat{a} A Combined Experimental and Density Functional Study. European Journal of Organic Chemistry, 2001, 2001, 2151-2160.	1.2	43
2399	Ab initio study of the mechanisms of intermolecular and intramolecular [4+2] cycloaddition reactions of conjugated enynes. Journal of Physical Organic Chemistry, 2001, 14, 109-121.	0.9	21
2400	Gauche, Ortho, Transoid and Anti Conformations of the Tetrasilanes SiMe ₃ SiX ₂ SiX ₂ SiMe ₃ (X=H, F, Cl). Tj ETQq0 0 0 rgBT /Overlock 10 T	1.8	8
2403	An Experimental and Theoretical Study of the Basicity of Tetra-tert-butyltetrahedrane. Chemistry - A European Journal, 2001, 7, 342-346.	1.7	27
2404	The Photohydration of N-Alkylpyridinium Salts: Theory and Experiment. Chemistry - A European Journal, 2001, 7, 1734-1742.	1.7	16
2405	Ab Initio Calculations on the Mechanism of the Oxidation of the Hydroxymethyl Radical by Molecular Oxygen in the Gas Phase: A Significant Reaction for Environmental Science. Chemistry - A European Journal, 2001, 7, 3377-3386.	1.7	35
2406	Thermal Rearrangements of 2-Vinylcyclopropylidene to Cyclopentadiene and Vinylallene: A Theoretical Investigation. Chemistry - A European Journal, 2001, 7, 3951-3960.	1.7	8
2407	Iron Bispentazole Fe(\hat{I} -5-N ₅) ₂ , a Theoretically Predicted High-Energy Compound: Structure, Bonding Analysis, Metal-Ligand Bond Strength and a Comparison with the Isoelectronic Ferrocene. Chemistry - A European Journal, 2001, 7, 4155-4163.	1.7	157
2408	C \hat{a} ~H Activation with Elemental Sulfur: Synthesis of Cyclic Thioureas from Formaldehyde Aminals and S ₈ . Chemistry - A European Journal, 2001, 7, 4477-4486.	1.7	53
2409	Medium Effects on ⁵¹ V NMR Chemical Shifts: A Density Functional Study. Chemistry - A European Journal, 2001, 7, 4487-4494.	1.7	108

#	ARTICLE	IF	CITATIONS
2410	Structure and Dynamics of the Host-Guest Complex of a Molecular Tweezer: Coupling Synthesis, Solid-State NMR, and Quantum-Chemical Calculations. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 717-720.	7.2	96
2411	Which Structural Elements Are Relevant for the Efficacy of Neocarzinostatin?. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 3833-3836.	7.2	11
2412	New integral transforms for molecular properties and application to a massively parallel GIAO-SCF implementation. <i>Computer Physics Communications</i> , 2001, 134, 150-166.	3.0	26
2413	Calculation of refractive indices and local electric field tensors in $\hat{1}\pm$ -sexithiophene crystal. <i>Chemical Physics Letters</i> , 2001, 336, 357-363.	1.2	15
2414	Non-ionic and zwitterionic forms of neutral arginine – an ab initio study. <i>Chemical Physics Letters</i> , 2001, 337, 143-150.	1.2	50
2415	Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model. <i>Chemical Physics Letters</i> , 2001, 338, 375-384.	1.2	430
2416	Multi-reference weak pairs local configuration interaction: efficient calculations of bond breaking. <i>Chemical Physics Letters</i> , 2001, 346, 177-185.	1.2	42
2417	Does SH really react with O ₃ in the ground state?. <i>Chemical Physics Letters</i> , 2001, 349, 123-130.	1.2	13
2418	Vibrational analysis of carbonyl modes in different stages of light-induced cyclopyrimidine dimer repair reactions. <i>Chemical Physics Letters</i> , 2001, 349, 342-348.	1.2	6
2419	Valence bond curve-crossing model of the 1,2-hydrogen shift in HCN and isovalent systems. <i>Chemical Physics Letters</i> , 2001, 350, 345-350.	1.2	7
2420	Spin-flip configuration interaction: an electronic structure model that is both variational and size-consistent. <i>Chemical Physics Letters</i> , 2001, 350, 522-530.	1.2	254
2422	Hybrid quantum mechanics/molecular mechanics studies of the active site of the blue copper proteins amicyanin and rusticyanin. <i>Inorganica Chimica Acta</i> , 2001, 324, 21-26.	1.2	30
2423	Polarization consistent basis sets: Principles. <i>Journal of Chemical Physics</i> , 2001, 115, 9113-9125.	1.2	571
2424	Title is missing!. <i>Russian Journal of Electrochemistry</i> , 2001, 37, 15-25.	0.3	8
2425	Conformational Analyses of Glycinal and Alaninal: A Computational Study. <i>Structural Chemistry</i> , 2001, 12, 45-58.	1.0	0
2426	Interactions between allosteric modulators and 4-DAMP and other antagonists at muscarinic receptors: potential significance of the distance between the N and carboxyl C atoms in the molecules of antagonists. <i>Neurochemical Research</i> , 2001, 26, 383-394.	1.6	9
2427	The nature of the O–O bond in hydroperoxides. <i>Russian Chemical Bulletin</i> , 2001, 50, 1539-1549.	0.4	15
2428	Low temperature matrix-isolation and solid state vibrational spectra of tetrazole. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3541-3547.	1.3	61

#	ARTICLE	IF	CITATIONS
2429	Reversible Carbon-Carbon Double Bond Cleavage of a Ketene Ligand at a Single Iridium(I) Center: A Theoretical Study. <i>Organometallics</i> , 2001, 20, 3938-3949.	1.1	45
2430	Calculated molecular properties for different alkanolic acid-alkylamine complexes: A comparison with measured FTIR and Raman spectra. <i>Chemical Physics</i> , 2001, 263, 127-138.	0.9	13
2431	An ab initio study of the enolboration of 3-pentanone mediated by boron monochlorides L2BCl. <i>Tetrahedron</i> , 2001, 57, 6239-6247.	1.0	8
2432	Theoretical Gibbs free energy study on $UO_2(H_2O)_n^{2+}$ and its hydrolysis products. <i>Chemical Physics Letters</i> , 2001, 334, 365-373.	1.2	74
2433	Influence of isomorphous substitution on acidity of zeolites: ab initio and density functional studies. <i>Computational and Theoretical Chemistry</i> , 2001, 535, 31-38.	1.5	14
2434	Structures and properties of nitrogen derivatives of tetrahedrane. <i>Computational and Theoretical Chemistry</i> , 2001, 536, 143-154.	1.5	8
2435	Multiconfigurational self-consistent and molecular mechanics simulation of solvent effects on the n π *-blue shift of pyrimidine. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 213-222.	1.5	25
2436	Stepwise hydrogenation of N_2 - a large-scale investigation of the performance and basis set convergence of DFT and conventional ab initio methods. <i>Computational and Theoretical Chemistry</i> , 2001, 541, 17-29.	1.5	15
2437	Calculation of static mean polarisability and polarisability anisotropy. Statistical comparison with the results of gases and influence of the geometrical parameters. <i>Computational and Theoretical Chemistry</i> , 2001, 542, 167-176.	1.5	11
2438	Reactions between the OH radical and oxygen-containing atmospheric pollutants: a theoretical description. <i>Computational and Theoretical Chemistry</i> , 2001, 542, 123-137.	1.5	17
2439	Ab initio MO GB analysis of the solvent effect on the electronic structure of push-pull diazenes in the cis-trans isomerization reaction. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 233-241.	1.5	3
2440	Solids modeled by ab initio crystal field methods. Part 19. Structure of yellow and light yellow form of dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate. <i>Computational and Theoretical Chemistry</i> , 2001, 546, 17-24.	1.5	9
2441	Quantum-chemical study of sulfoxide decomposition. <i>Computational and Theoretical Chemistry</i> , 2001, 545, 49-60.	1.5	2
2442	On the isomerization of β -pinene: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2001, 544, 213-220.	1.5	16
2443	Solids modeled by ab initio crystal field methods. Part 20. Charge transfer in white form of dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate. <i>Computational and Theoretical Chemistry</i> , 2001, 546, 25-32.	1.5	3
2444	Alkyl migration in vinylidene-acetylene rearrangement reactions: investigation of structural, activation thermodynamic energies and kinetics properties by density functional theory based method. <i>Computational and Theoretical Chemistry</i> , 2001, 546, 207-215.	1.5	6
2445	Ab initio study of structure, protonation and complex formation of novel pyrazolone-5 derivatives. <i>Computational and Theoretical Chemistry</i> , 2001, 571, 45-57.	1.5	17
2446	Structural studies on conformationally defined 6-s-trans UAB retinoids. <i>Computational and Theoretical Chemistry</i> , 2001, 549, 39-45.	1.5	1

#	ARTICLE	IF	CITATIONS
2447	Comparative study of the molecular structure of stilbene using molecular mechanics, Hartree-Fock and density functional theories. Computational and Theoretical Chemistry, 2001, 549, 63-67.	1.5	15
2448	Antimalarial activity of dihydroartemisinin derivatives against <i>P. falciparum</i> resistant to mefloquine: a quantum chemical and multivariate study. Computational and Theoretical Chemistry, 2001, 572, 35-44.	1.5	22
2449	What a difference a decade makes: progress in ab initio studies of the hydrogen bond. Computational and Theoretical Chemistry, 2001, 573, 11-23.	1.5	80
2450	Force field scale factors of effective core potential basis sets of some selenium and tellurium heterocyclic molecules, selenophene, 1,2,5-selenadiazole, tellurophene and 1,2,5-telluradiazole. Computational and Theoretical Chemistry, 2001, 572, 81-87.	1.5	17
2451	A CIS study of solvent effects on the electronic absorption spectrum of Reichardt's dye. Computational and Theoretical Chemistry, 2001, 572, 203-212.	1.5	22
2452	Calculation of electron affinities for small homonuclear and heteronuclear diatomic molecules with the CBS-QB3 and G3B3 method: basis set effects, and need for further development. Computational and Theoretical Chemistry, 2001, 574, 141-143.	1.5	5
2453	Ion-specificity for hydrogen-bonding hydration of polymer: an approach by ab initio molecular orbital calculations II. Computational and Theoretical Chemistry, 2001, 574, 195-211.	1.5	15
2454	Theoretical study on the structure and stability of the clusters of tropylium ion solvated by methanol molecules. Computational and Theoretical Chemistry, 2001, 574, 117-125.	1.5	1
2455	A Computational Study of the Effectiveness of the Frontier Molecular Orbital Formalism in Predicting Conformational Isomerism in (p-RC6H4NC)2W(dppe)2. Journal of Chemical Information and Computer Sciences, 2001, 41, 50-55.	2.8	6
2456	Spin uncoupling in chemical reactions. Advances in Quantum Chemistry, 2001, 40, 191-211.	0.4	11
2457	Formation of ammonium halide particles from pure ammonia and hydrogen halide gases: A theoretical study on small molecular clusters (NH3-HX) _n (n=1, 2, 4; X=F, Cl, Br). Journal of Chemical Physics, 2001, 114, 1720-1726.	1.2	22
2458	I. Three-center versus four-center HCl-elimination in photolysis of vinyl chloride at 193 nm: Bimodal rotational distribution of HCl ($v=7$) detected with time-resolved Fourier-transform spectroscopy. Journal of Chemical Physics, 2001, 114, 160.	1.2	52
2459	Excited states of ladder-type poly-p-phenylene oligomers. Physical Review B, 2001, 64, .	1.1	57
2460	Nuclear spin-state mixing in the NH ₂ radical. Physical Review A, 2001, 63, .	1.0	3
2461	The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269.	1.2	39
2462	Scanning tunneling microscope study of boron-doped highly oriented pyrolytic graphite. Journal of Applied Physics, 2001, 90, 5670-5674.	1.1	159
2463	Free energy of solvation for the reference interaction site model: Critical comparison of expressions. Journal of Chemical Physics, 2001, 115, 3724-3731.	1.2	69
2464	The reactions CH ₄ +OH ⁺ and CH ₄ +OD ⁺ as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526.	1.2	29

#	ARTICLE	IF	CITATIONS
2465	Intervallence transition in triarylamine mixed-valence systems: A time-dependent density functional theory study. <i>Journal of Chemical Physics</i> , 2001, 115, 10409.	1.2	41
2466	An ab initio direct-trajectory study of the kinetic isotope effect on the bifurcating reaction. <i>Journal of Chemical Physics</i> , 2001, 114, 6973-6982.	1.2	26
2467	The molecular structures and nature of interactions in CH ₃ +Ar _n (n=1-8) complexes. <i>Journal of Chemical Physics</i> , 2001, 115, 771-777.	1.2	17
2468	Infrared and density-functional-theory study of spherosiloxane-based model silicon/silicon oxide interfaces. <i>Physical Review B</i> , 2001, 64, .	1.1	11
2469	A crystalline orbital study of polydiacetylenes. <i>Journal of Chemical Physics</i> , 2001, 114, 9130-9141.	1.2	24
2470	MP2 correlation effects upon the electronic and vibrational properties of polyynes. <i>Journal of Chemical Physics</i> , 2001, 114, 5917-5922.	1.2	26
2471	Generation of full-dimensional potential energy surface of intramolecular hydrogen atom transfer in malonaldehyde and tunneling dynamics. <i>Journal of Chemical Physics</i> , 2001, 115, 10647-10655.	1.2	100
2472	Density functional theory predictions of anharmonicity and spectroscopic constants for diatomic molecules. <i>Journal of Chemical Physics</i> , 2001, 115, 2439-2448.	1.2	39
2473	Accurate core electron binding energy calculations using small 6-31G and TZV core hole optimized basis sets. <i>Journal of Chemical Physics</i> , 2002, 116, 3521-3532.	1.2	37
2474	Assessment of time-dependent density-functional theory for the calculation of critical features in the absorption spectra of a series of aromatic donor-acceptor systems. <i>Journal of Chemical Physics</i> , 2002, 116, 8761-8771.	1.2	98
2475	A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea. <i>Journal of Chemical Physics</i> , 2002, 117, 1031-1039.	1.2	75
2476	Bonding of NO to NiO(100) and Ni _x Mg _{1-x} O(100) surfaces: A challenge for theory. <i>Journal of Chemical Physics</i> , 2002, 117, 2299-2306.	1.2	38
2477	Time-dependent density-functional theory investigation of the formation of the charge transfer excited state for a series of aromatic donor-acceptor systems. Part I. <i>Journal of Chemical Physics</i> , 2002, 117, 4146-4156.	1.2	85
2478	A polarizable mixed Hamiltonian model of electronic structure for micro-solvated excited states. I. Energy and gradients formulation and application to formaldehyde (1A ₂). <i>Journal of Chemical Physics</i> , 2002, 117, 1242-1255.	1.2	36
2479	Molecular and Electronic Structure on n-Alkyl Cyanobiphenyl Nematogens. <i>Molecular Crystals and Liquid Crystals</i> , 2002, 373, 143-153.	0.4	3
2480	Rearrangement pathways of the water trimer and tetramer anions. <i>Journal of Chemical Physics</i> , 2002, 116, 3612-3616.	1.2	18
2481	The use of distributed partial wave basis for accurate atom-molecule statistical distributions. <i>Journal of Chemical Physics</i> , 2002, 117, 4087-4094.	1.2	16
2482	Density functional theory of spin-coupled models for diiron-oxo proteins: Effects of oxo and hydroxo bridging on geometry, electronic structure, and magnetism. <i>Journal of Chemical Physics</i> , 2002, 116, 6253-6270.	1.2	56

#	ARTICLE	IF	CITATIONS
2483	Energy correction to simulation of volume polarization in reaction field theory. <i>Journal of Chemical Physics</i> , 2002, 116, 10129-10138.	1.2	40
2484	High-spin electronic interaction of small lithium and sodium cluster formation in the excited states. <i>Journal of Chemical Physics</i> , 2002, 117, 142-152.	1.2	14
2485	Local weak-pairs pseudospectral multireference configuration interaction. <i>Journal of Chemical Physics</i> , 2002, 117, 1982-1993.	1.2	45
2486	Interaction of HOCl with a chlorinated ice surface to produce molecular chlorine: An ab-initio study. <i>Journal of Chemical Physics</i> , 2002, 116, 9856-9864.	1.2	20
2487	A generalized scaling of a chiral index for molecules. <i>Journal of Chemical Physics</i> , 2002, 116, 9875-9881.	1.2	46
2488	Can coupled cluster singles and doubles be approximated by a valence active space model?. <i>Journal of Chemical Physics</i> , 2002, 117, 3040-3048.	1.2	14
2489	Semiclassical initial value representation description of molecular structure problems: An elongated dihydrogen ruthenium complex. <i>Journal of Chemical Physics</i> , 2002, 117, 7094-7101.	1.2	5
2490	Practical failures from the inclusion of exact exchange: how much exact exchange is appropriate?. <i>Molecular Physics</i> , 2002, 100, 483-497.	0.8	22
2491	Nonlinear partial differential equations and applications: Peroxone chemistry: Formation of H ₂ O ₃ and ring-(HO ₂)(HO ₃) from O ₃ /H ₂ O ₂ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 15308-15312.	3.3	56
2492	Recent advances in electronic structure theory: Method of moments of coupled-cluster equations and renormalized coupled-cluster approaches. <i>International Reviews in Physical Chemistry</i> , 2002, 21, 527-655.	0.9	258
2493	An ab initio investigation of scandium chloro complexes. <i>Canadian Journal of Chemistry</i> , 2002, 80, 1331-1342.	0.6	7
2494	OH frequency calculations for the hydroxylated MgO(001) surface. <i>Molecular Simulation</i> , 2002, 28, 663-681.	0.9	5
2495	Incorporation of azides into recombinant proteins for chemoselective modification by the Staudinger ligation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 19-24.	3.3	855
2496	The gas phase reaction of singlet dioxygen with water: A water-catalyzed mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 3376-3381.	3.3	94
2497	Ab initio quantum mechanical modeling of infrared vibrational frequencies of the OH group in dioctahedral phyllosilicates. Part I: Methods, results and comparison to experimental data. <i>American Mineralogist</i> , 2002, 87, 1215-1223.	0.9	29
2498	From bifluorenylidene dianion to dibenzo[g,p]chrysene dianion: sensitivity of anisotropy changes to bonding structure. <i>Perkin Transactions II RSC</i> , 2002, , 449-454.	1.1	19
2499	Olefin Polymerization by Early Transition Metal Catalysts. <i>Catalysis By Metal Complexes</i> , 2002, , 23-56.	0.6	5
2500	Controlled Alcohol \rightleftharpoons Ketone Interconversion by Dihydrogen Transfer: An ab Initio Study of the Methanol \rightleftharpoons Formaldehyde Complex. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9512-9519.	1.1	11

#	ARTICLE	IF	CITATIONS
2501	Ureidosilanes on E-glass fibres: deposition and surface characteristics. <i>Journal of Adhesion Science and Technology</i> , 2002, 16, 429-448.	1.4	5
2502	Computation of pK _a from Dielectric Continuum Theory. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7413-7422.	1.1	204
2503	Comparison of Some Computational Methods for Geometry Optimisation of Phosphorus Acid Derivatives. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2002, 177, 2711-2724.	0.8	4
2504	Charge transfer in small hydrogen bonded clusters. <i>Journal of Chemical Physics</i> , 2002, 116, 7380-7388.	1.2	62
2505	Aggregation and Solvation of Steroid Molecules in Different Solvents. <i>Crystal Growth and Design</i> , 2002, 2, 121-126.	1.4	3
2506	An Investigation of the ¹⁷ O NMR Chemical Shifts in Oxiranes Using Magnetically Corrected Basis Sets. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4176-4180.	1.1	15
2507	Chlorination Chemistry. 3. Ab Initio Study of the Reaction of Chlorine Atom with Allene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1739-1745.	1.1	9
2508	Activation of Propargylic Alcohols Derived from Hormonal Steroids by the Indenyl ^π Ruthenium(II) Complex [RuCl(Indenyl)(PPh ₃) ₂]: Experimental and Theoretical Evidence of an Allenylidene ^π Vinylidene Equilibrium. <i>Organometallics</i> , 2002, 21, 203-209.	1.1	41
2509	Theoretical Study on the Structure, Stability, and Tautomerism of 2-Aza-21-carba-23-X(thia or Tj ETQq0 0 0 rgBT /Qverlock 10 Tf 50 422	1.1	9
2510	A DFT Study of SiH ₄ Activation by Cp ₂ LnH. <i>Inorganic Chemistry</i> , 2002, 41, 4355-4362.	1.9	75
2511	Relationships between basicity, structure, chemical shift and the charge distribution in resonance-stabilized iminoamines Electronic supplementary information (ESI) available: energies and N ⁺ -N distances in geometry-optimised iminoamine bases. See http://www.rsc.org/suppdata/p2/b2/b200899h/ . <i>Perkin Transactions II RSC</i> , 2002, , 899-905.	1.1	26
2512	Ab Initio and DFT Study of the Formation Mechanisms of Polycyclic Aromatic Hydrocarbons: The Phenanthrene Synthesis from Biphenyl and Naphthalene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6171-6182.	1.1	35
2513	Silicon ^π Carbon Unsaturated Compounds. 65. Thermal and Photochemical Isomerization of Trimethylsiloxy- and Bis(trimethylsilyl)-Substituted Silacyclobut-3-enes. <i>Organometallics</i> , 2002, 21, 2033-2035.	1.1	27
2514	Quantum Mechanical/Molecular Mechanical Studies of the Triosephosphate Isomerase-Catalyzed Reaction: Verification of Methodology and Analysis of Reaction Mechanisms. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1768-1798.	1.2	58
2515	Accurate Structures and Binding Energies for Stacked Uracil Dimers. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3850-3854.	1.1	71
2516	Quantum Mechanics/Molecular Mechanics Studies of Triosephosphate Isomerase-Catalyzed Reactions: Effect of Geometry and Tunneling on Proton-Transfer Rate Constants. <i>Journal of the American Chemical Society</i> , 2002, 124, 3093-3124.	6.6	123
2517	Structural effects influencing cis ^π trans isomerisation in methoxy and cyano substituted stilbene derivatives Electronic supplementary information (ESI) available: Cartesian coordinates for the calculated geometries of 1 ^π 3 and (E)- and (Z)-stilbene. See http://www.rsc.org/suppdata/p2/b2/b201623k/ . <i>Perkin Transactions II RSC</i> , 2002, , 1345-1351.	1.1	14
2518	Solid-State and Theoretical Model Structures of Monolithiated (Organosulfonyl)acetonitriles and the Characterization and Reactivity of Their Geminated Dithio Derivatives. <i>Organometallics</i> , 2002, 21, 606-616.	1.1	28

#	ARTICLE	IF	CITATIONS
2519	Mechanism of the Stereoselective Alkyl Group Exchange between Alkylboranes and Alkylzinc Compounds. Quest for Novel Types of Boron-Metal Exchange Reactions. <i>Organometallics</i> , 2002, 21, 2203-2207.	1.1	25
2520	Theoretical Study of the Quadrupolarity of Carbodiimide. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7950-7957.	1.1	14
2521	Sterically Induced Conformational Relaxation and Structure of meso-Diaryloctaalkyl Porphyrins in the Excited Triplet State: A Experimental and DFT Studies. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12613-12622.	1.2	32
2522	Oxygen Atom Reactions with Circumtrindene and Related Molecules: A Analogues for the Oxidation of Nanotube Caps. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2572-2579.	1.1	18
2523	Comparison of Nonlinear Transformation Methods for Electron Density Approximation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5504-5509.	1.1	17
2524	Local Spin III: A Wave Function Analysis along a Reaction Coordinate, H Atom Abstraction, and Addition Processes of Benzynes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6890-6896.	1.1	52
2525	Quantum Control of Molecular Chirality: A Optical Isomerization of Difluorobenzo[c]phenanthrene. <i>Journal of the American Chemical Society</i> , 2002, 124, 9265-9271.	6.6	31
2526	Theory Supplemented by Experiment. Electronic Effects on the Rotational Stability of the Amide Group in p-Substituted Acetanilides. <i>Journal of Organic Chemistry</i> , 2002, 67, 6210-6215.	1.7	27
2527	Silyl, Hydrido-Silylene, or Other Bonding Modes: A Some Unusual Structures of [(dhpe)Pt(SiHR ₂)] ⁺ (dhpe) ⁻ Tj ETQqO O O rgBT /Overlock 10 Calculations. <i>Inorganic Chemistry</i> , 2002, 41, 7105-7112.	1.9	28
2528	Synthesis of [5]-, [6]-, and [7]Helicene via Ni(0)- or Co(I)-Catalyzed Isomerization of Aromatic cis-Dienetriynes. <i>Journal of the American Chemical Society</i> , 2002, 124, 9175-9180.	6.6	153
2529	Role of Diagonal Silicon-Carbon Interaction in the [2 + 2] Cycloaddition of Silene and Acetylene. <i>Organometallics</i> , 2002, 21, 3271-3277.	1.1	24
2530	Conformational Change of Poly(N-isopropylacrylamide) during the Coil-Globule Transition Investigated by Attenuated Total Reflection/Infrared Spectroscopy and Density Functional Theory Calculation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3429-3435.	1.1	230
2531	Ab initio electronic structure calculations for metallic intermediate band formation in photovoltaic materials. <i>Physical Review B</i> , 2002, 65, .	1.1	122
2532	First-Principles Dynamics along the Reaction Path of CH ₃ CH ₂ + O ₂ → H ₂ C=CH ₂ + HOO: A Evidence for Vibronic State Mixing and Neutral Hydrogen Transfer. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9672-9685.	1.1	8
2533	Ultrafast UV Pump/IR Probe Studies of C-H Activation in Linear, Cyclic, and Aryl Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2002, 124, 10605-10612.	6.6	56
2534	Carbene Formation in Its Lower Singlet State from Photoexcited 3H-Diazirine or Diazomethane. A Combined CASPT2 and ab Initio Direct Dynamics Trajectory Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 1728-1735.	6.6	57
2535	Functional Specificities of Methylglyoxal Synthase and Triosephosphate Isomerase: A Combined QM/MM Analysis. <i>Journal of the American Chemical Society</i> , 2002, 124, 14871-14878.	6.6	43
2536	Conformational Studies on 1,2-Di- and 1,2,3-Trisubstituted Heterocycles. A Spectroscopic and Theoretical Study of 3-Acylaminopicolinic Acid Derivatives and Their N-Oxides. <i>Journal of Organic Chemistry</i> , 2002, 67, 370-382.	1.7	6

#	ARTICLE	IF	CITATIONS
2537	Molecular Recognition in Purine-Rich Internal Loops: Thermodynamic, Structural, and Dynamic Consequences of Purine for Adenine Substitutions in 5'-(rGGCAAGCCU)2'. <i>Biochemistry</i> , 2002, 41, 14978-14987.	1.2	10
2538	Experimental Rate Measurements for NS + NO, O2 and NO2, and Electronic Structure Calculations of the Reaction Paths for NS + NO2. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8406-8410.	1.1	4
2539	Do Auophilic Interactions Compete against Hydrogen Bonds? Experimental Evidence and Rationalization Based on ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 6781-6786.	6.6	83
2540	The Transition State for Intramolecular Atom Exchange between Hydride and Dihydrogen Ligands incis-[Fe(PR3)4H(H2)]+Complexes. Trishydride or Trihydrogen?. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6189-6192.	1.1	12
2541	Exploring the Mechanism for the Synthesis of Silsesquioxanes. 3. The Effect of Substituents and Water. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11347-11353.	1.1	38
2542	The Torsional Potential of Dimethyl Peroxide: Still a Difficult Case for Theory. <i>Journal of Physical Chemistry A</i> , 2002, 106, 438-446.	1.1	27
2543	The Prediction of Protein pKa's Using QM/MM: The pKa of Lysine 55 in Turkey Ovomuroid Third Domain. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3486-3494.	1.2	90
2544	Structures and Aggregation States of Fluoromethylithium and Chloromethylithium Carbenoids in the Gas Phase and in Ethereal Solvent. <i>Journal of Organic Chemistry</i> , 2002, 67, 7607-7612.	1.7	40
2545	Field-Modulating Modes of Solvents for Describing Electrostatic Intermolecular Vibrational Interactions in Solution. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1167-1172.	1.1	8
2546	Charge-Transfer Transitions in Triarylamine Mixed-Valence Systems: A Joint Density Functional Theory and Vibronic Coupling Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 10519-10530.	6.6	106
2547	Coordination Geometries of Zn(II) and Cd(II) in Phosphotriesterase: Influence of Water Molecules in the Active Site. <i>Journal of Physical Chemistry B</i> , 2002, 106, 9446-9453.	1.2	19
2548	³ J(15N- ³¹ P) Spin-Spin Coupling Constants across N-H...O...P Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 2002, 124, 6393-6397.	6.6	32
2549	Two- and Four-Electron Alkyne Ligands in Osmium-Cyclopentadienyl Chemistry: Consequences of the π - σ Interaction. <i>Organometallics</i> , 2002, 21, 305-314.	1.1	54
2550	Mechanistic Study on the Platinum-Catalyzed Reaction between Disilacyclobutene and Acetylene. <i>Organometallics</i> , 2002, 21, 150-160.	1.1	13
2551	Trithiolatomolybdenum Nitrides, (RS)3MoN Where R = iPr and tBu, Preparation, Characterization and Comparisons with Related Trialkoxymolybdenumnitrides. <i>Inorganic Chemistry</i> , 2002, 41, 3437-3443.	1.9	11
2552	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7448-7455.	1.1	162
2553	Insights into the Metathesis Reaction Involving M ² , C ² , and M ² C Triple Bonds from Computations Employing Density Functional Theory on Model Compounds M2(OH)6 and M2(SH)6, Where M = Mo and W. <i>Journal of the American Chemical Society</i> , 2002, 124, 15351-15358.	6.6	21
2554	Computational Study of Hydrogen-Bonded Complexes between the Most Stable Tautomers of Glycine and Uracil. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7423-7433.	1.1	49

#	ARTICLE	IF	CITATIONS
2555	Cyclic Carbon Cluster Dianions and Their Aromaticity. <i>Journal of the American Chemical Society</i> , 2002, 124, 3163-3168.	6.6	12
2556	Direct Addition of Alcohols to Organonitriles Activated by Ligation to a Platinum(IV) Center. <i>Inorganic Chemistry</i> , 2002, 41, 2041-2053.	1.9	53
2557	Optimization of Conical Intersections with Floating Occupation Semiempirical Configuration Interaction Wave Functions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4679-4689.	1.1	75
2558	Chlorination Chemistry 4. Ab Initio Study of the Addition, Metathesis, and Isomerization Channels Governing the Reaction of Chlorine Atom with Propargyl Chloride. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6143-6153.	1.1	5
2559	Diverse Evolution of $[\{\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2\}\text{Pt}(\text{I}/4\text{-S})_2\text{Pt}\{\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2\}]$ ($n = 2, 3$) Metalloligands in CH_2Cl_2 . <i>Inorganic Chemistry</i> , 2002, 41, 3218-3229.	1.9	50
2560	Tetracyanometalates of Ni, Pd, and Pt with Cyclic Diquaternary Cations of 2,2'-Bipyridine and 1,10-Phenanthroline. A Vibrational, Crystallographic, and Theoretical Study of Intermolecular Weak Interactions. <i>Inorganic Chemistry</i> , 2002, 41, 4396-4404.	1.9	24
2561	Chemisorption and Reactivity of Methanol on MgO Thin Films. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11961-11969.	1.2	59
2562	An Experimental Determination of the $\text{Cr}^{\text{III}}\text{-DMB}$ (DMB = 3,3-Dimethyl-1-butene) Bond Energy in $\text{Cr}(\text{CO})_5(\text{DMB})$: A Effects of Alkyl Substitution on Chromium ^{III} -Olefin Bond Energies in $\text{Cr}(\text{CO})_5(\text{olefin})$ Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4651-4660.	1.1	3
2563	Relative Stabilities of Three Low-Energy Tautomers of Cytosine: A Coupled Cluster Electron Correlation Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1381-1390.	1.1	115
2564	A Self-Consistent Charge-Embedding Methodology for ab Initio Quantum Chemical Cluster Modeling of Ionic Solids and Surfaces: A Application to the (001) Surface of Hematite (Fe_2O_3). <i>Journal of Physical Chemistry B</i> , 2002, 106, 8136-8141.	1.2	31
2565	A polarizable mixed Hamiltonian model of electronic structure for solvated excited states. II. Application to the blue shift of the $\text{H}_2\text{CO} \rightarrow \text{S}_1(\pi^* \rightarrow n)$ excitation in water. <i>Journal of Chemical Physics</i> , 2002, 117, 1256-1268.	1.2	24
2566	Quantum mechanical modelling of alkene hydroformylation as catalyzed by xantphos-Rh complexes Based on the presentation given at Dalton Discussion No. 4, 10 th 13th January 2002, Kloster Banz, Germany.. <i>Dalton Transactions RSC</i> , 2002, , 729-742.	2.3	47
2567	Structure and Proton Reactivity of the Semiquinone Anion and Dianion of Biphenol in Water. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8908-8916.	1.1	7
2568	Low temperature matrix-isolation and solid state vibrational spectra of 5-chlorotetrazole Electronic supplementary information (ESI) available: Calculated molecular geometries, rotational constants, energies and dipole moments. Definition of internal symmetry coordinates used in the normal mode analysis. Experimental spectrum of polycrystalline 5-chlorotetrazole and calculated spectrum for the 1H-tautomer. See http://www.rsc.org/suppdata/cp/b1/b111329c/ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 1725-1731.	1.3	24
2569	An ab initio study of conformations and sigmatropic shifts in triazene and its mono-, di-, and trimethyl derivatives. <i>Canadian Journal of Chemistry</i> , 2002, 80, 447-454.	0.6	16
2570	Parametrization of a Universal Solvation Model for Molecules Containing Silicon. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5160-5168.	1.1	26
2571	A hybrid density functional theory study of the low-temperature dimethyl ether combustion pathways. I: Chain-propagation. <i>Israel Journal of Chemistry</i> , 2002, 42, 245-260.	1.0	25
2572	Structure of a Metal Ion Binding Site in β -Lactamase: A Quantum Mechanical Study of the Influence of Hydrogen-Bonding Network and Backbone Constraints. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1046-1053.	1.1	16

#	ARTICLE	IF	CITATIONS
2573	Halogen Bond in (CH ₃) _n X (X = N, P, n= 3; X = S, n= 2) and (CH ₃) _n XO (X = N, P, n= 3; X = S, n= 2) Adducts with CF ₃ I. Structural and Energy Analysis Including Relativistic Zero-Order Regular Approximation Approach in a Density Functional Theory Framework. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9114-9119.	1.1	77
2574	A Comparative Theoretical Study on DMABN: Significance of Excited State Optimized Geometries and Direct Comparison of Methodologies. <i>Journal of Physical Chemistry A</i> , 2002, 106, 804-815.	1.1	65
2575	Two functions of the density matrix and their relation to the chemical bond. <i>Journal of Chemical Physics</i> , 2002, 116, 3184-3193.	1.2	115
2576	Intramolecular hydrogen bonding in ribonucleosides: an AIM topological study of the electronic density. Electronic supplementary information (ESI) available: Integrated properties of atomic basins, radii characterizing hydrogen bond interactions, and properties at bond critical points of hydrogen bonds (Tables 3-5). See http://www.rsc.org/suppdata/cp/b2/b201339h/ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3843-3848.	1.3	28
2577	Tetrazolypentazoles: Nitrogen-Rich Compounds. <i>Inorganic Chemistry</i> , 2002, 41, 906-912.	1.9	114
2578	The H⋯H interaction in the solid state structure of HMn(CO) ₅ . <i>CrystEngComm</i> , 2002, 4, 368-372.	1.3	11
2579	Charge Model 3: A Class IV Charge Model Based on Hybrid Density Functional Theory with Variable Exchange. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10707-10717.	1.1	48
2580	A density functional theory study of phosphorescence and triplet-triplet absorption for nonlinear absorption chromophores. <i>Journal of Chemical Physics</i> , 2002, 117, 7128-7136.	1.2	67
2581	Theoretical Evidence for the Singlet Diradical Character of Square Planar Nickel Complexes Containing Two o-Semiquinonato Type Ligands. <i>Inorganic Chemistry</i> , 2002, 41, 4179-4193.	1.9	313
2582	Thermal Stability of Primary S-Nitrosothiols: Roles of Autocatalysis and Structural Effects on the Rate of Nitric Oxide Release. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8963-8970.	1.1	126
2583	Perturbative corrections to the equation-of-motion spin-flip self-consistent field model: Application to bond-breaking and equilibrium properties of diradicals. <i>Journal of Chemical Physics</i> , 2002, 116, 3194-3203.	1.2	192
2584	Electrophilic Addition of Ph ₃ PAu ⁺ to Anionic Alkoxy Fischer-Type Carbene Complexes: A Novel Approach to Metal-Stabilized Bimetallic Vinyl Ether Complexes. <i>Organometallics</i> , 2002, 21, 3173-3181.	1.1	46
2585	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H ₂ O ₂ with HF, HCl, and HBr. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6406-6414.	1.1	23
2586	Chemistry Inside Carbon Nanotubes: The Menshutkin SN ₂ Reaction. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1921-1925.	1.2	131
2587	Multiconfigurational nuclear-electronic orbital approach: Incorporation of nuclear quantum effects in electronic structure calculations. <i>Journal of Chemical Physics</i> , 2002, 117, 4106-4118.	1.2	259
2588	Model Molecular Magnets. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7456-7461.	1.1	34
2589	A Theoretical Analysis of the Proton and Hydride Transfer in Liver Alcohol Dehydrogenase (LADH). <i>Journal of Physical Chemistry B</i> , 2002, 106, 2721-2740.	1.2	151
2590	The Elusive Oxidant Species of Cytochrome P450 Enzymes: Characterization by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Calculations. <i>Journal of the American Chemical Society</i> , 2002, 124, 8142-8151.	6.6	290

#	ARTICLE	IF	CITATIONS
2591	Structures, Metal-Ligand Bond Strength, and Bonding Analysis of Ferrocene Derivatives with Group-15 Heteroligands Fe(η -5-E ₅) ₂ and FeCp(η -5-E ₅) (E = N, P, As, Sb). A Theoretical Study. <i>Organometallics</i> , 2002, 21, 3351-3359.	1.1	129
2592	Cycloaddition Reactions of Acrylonitrile on the Si(100)-2 \times 1 Surface. <i>Journal of the American Chemical Society</i> , 2002, 124, 6162-6167.	6.6	43
2593	Theoretical Study of Toluene Adsorbed on Zeolites X and Y: Calculation of ¹³ C NMR Parameters. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10944-10954.	1.2	26
2594	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. <i>Journal of Chemical Physics</i> , 2002, 116, 5363-5373.	1.2	43
2595	On the thermochemical stability of the sextet CO ₂ anion: results from density functional theory. <i>Molecular Physics</i> , 2002, 100, 3691-3697.	0.8	0
2596	Analysis of the effect of changing the α parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 722-731.	1.3	51
2597	Structure and vibrational spectra of L-hydroxyisobutyric acid in the crystalline and glassy phases and isolated in inert gas matrixes. Electronic supplementary information (ESI) available: Predicted geometries for high energy conformers of HIBA (Table S1), definition of symmetry coordinates used in the vibrational calculations (Table S2) and calculated spectra for the experimentally relevant conformers and potential energy distributions (Tables S3-S5). See http://www.rsc.org/suppdata/cp/b1/b110949a/ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 1555-1563.	1.3	10
2598	On the 6-Exo Atom Transfer Radical Cyclization Reactions of 3-Butenyl 2-Iodoalkanoates. <i>Journal of Organic Chemistry</i> , 2002, 67, 8481-8488.	1.7	21
2599	On the Electronic Structure of Bis(η -5-cyclopentadienyl) Titanium. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7921-7926.	1.1	16
2600	Computational Exploration of Rearrangements Related to the Vitamin B12-Dependent Ethanolamine Ammonia Lyase Catalyzed Transformation. <i>Journal of the American Chemical Society</i> , 2002, 124, 8974-8983.	6.6	37
2601	Theoretical study of adsorption sites and thermodynamics of thionine in zeolite NaY. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 4212-4217.	1.3	1
2602	Counter-ion effects switch ligand binding from C-2 to C-5 in kinetic carbenes formed from an imidazolium salt and IrH ₅ (PPh ₃) ₂ . <i>Chemical Communications</i> , 2002, , 2580-2581.	2.2	82
2603	New Cu(I) and Ag(I) binuclear complexes containing the dppa ligand. <i>Dalton Transactions RSC</i> , 2002, , 4365-4374.	2.3	25
2604	Exocyclic coordination of the η -3-fluorenyl, η -3-cyclopenta[def]phenanthrenyl and η -3-8,9-dihydrocyclopenta[def]phenanthrenyl anions: X-ray crystal structures, NMR fluxionality and theoretical studies. <i>New Journal of Chemistry</i> , 2002, 26, 1552-1558.	1.4	6
2605	Low barrier hydrogen bonds in sterically modified Schiff bases. <i>Perkin Transactions II RSC</i> , 2002, , 835-842.	1.1	86
2606	A solid state and theoretical study of the solvent effects controlling the mono- and di-lithiation of aromatic primary amines. <i>Dalton Transactions RSC</i> , 2002, , 2505.	2.3	12
2607	Thermal and solvent effects on ⁵⁷ Fe NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5508-5514.	1.3	50
2608	A hybrid quantum mechanical and empirical model for the prediction of isotropic ¹³ C shielding constants of organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5498-5507.	1.3	56

#	ARTICLE	IF	CITATIONS
2609	The structures of borane carbonyl compounds B ₄ X ₆ CO (X = F, Cl, Br and I) by gas-phase electron diffraction and ab initio calculations. Electronic supplementary information (ESI) available: least-squares correlation matrix for electron diffraction structure refinement for B(BF ₂) ₃ CO; tables of geometric parameters for B ₄ X ₆ CO and B ₂ X ₄ (X = F, Cl, Br and I). See http://www.rsc.org/suppdata/dt/b2/b207192d/ . Dalton Transactions RSC, 2002, , 4162-4167.	2.3	5
2610	Carbon- π hydrogen bond activation in cyclopentadienyl dimethyl tungsten nitrosyl and carbonyl complexes. Based on the presentation given at Dalton Discussion No. 4, 10 th 13th January 2002, Kloster Banz, Germany. Theoretical studies of inorganic and organometallic reaction mechanisms. Part 21.1. Dalton Transactions RSC, 2002, , 713-718.	2.3	11
2611	The self-exchange of a nonbonding electron via the outer-sphere pathway: reorganizational energy and electronic coupling matrix element for the V(OH ₂) ₆ ²⁺ / ₃ ⁺ , Ru(OH ₂) ₆ ²⁺ / ₃ ⁺ , V(OH ₂) ₆ ³⁺ / ₄ ⁺ , and Ru(OH ₂) ₆ ³⁺ / ₄ ⁺ couples. Dalton Transactions RSC, 2002, , 719.	2.3	17
2612	P=O bond cleavage; energetics and structural changes in tetramethyldiphosphine and tetrasilyldiphosphine from ab initio MO calculations. Dalton Transactions RSC, 2002, , 3135.	2.3	11
2613	H-bridged A ₃ H ₃ ⁺ (A = Si and Ge): A π -ligand in organometallic chemistry. Dalton Transactions RSC, 2002, , 1857.	2.3	2
2614	Adsorption of CS ₂ on MgO microcrystals: formation of a S-doped MgO surface. Physical Chemistry Chemical Physics, 2002, 4, 366-374.	1.3	13
2615	A study of the asymmetry of ligands in bis(trichlorosilyl)tert-butylphosphine, PBut(SiCl ₃) ₂ : molecular structure by gas-phase electron diffraction and ab initio calculations. Dalton Transactions RSC, 2002, , 3787.	2.3	6
2616	Bis(tert-butyl)sulfur diimide, S(NBut) ₂ , and tris(tert-butyl)sulfur triimide, S(NBut) ₃ : structures by gas electron diffraction, X-ray crystallography and ab initio calculations. Dalton Transactions RSC, 2002, , 4607.	2.3	15
2617	An unexpected transamination of bis[bis(trimethylsilyl)amido]zinc with dibenzylamine to form bis(dibenzylamido)zinc: structural studies by NMR spectroscopy, X-ray crystallography and theoretical calculations. Dalton Transactions RSC, 2002, , 1656-1661.	2.3	19
2618	On the electronic structure of main group diazadiene complexes, with boron, aluminium, gallium and indium, a density functional evaluation. Dalton Transactions RSC, 2002, , 405-409.	2.3	26
2619	What to do about unpaired electrons? A hydrocarbon hexaradical with three Closs diradicals linked by 1,3,5-trimethylbenzene as ferromagnetic coupler. Journal of Chemical Physics, 2002, 117, 7147-7152.	1.2	5
2620	Hydrophobic Ion Hydration and the Magnitude of the Dipole Potential. Biophysical Journal, 2002, 82, 3081-3088.	0.2	78
2621	Hybrid Density Functional Theory Studies on the Magnetic Interactions and the Weak Covalent Bonding for the Phenalenyl Radical Dimeric Pair. Journal of the American Chemical Society, 2002, 124, 11122-11130.	6.6	118
2622	Density-functional theory of linear and nonlinear time-dependent molecular properties. Journal of Chemical Physics, 2002, 117, 9630-9645.	1.2	359
2623	Theoretical Investigation of the Ground and Excited States of Coumarin 151 and Coumarin 120. Journal of Physical Chemistry A, 2002, 106, 9294-9305.	1.1	156
2624	Metal Ion Binding: An Electronic Structure Study of M+(Dimethyl Ether) _n , M = Cu, Ag, and Au and (n-) Tj ETQq1 1,0.784314 rgBT /Ove 1,1	1.1	18
2625	The Fourier transform Coulomb method: Efficient and accurate calculation of the Coulomb operator in a Gaussian basis. Journal of Chemical Physics, 2002, 117, 7827-7835.	1.2	91
2626	Energetic, Structural, and Dynamic Aspects of Ethylene Polymerization Mediated by Homogeneous Single-Site π -Constrained Geometry Catalysts in the Presence of Cocatalyst and Solvation: An Investigation at the ab Initio Quantum Chemical Level. Organometallics, 2002, 21, 5594-5612.	1.1	109

#	ARTICLE	IF	CITATIONS
2627	Comparison of ab Initio and DFT Methods for Studying Chain Propagation and Chain Termination Processes with Group 4 Polymerization Catalysts. 1. The ansa-Bis(cyclopentadienyl)zirconium Catalyst. <i>Organometallics</i> , 2002, 21, 4939-4949.	1.1	49
2628	Why Is the Nickel(II) Diphenyldiimine Complex the Best Catalyst for Polymerization of Ethylene in Three Kinds of Cationic Nickel(II) Complexes, [Ni(CH ₃)L] ⁺ (L = Diphenyldiimine, 2,2'-Bipyridine, or Tj ETQq1 1 0.7843141rgBT /Oæerlock 1	1.1	49
2629	Ab initio and density functional theory studies of peri- and regioselectivity in 1,3-dipolar cycloaddition reaction of 1,2-diazepine with nitrile oxide. <i>Computational and Theoretical Chemistry</i> , 2002, 580, 183-192.	1.5	9
2630	How accurately can we calculate molecular CH and CC re distances by DFT methods? Dependence on basis sets and functionals, estimations of experimentally inaccessible re distances and distance-dependent scaling factors for approximations of triple-zeta quality. <i>Computational and Theoretical Chemistry</i> , 2002, 578, 229-247.	1.5	16
2632	Fluxional Processes in Diamagnetic and Paramagnetic Allyl Dicarbonyl and 2-Methylallyl Dicarbonyl Molybdenum Histidinato Complexes as Revealed by Spectroscopic Data and Density Functional Calculations. <i>Chemistry - A European Journal</i> , 2002, 8, 1649-1662.	1.7	30
2633	A Four-Step Alternating Reductive Dimerization/Bond Cleavage of Indenocorannulene. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1712-1715.	7.2	44
2634	Synthesis and Photophysical Characterization of a New, Highly Hydrophilic Caging Group. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 1037-1046.	1.2	25
2635	Silylation of an OH-terminated self-assembled monolayer surface through low-energy collisions of ions: a novel route to synthesis and patterning of surfaces. <i>Journal of Mass Spectrometry</i> , 2002, 37, 591-602.	0.7	26
2636	Interpreting 2hJ(F,N), 1hJ(H,N) and 1J(F,H) in the hydrogen-bonded FH-collidine complex. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, 767-771.	1.1	54
2637	Study of gallium(III) nitrate hydrate and aqueous solutions: Raman spectroscopy and ab initio molecular orbital calculations of gallium(III) water clusters. <i>Journal of Raman Spectroscopy</i> , 2002, 33, 177-190.	1.2	29
2638	A new molecular mechanics force field for the oxidized form of blue copper proteins. <i>Journal of Computational Chemistry</i> , 2002, 23, 697-705.	1.5	79
2639	Vibrational spectra and structure of 1-phenyltetrazole and 5-chloro-1-phenyltetrazole. <i>Vibrational Spectroscopy</i> , 2002, 30, 213-225.	1.2	23
2640	Assignment of the in-plane molecular vibrations of the electron-donor molecule BDT-TTP based on polarized Raman and infrared spectra, in which BDT-TTP is 2,5-bis(1,3-dithiol-2-ylidene)-1,3,4,6-tetrathiapentalene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 1643-1656.	2.0	16
2641	Structural and vibrational study of the Ci(1) conformation of 18-crown-6. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 2877-2884.	2.0	8
2642	Gas phase nucleophilic substitution. <i>International Journal of Mass Spectrometry</i> , 2002, 214, 277-314.	0.7	211
2643	Proton affinities of methyl esters of N-acetylated amino acids. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 101-114.	0.7	29
2644	Silicon- versus carbon-containing ions: 1,3-CH ₃ ⁺ transfers. <i>International Journal of Mass Spectrometry</i> , 2002, 217, 245-255.	0.7	3
2645	Silicon vs. carbon containing ions: 1,3-proton transfers within the (CH ₃)(X)Si(OR)(+OHR ⁺) units. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 537-547.	0.7	6

#	ARTICLE	IF	CITATIONS
2646	Tetrasulfur tetranitride and its selenium analogs: ab initio and DFT calculations. Computational and Theoretical Chemistry, 2002, 582, 85-90.	1.5	9
2647	Conformation and parity-violating energy of hydrated d-glyceraldehyde in aqueous solution. Computational and Theoretical Chemistry, 2002, 586, 1-7.	1.5	4
2648	Peptide models XXXIV. Side-chain conformational potential energy surfaces associated with all major backbone folds of neutral tautomers of N- and C-protected l-histidine. An ab initio study on ethylimidazole and N-formyl-l-histidinamide. Computational and Theoretical Chemistry, 2002, 583, 117-135.	1.5	11
2649	Peptide models XXXV. Protonated and deprotonated N-Formyl-l-histidinamide: an ab initio study on side-chain potential energy surfaces of all major backbone conformers. Computational and Theoretical Chemistry, 2002, 583, 199-213.	1.5	9
2650	Parity-violating energy for the chirality-producing step in Strecker synthesis of l-alanine. Computational and Theoretical Chemistry, 2002, 584, 89-94.	1.5	5
2651	Reliability of ab initio (HF, post HF and DFT) methods and basis set dependencies for accurate prediction of equilibrium r e distances of CO bond lengths. Computational and Theoretical Chemistry, 2002, 585, 35-47.	1.5	11
2652	A theoretical study of the catalytic properties of Pt/Fe nanoclusters. Computational and Theoretical Chemistry, 2002, 586, 17-27.	1.5	19
2653	Part II. Ionization energies, hardness, softness, and absolute electronegativity of heteronuclear and homonuclear diatomic molecules by the CBS-QB3 and G3B3 methods. Computational and Theoretical Chemistry, 2002, 585, 205-208.	1.5	10
2654	Density functional theory characterization of the structure and gas-phase, mid-infrared absorption spectrum of 2-azido-N,N-dimethylethanamine (DMAZ). Computational and Theoretical Chemistry, 2002, 587, 199-218.	1.5	20
2655	Ab initio spin-orbit coupling SCF calculation of parity-violating energy of chiral molecules. Computational and Theoretical Chemistry, 2002, 589-590, 183-193.	1.5	16
2656	Density functional theory calculation of hyperfine coupling constants of small radicals using Becke97-type exchange-correlation functionals. Computational and Theoretical Chemistry, 2002, 617, 47-52.	1.5	7
2657	Synthesis, X-ray crystal structure and solution behaviour of $[Zn\{\{\text{I-5-C5H5}\}\text{Fe}\{\{\text{I-5-C5H4}\}\text{I-CH}_2\text{...Nf-(CH}_2\text{)}_3\text{I-NMe}_2\}\}\text{Cl}_2]$. Polyhedron, 2002, 21, 2361-2367.	1.0	4
2658	Classifications of families of homologous organic compounds based on energy by means of ab initio HF, MP2 and DFT optimizations. Journal of Physical Organic Chemistry, 2002, 15, 677-688.	0.9	14
2659	Coupled-perturbed Hartree-Fock treatment of infinite periodic systems: Application to static polarizabilities and hyperpolarizabilities of polydiacetylene, polybutatriene, and interacting pairs of polyacetylene chains. International Journal of Quantum Chemistry, 2002, 90, 709-718.	1.0	25
2660	Interplay of intra- and intermolecular H-bonds for the addition of a water molecule to the neutral and N-protonated forms of noradrenaline. International Journal of Quantum Chemistry, 2002, 90, 641-656.	1.0	38
2661	5-fluorouracil dimers in aqueous solution: molecular dynamics in water and continuum solvation. International Journal of Quantum Chemistry, 2002, 88, 133-146.	1.0	17
2662	Ab initio calculation of the Young's modulus of β -polyamides. International Journal of Quantum Chemistry, 2002, 87, 303-310.	1.0	8
2663	Investigation of the frequency-dispersion effects on the Raman spectra of small polyenes. International Journal of Quantum Chemistry, 2002, 89, 341-348.	1.0	14

#	ARTICLE	IF	CITATIONS
2664	Theoretical studies on heats of formation for cubyl nitrates using density functional theory B3LYP method and semiempirical MO methods. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 305-312.	1.0	26
2665	An analysis of the topology of the electron charge density and the reactant-product electronic structure variation along the intrinsic reaction coordinate. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 151-166.	1.0	1
2666	Method/basis set dependence of the traceless quadrupole moment calculation for N ₂ , CO ₂ , SO ₂ , HCl, CO, NH ₃ , PH ₃ , HF, and H ₂ O. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 199-217.	1.0	19
2667	Equilibrium structures of isolated (halogenated) fluorolithiomethanes. <i>Journal of Fluorine Chemistry</i> , 2002, 113, 147-154.	0.9	13
2668	Etude DFT du mécanisme des réactions de cycloaddition dipolaire-1,3 de la C,N-diphénylnitrone avec des dipolarophiles fluorés de type éthylénique et acétylénique. <i>Journal of Fluorine Chemistry</i> , 2002, 114, 81-89.	0.9	14
2669	The NMR shifts are not a measure for the nakedness of the fluoride anion. <i>Journal of Fluorine Chemistry</i> , 2002, 116, 49-58.	0.9	57
2670	Computational analysis of side-chain conformations in polyaspartates exhibiting reversible helical sense inversion in the solid state. <i>Journal of Molecular Structure</i> , 2002, 610, 197-205.	1.8	2
2671	Hydrogen bonding. Part 80. Molecular orbital evaluation of C-H hydrogen bonding in tetramethylammonium tetrahydroborate. <i>Journal of Molecular Structure</i> , 2002, 616, 181-186.	1.8	0
2672	On the mechanism of olefin polymerisation with titanium η^2 -diketonato complexes. A model density functional study. <i>Journal of Organometallic Chemistry</i> , 2002, 648, 126-133.	0.8	3
2673	Density functional study on the adsorption and surface reactions on SiO ₂ in TiN-CVD using TiCl ₄ and NH ₃ . <i>Thin Solid Films</i> , 2002, 409, 51-57.	0.8	13
2674	Ab initio infra-red spectra of iron-polycyclic aromatic hydrocarbon compounds: a model case. <i>Planetary and Space Science</i> , 2002, 50, 871-876.	0.9	8
2675	On the evaluation of thermal corrections to gas phase ab initio relative energies: implications to the conformational analysis study of cyclooctane. <i>Chemical Physics</i> , 2002, 280, 31-42.	0.9	35
2676	Efficient computer implementation of the renormalized coupled-cluster methods: The R-CCSD[T], R-CCSD(T), CR-CCSD[T], and CR-CCSD(T) approaches. <i>Computer Physics Communications</i> , 2002, 149, 71-96.	3.0	443
2677	Impact of conformation on the dipole moment of bis-triarylamine derivatives. <i>Chemical Physics Letters</i> , 2002, 354, 283-290.	1.2	33
2678	Time-dependent density functional theory simulation of UV/visible absorption spectra of zirconocene catalysts. <i>Chemical Physics Letters</i> , 2002, 354, 449-457.	1.2	62
2679	The N-H...O...C proton transfer in aqueous solution: a suitable procedure for extracting atomic charges. <i>Chemical Physics Letters</i> , 2002, 357, 279-286.	1.2	15
2680	Effective exchange integrals and chemical indices for a phenalenyl radical dimeric pair. <i>Chemical Physics Letters</i> , 2002, 358, 17-23.	1.2	31
2681	Theoretical study of C ₂₀ fullerene dimerization: a facile [2+2] cycloaddition. <i>Chemical Physics Letters</i> , 2002, 359, 446-452.	1.2	22

#	ARTICLE	IF	CITATIONS
2682	1,3,5-Cyclohexatriene captured in computro; the importance of resonance. Chemical Physics Letters, 2002, 361, 203-208.	1.2	24
2683	A stable unconventional structure of Sc ₂ @C ₆₆ found by density functional calculations. Chemical Physics Letters, 2002, 362, 373-379.	1.2	67
2684	An excess electron binding to the 'purple' zwitterion quinonoid. Chemical Physics Letters, 2002, 362, 527-533.	1.2	24
2685	Energetics for the reaction of CBr ₂ O with water. Chemical Physics Letters, 2002, 363, 275-282.	1.2	5
2686	Is density functional theory free of spatial symmetry breaking? The case of the linear carbon radical cations: C ₃ ⁺ , C ₅ ⁺ , C ₇ ⁺ , and C ₉ ⁺ . Chemical Physics Letters, 2002, 363, 486-491.	1.2	18
2687	A quadratic configuration interaction study of the proton affinity of acetic acid. Chemical Physics Letters, 2002, 364, 427-431.	1.2	7
2688	Kinetics of Reductive N=O Bond Fragmentation: The Role of a Conical Intersection. Journal of the American Chemical Society, 2002, 124, 15225-15238.	6.6	83
2689	Title is missing!. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2002, 28, 191-200.	0.3	7
2690	Title is missing!. Journal of Cluster Science, 2002, 13, 165-187.	1.7	10
2691	¹³ C- ¹³ C Spin-Spin Coupling Constants in Structural Studies: XXXIV. Nonempirical Calculations: Small Heterocycles. Russian Journal of Organic Chemistry, 2003, 39, 1618-1628.	0.3	4
2692	Quantum Mechanical Study of the Syn and Anti Conformations of Solvated Cyclic GMP. Structural Chemistry, 2003, 14, 527-533.	1.0	6
2693	Ab Initio Study of Cis-Trans Photoisomerization in Stilbene and Ethylene. Journal of Physical Chemistry A, 2003, 107, 829-837.	1.1	251
2694	Accuracy assessment of semiempirical molecular electrostatic potential of proteins. Theoretical Chemistry Accounts, 2003, 109, 213-219.	0.5	4
2695	Ion-specific swelling behavior of uncharged poly(acrylic acid) gel. Colloid and Polymer Science, 2003, 282, 149-155.	1.0	25
2696	AM1* parameters for phosphorus, sulfur and chlorine. Journal of Molecular Modeling, 2003, 9, 408-414.	0.8	74
2697	Modeling zinc in biomolecules with the self consistent charge-density functional tight binding (SCC-DFTB) method: Applications to structural and energetic analysis. Journal of Computational Chemistry, 2003, 24, 565-581.	1.5	150
2698	A flexible nudged elastic band program for optimization of minimum energy pathways using ab initio electronic structure methods. Journal of Computational Chemistry, 2003, 24, 990-996.	1.5	34
2699	Parameterization of charge model 3 for AM1, PM3, BLYP, and B3LYP. Journal of Computational Chemistry, 2003, 24, 1291-1304.	1.5	107

#	ARTICLE	IF	CITATIONS
2700	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-Cl study. <i>Journal of Computational Chemistry</i> , 2003, 24, 1421-1431.	1.5	83
2701	Ab initio quality properties for macromolecules using the ADMA approach. <i>Journal of Computational Chemistry</i> , 2003, 24, 1980-1986.	1.5	105
2702	A Solid-State, Solution, and Theoretical Structural Study of Kinetic and Thermodynamic Lithiated Derivatives of a Simple Diazomethane and Their Reactivities Towards Aryl Isothiocyanates. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 3363-3375.	1.0	18
2703	Sodium-1,2-Diphosphonate Carbanions: Characterization of the Tetrameric Cubane and the Hexameric Ladder Complexes $[(iPrO)_2P(O)]_2CHNa_4$ and $[(EtO)_2P(O)]_2CHNa_6$. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 3325-3331.	1.0	8
2704	Synthesis, Structure and Theoretical Studies of the Hydrido Inverse Crown $[K_2Mg_2(NiPr_2)_4(\frac{1}{4}H)_2(\text{toluene})_2]$: a Rare Example of a Molecular Magnesium Hydride with a $Mg-(\frac{1}{4}H)-Mg$ Double Bridge. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 3354-3362.	1.0	71
2705	Reactions of cis-2,3-Dimethylaziridine, 3-Pyrroline and Pyrrolidine with Me_3Al and Me_3Ga : Adducts and Dimeric Amides. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 656-665.	1.0	12
2706	Reactions of a Stable (Phosphanyl)(silyl)carbene with Aliphatic Aldehydes: [2+1] versus [2+2] Addition to a Carbonyl Group. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 3147-3152.	1.2	24
2707	Diradical versus Concerted Mechanisms for the Dihydroxylation of Protoanemonin by OsO_4 and NH_3 - The Effect of the Base in the Reaction. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 833-839.	1.2	8
2708	Experimental Assessment of the Effect of a Bicyclo[1.1.0]butane System in Strain-Induced Localisation of Aromatic π -Bonds. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 901-906.	1.2	7
2709	On the Electronic Structures of the 1,3-Diboracyclobutane-1,3-diyls and Their Valence Isomers with a B ₂ E ₂ Skeleton (E=N, P, As). <i>Chemistry - A European Journal</i> , 2003, 9, 3611-3617.	1.7	53
2710	The 11^{th} Dioxygen Ene Reaction with Propene: A Density Functional and Multireference Perturbation Theory Mechanistic Study. <i>Chemistry - A European Journal</i> , 2003, 9, 2616-2626.	1.7	21
2711	The Evolution of $[Ph_2P(CH_2)_nPPh_2]Pt(\frac{1}{4}S)_2Pt\{Ph_2P(CH_2)_nPPh_2\}$ (n=2, 3) Metalloligands in Protic Acids: A Cascade of Sequential Reactions. <i>Chemistry - A European Journal</i> , 2003, 9, 5023-5035.	1.7	38
2712	Theoretical Investigation of the Photochemical C ₂ -C ₆ Cyclisation of Enyne-Heteroallenes. <i>Chemistry - A European Journal</i> , 2003, 9, 4670-4677.	1.7	11
2713	Carâ€Parrinello Molecular Dynamics Study of the Rearrangement of the Valeramide Radical Cation. <i>Chemistry - A European Journal</i> , 2003, 9, 4396-4404.	1.7	8
2714	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. <i>Chemistry - A European Journal</i> , 2003, 9, 1113-1122.	1.7	125
2715	Synthesis, Biological Activity, and Docking Studies of New Acetylcholinesterase Inhibitors of the Bispyridinium Type. <i>Archiv Der Pharmazie</i> , 2003, 336, 523-540.	2.1	37
2716	Numerical simulations of Raman spectra of guanine-cytosine Watson-Crick and protonated Hoogsteen base pairs. <i>Biopolymers</i> , 2003, 72, 339-344.	1.2	15
2717	Electron pairing analysis of the Fischer-type chromium carbene complexes $(CO)_5Cr^{\eta^6}C(X)R$ (X=H, OH). <i>Journal of Organometallic Chemistry</i> , 2003, 678, 1-14.	0.9	18

#	ARTICLE	IF	CITATIONS
2718	Theoretical study of stability of graphite intercalation compounds with Brønsted acids. <i>Carbon</i> , 2003, 41, 2757-2760.	5.4	17
2719	On the structure and torsional potential of trifluoromethoxybenzene: an ab initio and density functional study. <i>Chemical Physics Letters</i> , 2003, 367, 566-575.	1.2	41
2720	A time-dependent density-functional theory investigation of the fluorescence behavior of related cyano and di-cyano isomers of 4-(N,N-dimethylamino) benzonitrile. <i>Chemical Physics Letters</i> , 2003, 368, 561-567.	1.2	15
2721	Improved coupled perturbed Hartree-Fock and Kohn-Sham convergence acceleration. <i>Chemical Physics Letters</i> , 2003, 370, 99-105.	1.2	8
2722	Evidence of ultra-fast dissociation in ammonia observed by resonant Auger electron spectroscopy. <i>Chemical Physics Letters</i> , 2003, 370, 781-788.	1.2	33
2723	Relativistically corrected geometries obtained with analytical gradients: normalized elimination of the small component using an effective potential. <i>Chemical Physics Letters</i> , 2003, 370, 647-653.	1.2	17
2724	Magnetic response of dithiin molecules: is there anti-aromaticity in nature?. <i>Chemical Physics Letters</i> , 2003, 375, 583-590.	1.2	27
2725	A theoretical study of spin density distributions and isotropic hyperfine couplings of N and P atoms in N@C60, P@C60, N@C70, N@C60(CH2)6, and N@C60(SiH2)6. <i>Chemical Physics Letters</i> , 2003, 377, 93-98.	1.2	27
2726	A theoretical study of structure and stability of various Ge ₂ H _m ^{m+} (m=0-5) ions. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 1-7.	1.5	6
2727	Theoretical study of the relative stability of isomeric forms of platinum carboxamide complexes. <i>Inorganica Chimica Acta</i> , 2003, 350, 245-251.	1.2	3
2728	Structural preferences of 20-electron bisindenyl complexes of Group 6 metals: a DFT study. <i>Inorganica Chimica Acta</i> , 2003, 350, 547-556.	1.2	7
2729	1,3-Dipolar cycloaddition of nitrile oxides to free and Pt-bound nitriles: a theoretical study of the activation effect, reactivity and mechanism. <i>Inorganica Chimica Acta</i> , 2003, 356, 85-94.	1.2	36
2730	Te ⁺ -Te interactions in inorganic rings with sulfur donors. <i>Inorganica Chimica Acta</i> , 2003, 356, 319-327.	1.2	8
2731	Synthesis and characterization of [W(NC4Me4)2Cl2] and [W(NC4Me4)2(CH3)2], the first azametallocene tungsten complexes with pyrrolyl ligands. Electronic structure and bonding of tungsten bispyrrolyl complexes. <i>Inorganica Chimica Acta</i> , 2003, 356, 249-258.	1.2	12
2732	Theoretical prediction of spectroscopic constants of 1-alkoxy radicals. <i>Journal of Molecular Spectroscopy</i> , 2003, 220, 276-290.	0.4	34
2733	Structure and hydrogen bonding in ortho-hydroxy Ketimines. <i>Journal of Molecular Structure</i> , 2003, 644, 187-195.	1.8	37
2734	A theoretical study of the structure and vibrations of 2,4,6-trinitrotoluene. <i>Journal of Molecular Structure</i> , 2003, 648, 203-214.	1.8	107
2735	A DFT analysis of the vibrational spectra of nitrobenzene. <i>Journal of Molecular Structure</i> , 2003, 655, 413-422.	1.8	112

#	ARTICLE	IF	CITATIONS
2736	Theoretical determination of $\hat{\Gamma}$ in 18+ $\hat{\Gamma}$ organometallic complexes. <i>Journal of Organometallic Chemistry</i> , 2003, 677, 96-100.	0.8	4
2737	Mechanism of copper(I)-catalyzed cyclopropanation: a DFT study calibrated with copper(I) alkene complexes. <i>Journal of Organometallic Chemistry</i> , 2003, 684, 124-143.	0.8	62
2738	Ab initio gas-phase bond energies of CNH _x isomers and the reactivity and stability of aminomethylidyne (CNH ₂) on metal surfaces: UBI-QEP analysis. <i>Surface Science</i> , 2003, 524, 15-28.	0.8	5
2739	Theoretical study of the chemisorption of CO on bimetallic RhCu surfaces and nanoparticles. <i>Surface Science</i> , 2003, 531, 39-52.	0.8	25
2740	Reactivity of (H ⁺)(e ⁻) color centers at the MgO surface: formation of O ₂ ⁻ and N ₂ ⁻ radical anions. <i>Surface Science</i> , 2003, 542, 293-306.	0.8	30
2741	A DFT study of the magnetic properties and the iron-iron interaction in the Cp ₂ Fe ₂ ($\hat{\Gamma}$ _{1/4} $\hat{\Gamma}$ ₁ $\hat{\Gamma}$ _{1/4} $\hat{\Gamma}$ ₂) and Cp ₂ Fe ₂ ($\hat{\Gamma}$ _{1/4} $\hat{\Gamma}$ ₂ $\hat{\Gamma}$ ₁) $\hat{\Gamma}$ ₂ isomers of the Cp ₂ Fe ₂ S ₄ complex. <i>Computational and Theoretical Chemistry</i> , 2003, 1.5 621, 113-118.		2
2742	A theoretical study of tautomerism in hexa-aza macrocycles containing 2,2'-bipyridine and 1,10-phenanthroline and their ability to form lithium complexes. <i>Computational and Theoretical Chemistry</i> , 2003, 620, 49-63.	1.5	6
2743	Ion effects on hydrogen-bonding hydration of polymer an approach by $\hat{\Gamma}$ -induced force model $\hat{\Gamma}$ TM . <i>Computational and Theoretical Chemistry</i> , 2003, 620, 65-76.	1.5	18
2744	Ab initio and DFT studies on the mechanism of the 1,3-dipolar cycloaddition reaction between nitrene and sulfonylene chloride. <i>Computational and Theoretical Chemistry</i> , 2003, 620, 271-281.	1.5	15
2745	Thermal reactions of 3-Furyl Fulgide and 3-Thienyl Fulgide. Ab initio molecular orbital and CASSCF studies. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 167-178.	1.5	10
2746	A density functional study on the Pt(0)-catalysed hydrosilylation of ethylene. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 277-288.	1.5	11
2747	DFT study of metal-tetrahydroborato ligand interactions in [Ti(CO) ₄ (BH ₄)] ⁻ . <i>Computational and Theoretical Chemistry</i> , 2003, 625, 305-314.	1.5	7
2748	DFT and CASPT2 study of two thermal reactions of nitromethane: C-N bond cleavage and nitro-to-nitrite isomerization. An example of the inverse symmetry breaking deficiency in density functional calculations of an homolytic dissociation. <i>Computational and Theoretical Chemistry</i> , 2003, 630, 17-23.	1.5	32
2749	An ab initio/hybrid (ONIOM) investigation of biliverdin isomers and metal-biliverdin analogue complexes. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 21-33.	1.5	12
2750	The ring closure of ethylene phosphites is a new P(III)-insertion reaction. A computational study. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 35-48.	1.5	1
2751	Electronic against steric effects in distorted amides. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 131-144.	1.5	22
2752	Potentials of mean force with ab initio mixed Hamiltonian models of solvation. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 173-183.	1.5	10
2753	An averaged solvent electrostatic potential/molecular dynamics study of the influence of the electron correlation on the properties of liquid hydrogen fluoride. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 227-234.	1.5	3

#	ARTICLE	IF	CITATIONS
2754	Conformation of protonated trans-N-benzylideneaniline: a revisit. Computational and Theoretical Chemistry, 2003, 634, 311-314.	1.5	7
2755	Regioselectivity in the interaction of rhodium hydridotricarbonyl with propene: a theoretical study. Computational and Theoretical Chemistry, 2003, 634, 95-106.	1.5	8
2756	A computational study of the formation of a boron-oxygen-carbon linkage. The reaction of monohydroxy borane with methanol. Computational and Theoretical Chemistry, 2003, 638, 107-117.	1.5	12
2757	An investigation into the relative influence of alkoxide and thiolate ligands on the metal-carbon triple bond in $X_3M\uparrow CH$ compounds, where $M=Cr, Mo$ and W and $X=OH, SH, OCH_3, SCH_3, OCF_3$ and SCF_3 from electronic structure calculations. Polyhedron, 2003, 22, 145-152.	1.0	3
2758	Thermodynamic and dielectric properties of aqueous solutions using ESIE charges to describe small solutes. Chemical Physics, 2003, 293, 193-202.	0.9	11
2759	Progress on the two-dimensional filter diagonalization method. An efficient doubling scheme for two-dimensional constant-time NMR. Journal of Magnetic Resonance, 2003, 162, 74-89.	1.2	39
2760	Electrostatic interaction of \uparrow -Acidic amides with hydrogen-Bond acceptors. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3261-3266.	1.0	20
2761	Pharmacophoric features of nucleosidic HIV-1RT inhibitors. Bioorganic and Medicinal Chemistry, 2003, 11, 1801-1807.	1.4	4
2762	Synthesis, molecular modeling and biological evaluation of aza-proline and aza-pipecolic derivatives as FKBP12 ligands and their in vivo neuroprotective effects. Bioorganic and Medicinal Chemistry, 2003, 11, 4815-4825.	1.4	24
2763	Structure and vibrational frequencies of 2-butanimine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2593-2601.	2.0	1
2764	Response calculations of electronic and vibrational transitions in molecular oxygen induced by interaction with noble gases. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 3387-3410.	2.0	29
2765	Active copper species in 1-butene skeletal isomerization: comparison between copper-modified MCM-41 and beta catalysts. Microporous and Mesoporous Materials, 2003, 60, 159-171.	2.2	35
2766	Density functional theory study on the structure of bis(1,1-diethyl-3-benzoyl-thioureato) copper(II). Planar or distorted tetrahedral CuS_2O_2 conformation?. Inorganic Chemistry Communication, 2003, 6, 149-153.	1.8	12
2767	Solvent effects in enantioselective hydrogenation of 1-phenyl-1,2-propanedione. Journal of Molecular Catalysis A, 2003, 192, 135-151.	4.8	64
2768	Bonding of NO on $NixMg_{1-x}O$ powders: an EPR and computational study. Journal of Molecular Catalysis A, 2003, 204-205, 779-786.	4.8	16
2769	Two derivatives of 5-aminotetrazole: 5-amino-1-phenyltetrazole and 5-amino-1-(1-naphthyl)tetrazole. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o690-o693.	0.4	16
2770	Computational analysis of 1-methoxybicyclo[3.2.0]hepta-3,6-dien-2-one and its enantiomeric separation. Journal of Physical Organic Chemistry, 2003, 16, 114-120.	0.9	0
2771	Competing nature of intramolecular $[4+2]$ and $[3+2]$ cycloaddition reactions: a theoretical study. Journal of Physical Organic Chemistry, 2003, 16, 253-263.	0.9	10

#	ARTICLE	IF	CITATIONS
2772	An experimental and theoretical study of the preferred hydrogen bonding site of methyl isothiocyanate. <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 608-614.	0.9	6
2773	Artemisinin Derivatives with Antimalarial Activity against <i>Plasmodium falciparum</i> Designed with the Aid of Quantum Chemical and Partial Least Squares Methods. <i>QSAR and Combinatorial Science</i> , 2003, 22, 830-842.	1.5	27
2774	Ab initio investigation of the Young's modulus of polyamide-6. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 32-38.	1.0	8
2775	Valence bond descriptions of benzene and cyclobutadiene and their counterparts with localized bonds. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 566-574.	1.0	21
2776	Global optimization of SixHy at the ab initio level via an iteratively parametrized semiempirical method. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 617-626.	1.0	12
2777	Title is missing!. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2003, 629, 803-815.	0.6	8
2778	Fast hydrogen elimination from the [Ru(PH ₃) ₃ (CO)(H) ₂] complex in the first singlet excited states. A quantum dynamics study. <i>Chemical Physics</i> , 2003, 286, 149-163.	0.9	2
2779	Proton transfer and self-association of sterically modified Schiff bases. <i>Chemical Physics</i> , 2003, 287, 113-124.	0.9	56
2780	Synthesis and testing of novel classical cannabinoids: exploring the side chain ligand binding pocket of the CB1 and CB2 receptors. <i>Bioorganic and Medicinal Chemistry</i> , 2003, 11, 3121-3132.	1.4	33
2781	Coherent Three-Pulse Spectroscopy of Coupled Vibrations in a Rigid Dipeptide: A Density Functional Theory Simulations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5967-5985.	1.2	22
2782	Molecular Structures, Bond Energies, and Bonding Analysis of Group 11 Cyanides TM(CN) and Isocyanides TM(NC) (TM = Cu, Ag, Au). <i>Inorganic Chemistry</i> , 2003, 42, 4977-4984.	1.9	70
2783	Predicting aqueous solubilities from aqueous free energies of solvation and experimental or calculated vapor pressures of pure substances. <i>Journal of Chemical Physics</i> , 2003, 119, 1661-1670.	1.2	97
2784	Full configuration interaction potential energy curves for breaking bonds to hydrogen: An assessment of single-reference correlation methods. <i>Journal of Chemical Physics</i> , 2003, 118, 1610-1619.	1.2	115
2785	Solvated Succinate Dianion: Structures, Electron Binding Energies, and Dyson Orbitals. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10360-10369.	1.1	13
2786	A Silsesquioxane-Based Diphosphinite Ligand: Synthesis, DFT Study, and Coordination Chemistry. <i>Organometallics</i> , 2003, 22, 5297-5306.	1.1	17
2787	Energy Partitioning Analysis of the Bonding in L ₂ TM(C ₂ H ₂) and L ₂ TM(C ₂ H ₄) (TM = Ni, Pd, Pt; L ₂ = (PH ₃) ₂). <i>J. Phys. Chem. B</i> , 2003, 107, 10360-10369.	1.1	11
2788	Observation and Interpretation of Annulated Porphyrins: Studies on the Photophysical Properties of meso-Tetraphenylmetalporphyrins. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11331-11339.	1.1	160
2789	Mechanism of Ethene Trimerization at anansa-(Arene)(cyclopentadienyl) Titanium Fragment. <i>Organometallics</i> , 2003, 22, 2564-2570.	1.1	124

#	ARTICLE	IF	CITATIONS
2790	Pi Bonding and Negative Hyperconjugation in Mono-, Di-, and Triaminoborane, -alane, -gallane, and -indane. <i>Inorganic Chemistry</i> , 2003, 42, 6691-6700.	1.9	22
2791	Origins of Opposite Absolute Stereoselectivities in Proline-Catalyzed Direct Mannich and Aldol Reactions. <i>Organic Letters</i> , 2003, 5, 1249-1251.	2.4	154
2792	An improved 6-31G* basis set for first-row transition metals. <i>Journal of Chemical Physics</i> , 2003, 118, 7775-7782.	1.2	151
2793	Mechanism for the Cyclotrimerization of Alkynes and Related Reactions Catalyzed by CpRuCl. <i>Journal of the American Chemical Society</i> , 2003, 125, 11721-11729.	6.6	168
2794	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1384-1388.	1.1	688
2795	The role of the basis set: Assessing density functional theory. <i>Journal of Chemical Physics</i> , 2003, 119, 3005-3014.	1.2	181
2796	Lactam Hydrolysis Catalyzed by Mononuclear Metallo- β -lactamases: A Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2366-2375.	1.2	29
2797	Some structural and electronic properties of MX ₃ (M = Ln, Sc, Y, Ti ⁺ , Zr ⁺ , Hf ⁺ ; X = H, Me, Hal, NH ₂) from DFT calculations. <i>Faraday Discussions</i> , 2003, 124, 25-39.	1.6	59
2798	Electronic properties of para-substituted thiophenols and disulfides from ¹³ C NMR spectroscopy and ab initio calculations: relations to the Hammett parameters and atomic charges. Electronic supplementary information (ESI) available: all characterization data are tabulated in Table S1. A figure showing the dependence of the natural charge of the C1 atom of the disulfides on the ¹³ C NMR chemical shift is also provided. See http://www.rsc.org/suppdata/nj/b3/b300048f/ . <i>New Journal of Chemistry</i> , 2003, 27, 1115.	1.4	37
2799	Calculation of Physical and Chemical Data. , 0, , 319-400.		0
2800	Ab Initio Study of the Catalytic Reactivity of Titanosilsesquioxanes and Titanosiloxanes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8756-8762.	1.1	14
2801	DFT Analysis of NMR Scalar Interactions Across the Glycosidic Bond in DNA. <i>Journal of the American Chemical Society</i> , 2003, 125, 3649-3658.	6.6	35
2802	A Novel Facet of Carbonyliron-Diene Photochemistry: The β -4-s-transomer of the Classical Fe(CO) ₃ (β -4-s-cis-1,3-butadiene) Discovered by Time-Resolved IR Spectroscopy and Theoretically Examined by Density Functional Methods. <i>Organometallics</i> , 2003, 22, 1696-1711.	1.1	26
2803	Properties of the phosphorus oxide radical, PO, its cation and anion in their ground electronic states: comparison of theoretical and experimental data. <i>International Reviews in Physical Chemistry</i> , 2003, 22, 641-675.	0.9	22
2804	Characterization of Hydrogen Bonds in the Interactions between the Hydroperoxyl Radical and Organic Acids. <i>Journal of the American Chemical Society</i> , 2003, 125, 15614-15622.	6.6	32
2805	Anion electric field is related to hydration energy. <i>Journal of Chemical Physics</i> , 2003, 118, 9937-9942.	1.2	34
2806	Ortho-CH Activation of Aromatic Ketones, Partially Fluorinated Aromatic Ketones, and Aromatic Imines by a Trihydride-Stannyl-Osmium(IV) Complex. <i>Organometallics</i> , 2003, 22, 3753-3765.	1.1	52
2807	Effect of Substituents on the Thermal Decomposition of Diazirines: Experimental and Computational Studies. <i>Journal of Organic Chemistry</i> , 2003, 68, 7471-7478.	1.7	32

#	ARTICLE	IF	CITATIONS
2808	Two-Bond ^{15}N - ^{19}F Spin-Spin Coupling Constants ($2h_{\text{JN-F}}$) across $\text{N-H}\cdots\text{F}$ Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3126-3131.	1.1	23
2809	Rational classification of a series of aromatic donor-acceptor systems within the twisting intramolecular charge transfer model, a time-dependent density-functional theory investigation. <i>Journal of Chemical Physics</i> , 2003, 119, 12852-12865.	1.2	32
2810	Internal Degrees of Freedom, Structural Motifs, and Conformational Energetics of the $5'$ -Deoxyadenosyl Radical: Implications for Function in Adenosylcobalamin-Dependent Enzymes. A Computational Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 570-579.	6.6	26
2811	Molecular Orbital Interactions in the Nanostar Dendrimer. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14204-14210.	1.2	34
2812	Two-Bond ^{19}F - ^{15}N Spin-Spin Coupling Constants ($2h_{\text{JF-N}}$) across $\text{F-H}\cdots\text{N}$ Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3121-3125.	1.1	42
2813	1,3-Dipolar Cycloaddition of Nitrones to Free and Pt-Bound Nitriles. A Theoretical Study of the Activation Effect, Reactivity, and Mechanism. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6108-6120.	1.1	56
2814	Structural Changes, P-P Bond Energies, and Homolytic Dissociation Enthalpies of Substituted Diphosphines from Quantum Mechanical Calculations. <i>Inorganic Chemistry</i> , 2003, 42, 7129-7136.	1.9	14
2815	Preparation and Characterization of Osmium-Stannyl Polyhydrides: d^4d^2 Oxidative Addition of Neutral Molecules in a Late Transition Metal. <i>Organometallics</i> , 2003, 22, 2087-2096.	1.1	46
2816	Collision-Induced Dissociation and Theoretical Studies of $\text{Ag}^+(\text{methanol})_n$, $n = 1-4$. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2829-2838.	1.1	18
2817	Theoretical Thermochemistry: Ab Initio Heat of Formation for Hydroxylamine. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1077-1081.	1.1	26
2818	Excess Electron Attachment Induces Barrier-Free Proton Transfer in Binary Complexes of Uracil with H_2Se and H_2S but Not with H_2O . <i>Journal of Physical Chemistry B</i> , 2003, 107, 7889-7895.	1.2	53
2819	Theoretical Study of the Reactivity of (η -Allyl)molybdenum Complexes. <i>Organometallics</i> , 2003, 22, 3649-3658.	1.1	14
2820	Direct Dynamics Study on the Hydrogen Abstraction Reaction $\text{N}_2\text{H}_4 + \text{H} \rightarrow \text{N}_2\text{H}_3 + \text{H}_2$. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6055-6061.	1.1	14
2821	Dynamics of an Excess Electron at Metal/Polar Interfaces. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13608-13615.	1.2	6
2822	Ab Initio Study of the Thermal Isomerization of Tricyclo[3.1.0.0 ^{2,6}]hexane to (Z,Z)-1,3-Cyclohexadiene through the (E,Z)-1,3-Cyclohexadiene Intermediate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 198-203.	1.1	14
2823	Proton-Coupled Electron Transfer in a Model for Tyrosine Oxidation in Photosystem II. <i>Journal of the American Chemical Society</i> , 2003, 125, 10429-10436.	6.6	100
2824	Theoretical Study of the Initial Decomposition Process of the Energetic Material Urea Nitrate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6444-6450.	1.1	11
2825	Electronic and Vibrational Polarizabilities and Hyperpolarizabilities of Azoles: A Comparative Study of the Structure-Polarization Relationship. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4172-4183.	1.1	60

#	ARTICLE	IF	CITATIONS
2826	Density Functional Investigation of Hydrated V(II) and V(III) Ions: Influence of the Second Coordination Sphere; Water Exchange Mechanism. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4122-4129.	1.1	29
2827	Highly Asymmetric Coordination in Alkenes: Gas-Phase Structures of <i>trans</i> -1,2-Dichloro-1,2-disilylethene and 1-Bromo-1-silylethene. <i>Inorganic Chemistry</i> , 2003, 42, 6539-6544.	1.9	3
2828	Density Functional Study on the Effect of the <i>trans</i> Axial Ligand of B12 Cofactors on the Heterolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 306-315.	1.2	48
2829	First X-ray Characterization and Theoretical Study of η^5 -Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp* <i>Ru</i> (PEt ₃) ₂] ⁺ . <i>Journal of the American Chemical Society</i> , 2003, 125, 3311-3321.	6.6	90
2830	Aggregation Patterns in \hat{I}^{\pm} -Stabilized Carbanions: Assembly of a Sodium Cage Polymer by Slip-Stacking of Dimers. <i>Inorganic Chemistry</i> , 2003, 42, 2736-2741.	1.9	14
2831	Benchmark Study of Isotropic Hyperfine Coupling Constants for Hydrogen: Influence of Geometry, Correlation Method, and Basis Set. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6656-6667.	1.1	47
2832	Adsorbed Water Molecules on a K-Promoted Catalyst Surface Studied by Stimulated Micro-Raman Spectroscopy. <i>Langmuir</i> , 2003, 19, 5756-5762.	1.6	20
2833	Platinum(IV)-Mediated Nitrile-Sulfimide Coupling: A Route to Heterodiazadienes. <i>Inorganic Chemistry</i> , 2003, 42, 301-311.	1.9	62
2834	Hybrid Density Functional Theory Predictions of Low-Temperature Dimethyl Ether Combustion Pathways. II. Chain-Branching Energetics and Possible Role of the Criegee Intermediate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9463-9478.	1.1	64
2835	D _{3d} Ground-State Structure of V(CO) ₆ : A Combined Matrix Isolation and <i>ab Initio</i> Study of the Jahn-Teller Effect. <i>Journal of Physical Chemistry A</i> , 2003, 107, 859-868.	1.1	29
2836	Irradiation of Imine-Group VI Carbene Complexes in the Presence of Alkynes: A Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 2003, 68, 4674-4683.	1.7	26
2837	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of <i>Rhodospseudomonas Viridis</i> : Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 838-847.	1.2	19
2838	Adsorption of Small Palladium Clusters on the Relaxed \hat{I}^{\pm} -Al ₂ O ₃ (0001) Surface. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6411-6424.	1.2	39
2839	Insertion of Isocyanides into Group 4 Metal-Carbon and Metal-Nitrogen Bonds. Syntheses and DFT Calculations. <i>Organometallics</i> , 2003, 22, 4218-4228.	1.1	39
2840	2-Thia-1,3,5-triaza-7-phosphaadamantane 2,2-Dioxide (PASO ₂). Comparative Structural and Reactivity Investigation with the Water-Soluble Phosphine Ligand 1,3,5-triaza-7-phosphaadamantane (PTA). <i>Organometallics</i> , 2003, 22, 2050-2056.	1.1	24
2841	Prediction of Cellular Toxicity of Halocarbons from Computed Chemodescriptors: A Hierarchical QSAR Approach. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1103-1109.	2.8	43
2842	Computational Studies of the Chemistry of Syn Acetaldehyde Oxide. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11525-11532.	1.1	37
2843	On the Origin of Higher Rotational Barriers in Thioamides than in Amides. Remote Substituent Effects on the Conformational Stability of the Thioamide Group in Thioacetanilides. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5854-5861.	1.1	26

#	ARTICLE	IF	CITATIONS
2844	Pseudo-Jahn-Teller Distortion from Planarity in Heterocyclic Seven- and Eight-Membered Ring Systems with Eight π Electrons. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2749-2756.	1.1	14
2845	Thermal Isomerization of Tricyclo[4.1.0.0 ^{2,7}]heptane and Bicyclo[3.2.0]hept-6-ene through the (E,Z)-1,3-Cycloheptadiene Intermediate. <i>Journal of Organic Chemistry</i> , 2003, 68, 9081-9087.	1.7	10
2846	Olefin Insertion and Subsequent β -X Elimination from a Pentacoordinate Tantalum Complex. A Density Functional Theory Study. <i>Organometallics</i> , 2003, 22, 4047-4059.	1.1	22
2847	Cycloaddition Reactions of 1-Pyrazoline on the Si(100) 2×1 Surface: A Possible Route to an SiN Interfacial Double Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6853-6858.	1.2	3
2848	Outer sphere anion participation can modify the mechanism for conformer interconversion in Pd pincer complexes. <i>Dalton Transactions</i> , 2003, , 831-838.	1.6	84
2849	Cumulant approach to the direct calculation of reduced density matrices: A critical analysis. <i>Journal of Chemical Physics</i> , 2003, 118, 4832-4848.	1.2	34
2850	Basis set and electron correlation effects on ab initio electronic and vibrational nonlinear optical properties of conjugated organic molecules. <i>Journal of Chemical Physics</i> , 2003, 118, 711-718.	1.2	105
2851	The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. <i>Journal of Chemical Physics</i> , 2003, 118, 10584-10592.	1.2	67
2852	Theoretical Study of the Amazing Firefly Bioluminescence: The Formation and Structures of the Light Emitters. <i>Journal of the American Chemical Society</i> , 2003, 125, 6962-6971.	6.6	132
2853	Charge-Transfer Mechanism for Electrophilic Aromatic Nitration and Nitrosation via the Convergence of (ab Initio) Molecular-Orbital and Marcus-Hush Theories with Experiments. <i>Journal of the American Chemical Society</i> , 2003, 125, 3273-3283.	6.6	88
2854	The glass forming ability of tellurites: a rigid polytope approach. <i>Journal of Non-Crystalline Solids</i> , 2003, 316, 273-280.	1.5	15
2855	Hydrogen isotope exchange kinetics between H ₂ O and H ₄ SiO ₄ from ab initio calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2003, 67, 1259-1276.	1.6	20
2856	The Effect of Protein Conformational Flexibility on the Electronic Properties of a Chromophore. <i>Biophysical Journal</i> , 2003, 84, 2805-2813.	0.2	36
2857	Solvation Effects on Alternative Nucleophilic Substitution Reaction Paths for Chloride/Allyl Chloride and β -Methylated Congeners. <i>Journal of Organic Chemistry</i> , 2003, 68, 6375-6386.	1.7	30
2858	Density Functional Study on the Mechanism of the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. <i>Journal of Organic Chemistry</i> , 2003, 68, 4265-4274.	1.7	57
2859	Are both symmetric and buckled dimers on Si(100) minima? Density functional and multireference perturbation theory calculations. <i>Journal of Chemical Physics</i> , 2003, 119, 10917-10923.	1.2	42
2860	On the Transferability of Force Field Parameters With an ab Initio Force Field Developed for Sulfonamides. <i>Journal of Physical Chemistry A</i> , 2003, 107, 248-257.	1.1	23
2861	A quantum chemical mechanism for the water-initiated decomposition of silica. <i>Computational Materials Science</i> , 2003, 27, 102-108.	1.4	25

#	ARTICLE	IF	CITATIONS
2862	Influence of Media and Homoconjugate Pairing on Transition Metal Hydride Protonation. An IR and DFT Study on Proton Transfer to CpRuH(CO)(PCy ₃). <i>Journal of the American Chemical Society</i> , 2003, 125, 7715-7725.	6.6	74
2863	Theoretical identification of C ₂₀ carbon clusters: Prevalence of the monocyclic isomer and existence of the smallest fullerene and bowl isomer. <i>Physical Review B</i> , 2003, 67, .	1.1	22
2864	An experimental and theoretical study of the valence shell photoelectron spectra of purine and pyrimidine molecules. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2003, 36, 3129-3143.	0.6	69
2865	Time-Dependent Density Functional Theory (TDDFT) Study of the Excited Charge-Transfer State Formation of a Series of Aromatic Donor-Acceptor Systems. <i>Journal of the American Chemical Society</i> , 2003, 125, 252-264.	6.6	164
2866	Formation of Alkali Metal/Alkaline Earth Cation Water Clusters, M(H ₂ O) ₁₋₆ , M = Li ⁺ , Na ⁺ , K ⁺ , Mg ²⁺ , and Ca ²⁺ : An Effective Fragment Potential (EFP) Case Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 386-396.	1.1	74
2867	Experimental and Theoretical Studies of Bonding and Oxidative Addition of Germanes and Silanes, EH _{4-n} Ph _n (E = Si, Ge; n = 0-3), to Mo(CO)(diphosphine) ₂ . The First Structurally Characterized Germane-η ⁵ Complex. <i>Organometallics</i> , 2003, 22, 5307-5323.	1.1	68
2868	Theoretical Prediction of the Co-C Bond Strength in Cobalamins. <i>Journal of Physical Chemistry A</i> , 2003, 107, 7539-7545.	1.1	168
2869	Density Functional Theory Study of Fe(CO) ₃ (η ² -C ₃ H ₆), HFe(CO) ₃ (η ³ -C ₃ H ₅), and the Iron-Allyl Bond Energy. <i>Organometallics</i> , 2003, 22, 2652-2659.	1.1	28
2870	Ruthenium(II) and Ruthenium(IV) Complexes Containing η ¹ -P-, η ² -P,O-, and η ³ -P,N,O-Iminophosphorane-Phosphine Ligands Ph ₂ PCH ₂ P{NP(O)(OR) ₂ }Ph ₂ (R = Et, Ph): Synthesis, Reactivity, Theoretical Studies, and Catalytic Activity in Transfer Hydrogenation of Cyclohexanone. <i>Inorganic Chemistry</i> , 2003, 42, 3293-3307.	1.9	49
2871	The hydration structures of F ⁻ and Cl ⁻ investigated by ab initio QM/MM molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 357-362.	1.3	81
2872	Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-Catalyzed Reduction of Acetophenone. <i>Journal of the American Chemical Society</i> , 2003, 125, 10027-10039.	6.6	37
2873	Two-Bond ¹³ C- ¹⁵ N Spin-Spin Coupling Constants (2h _J C-N) Across C-H-N Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3222-3227.	1.1	25
2874	Paramagnetic Defect Centers at the MgO Surface. An Alternative Model to Oxygen Vacancies. <i>Journal of the American Chemical Society</i> , 2003, 125, 738-747.	6.6	134
2875	An Analysis of the Interactions between Nucleic Acid Bases: A Hydrogen-Bonded Base Pairs. <i>Journal of Physical Chemistry A</i> , 2003, 107, 418-426.	1.1	35
2876	Intra- and Intermolecular 1,3-Dipolar Cycloaddition of Sugar Ketonitrone with Mono-, Di-, and Trisubstituted Dipolarophiles. <i>Journal of Organic Chemistry</i> , 2003, 68, 4772-4783.	1.7	37
2877	Ga ₂ I ₂ [C(SiMe ₃) ₃] ₂ - an organogallium(II) halide containing a Ga-Ga single bond. <i>Dalton Transactions</i> , 2003, , 1360-1364.	1.6	28
2878	Molecular structure of trimethylphosphine-gallane, Me ₃ P·GaH ₃ : gas-phase electron diffraction, single-crystal X-ray diffraction, and quantum chemical studies. <i>Dalton Transactions</i> , 2003, , 3526-3533.	1.6	20
2879	Magnesium aryloxides: synthesis, structure, solution behavior and magnesiate ion formation. <i>Dalton Transactions</i> , 2003, , 1365-1372.	1.6	42

#	ARTICLE	IF	CITATIONS
2880	CF ₄ defluorination by Cp ₂ LnH: a DFT study. Dalton Transactions, 2003, , 4313-4318.	1.6	28
2881	Nucleophilic identity substitution reactions. The reaction between water and protonated alcohols Part I. For Part II, see following paper (DOI: 10.1039/b302270f). Electronic supplementary information (ESI) available: Cartesian co-ordinates for all species together with analytical imaginary frequencies for the transition structures. See http://www.rsc.org/suppdata/ob/b3/b302268d/ . Organic and Biomolecular Chemistry, 2003, 1, 2935.	1.5	25
2882	Synthesis, reactivity and catalytic activity in transfer hydrogenation of ketones of ruthenium(ii) and ruthenium(iv) complexes containing the novel N-thiophosphorylated iminophosphorane-phosphine ligands Ph ₂ PCH ₂ P(=NP(=S)(OR) ₂)Ph ₂ (R = Et, Ph). Dalton Transactions, 2003, , 3240-3249.	1.6	51
2883	C-H and C-C agostic interactions in cycloalkyl tris(pyrazolyl)boratoniobium complexes. Dalton Transactions, 2003, , 4057-4064.	1.6	49
2884	³ Agostic C-H or ² agostic Si-C bonds in La{CH(SiMe ₃) ₂ } ₃ ? A DFT study of the role of the ligand. New Journal of Chemistry, 2003, 27, 121-127.	1.4	88
2885	Theoretical study of the reaction mechanism of the uncatalyzed epoxidation of alkenes by iodosylbenzene Electronic supplementary information (ESI) available: B3LYP optimized geometries (Cartesian coordinates) and total energies for compounds 1 to 9. See http://www.rsc.org/suppdata/ni/b2/b203861g/ . New Journal of Chemistry, 2003, 27, 811-817.	1.4	18
2886	Quantum chemical study of Ln ⁱⁱⁱ (pyridine-dicarboxy-amide) ₁ complexes. Physical Chemistry Chemical Physics, 2003, 5, 2499.	1.3	11
2887	Structure, Bonding, and Vibrational Frequencies of CH ₃ CN~BF ₃ : New Insight into Medium Effects and the Discrepancy between the Experimental and Theoretical Geometries. Journal of Physical Chemistry A, 2003, 107, 4009-4018.	1.1	56
2888	EXAFS and Density Functional Study of Gold(I) Thiosulfate Complex in Aqueous Solution. Journal of Physical Chemistry A, 2003, 107, 2516-2523.	1.1	46
2889	Alkali Metal Doping of MgO: Mechanisms of Formation of Paramagnetic Surface Centers. Journal of Physical Chemistry B, 2003, 107, 8498-8506.	1.2	32
2890	Photolysis of Chiral 1-Pyrazolines to Cyclopropanes: Mechanism and Stereospecificity. Journal of Organic Chemistry, 2003, 68, 4906-4911.	1.7	19
2891	Ab Initio and Molecular Dynamics Study of the Active Site of the Reaction between Ribonuclease A and Cytidyl-3',5'-Adenosine. Journal of Physical Chemistry B, 2003, 107, 4871-4878.	1.2	2
2892	Valence bond analysis of the bonding in transition metal compounds: the RuNO group in nitrosyl complexes. Molecular Physics, 2003, 101, 715-720.	0.8	8
2893	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. Journal of Chemical Physics, 2003, 119, 11024-11034.	1.2	79
2894	Polarization propagator calculations of the polarizability tensor at imaginary frequencies and long-range interactions for the noble gases and n-alkanes. Journal of Chemical Physics, 2003, 118, 9167-9174.	1.2	48
2895	Electronic structure of paraaminophenoxyl radical in water. Journal of Chemical Physics, 2003, 118, 1378-1391.	1.2	10
2896	An ab initio study of conformations and IR spectra of 5-substituted 1,3-cyclopentadienes. Canadian Journal of Chemistry, 2003, 81, 14-30.	0.6	10
2897	A theoretical analysis of the conformational behaviour of substituted methylenecyclohexanes. Canadian Journal of Chemistry, 2003, 81, 1101-1107.	0.6	2

#	ARTICLE	IF	CITATIONS
2898	Computational Study on Mechanistic Details of the Aminoethanol Rearrangement Catalyzed by the Vitamin B12-Dependent Ethanolamine Ammonia Lyase: A His and Asp/Glu Acting Simultaneously as Catalytic Auxiliaries. <i>Journal of Organic Chemistry</i> , 2003, 68, 6967-6983.	1.7	24
2899	The treatment of the spin coupling in the bonding of NO to the Ni-doped MgO (100) surface. <i>Molecular Physics</i> , 2003, 101, 241-247.	0.8	9
2900	Multiconfigurational self-consistent field study of the silicon carbide (001) surface. <i>Journal of Chemical Physics</i> , 2003, 119, 10318-10324.	1.2	15
2901	A path integral approach to molecular thermochemistry. <i>Journal of Chemical Physics</i> , 2003, 118, 1596-1603.	1.2	23
2902	Combustion and atmospheric oxidation of hydrocarbons: Theoretical study of the methyl peroxy self-reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 10575-10583.	1.2	47
2903	Local correlation in the virtual space in multireference singles and doubles configuration interaction. <i>Journal of Chemical Physics</i> , 2003, 118, 8127-8139.	1.2	62
2904	Wavepacket dynamics and quantum mechanical energy densities in the quartet N+2+ O2 system. <i>Molecular Physics</i> , 2003, 101, 295-307.	0.8	6
2905	Emission spectra of Rb*He complexes in a cold He gas. <i>Physical Review A</i> , 2003, 68, .	1.0	38
2906	Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters. <i>Journal of Chemical Physics</i> , 2003, 119, 6560-6570.	1.2	8
2907	Ground- and excited-state properties of M-center oxygen vacancy aggregates in the bulk and surface of MgO. <i>Physical Review B</i> , 2003, 68, .	1.1	35
2908	New developments in the Fourier transform Coulomb method: Efficient and accurate localization of the filtered core functions and implementation of the Coulomb energy forces. <i>Journal of Chemical Physics</i> , 2003, 119, 11080-11087.	1.2	25
2909	Jahn-Teller triplet excited state structures and spectra of zinc complexes of porphyrin and phthalocyanine: A density functional theory study. <i>Journal of Chemical Physics</i> , 2003, 118, 5802-5810.	1.2	50
2910	Electron attachment to CO2 clusters. <i>Journal of Chemical Physics</i> , 2003, 119, 7714-7724.	1.2	22
2911	Vibrational analysis for the nuclear-electronic orbital method. <i>Journal of Chemical Physics</i> , 2003, 118, 9489-9496.	1.2	52
2912	DYNGA: a general purpose QM-MM-MD program. I. Application to water. <i>Molecular Physics</i> , 2003, 101, 2659-2668.	0.8	8
2913	Ab initio modelling of transition metals in diamond. <i>Journal of Physics Condensed Matter</i> , 2003, 15, S2913-S2927.	0.7	8
2914	Quantum Energy Flow and trans-Stilbene Photoisomerization: An Example of a Non-RRKM Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 10706-10716.	1.1	94
2915	Changing the Properties of N+5 and N~5 by Substitution. <i>Theoretical and Computational Chemistry</i> , 2003, , 441-455.	0.2	3

#	ARTICLE	IF	CITATIONS
2916	Does the Hydroperoxo Species of Cytochrome P450 Participate in Olefin Epoxidation with the Main Oxidant, Compound I? Criticism from Density Functional Theory Calculations. Bulletin of the Chemical Society of Japan, 2003, 76, 721-732.	2.0	77
2917	A Proposed Mechanism of [closo-CB11H12]- Formation by Dichlorocarbene Insertion Into [nido-B11H14]-. A Computational Study by Density Functional Theory. Collection of Czechoslovak Chemical Communications, 2003, 68, 644-662.	1.0	10
2918	Computed EOM-CCSD 19F-19F Spin-Spin Coupling Constants in Small Organic Molecules. Zeitschrift Fur Physikalische Chemie, 2003, 217, 1565-1576.	1.4	19
2919	Electric Field Effects on 2JHH Spin-Spin Coupling Constants. International Journal of Molecular Sciences, 2003, 4, 218-230.	1.8	10
2920	Estimation of Electron Spectra Transitions of Free-Based Porphin and Mg-Porphin Using Various Quantum Chemical Approaches. International Journal of Molecular Sciences, 2004, 5, 196-213.	1.8	10
2921	A Computational Model Relating Structure and Reactivity in Enantioselective Oxidations of Secondary Alcohols by (âˆ™)-Sparteineâˆ™PdII Complexes. Journal of the American Chemical Society, 2004, 126, 7967-7974.	6.6	89
2922	Local properties of quantum chemical systems: The LoProp approach. Journal of Chemical Physics, 2004, 121, 4494-4500.	1.2	320
2923	Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] and [Ru(PH3)4(H)2] complexes in the first singlet excited states: A diabatic quantum dynamics study. Journal of Chemical Physics, 2004, 121, 6258-6267.	1.2	4
2924	Simple minimum principle to derive a quantum-mechanical/ molecular-mechanical method. Journal of Chemical Physics, 2004, 121, 3964-3972.	1.2	23
2925	Simple and accurate method to evaluate tunneling splitting in polyatomic molecules. Journal of Chemical Physics, 2004, 120, 5036-5045.	1.2	62
2926	Barrier-free intermolecular proton transfer induced by excess electron attachment to the complex of alanine with uracil. Journal of Chemical Physics, 2004, 120, 6064-6071.	1.2	55
2927	Atomic and molecular intracules for excited states. Journal of Chemical Physics, 2004, 120, 7290-7297.	1.2	19
2928	A computational strategy for geometry optimization of ionic and covalent excited states, applied to butadiene and hexatriene. Journal of Chemical Physics, 2004, 120, 7849-7860.	1.2	72
2929	Quantitative Analysis of Electronic Properties of Carbon Nanotubes by Scanning Probe Microscopy: From Atomic to Mesoscopic Length Scales. Physical Review Letters, 2004, 93, 246801.	2.9	22
2930	19Fâ€™19F spinâ€™spin coupling constant surfaces for (HF)2 clusters: The orientation and distance dependence of the sign and magnitude of JFâ€™F. Journal of Chemical Physics, 2004, 120, 3237-3243.	1.2	31
2931	Ab initio many-body investigation of structure and stability of two-fold rings in silicates. Journal of Chemical Physics, 2004, 120, 8734-8739.	1.2	12
2932	Theoretical investigation of substituted anthraquinone dyes. Journal of Chemical Physics, 2004, 121, 1736-1743.	1.2	113
2933	Electric field gradient calculations for LiTiS2 and comparison with Li7NMR results. Physical Review B, 2004, 70, .	1.1	79

#	ARTICLE	IF	CITATIONS
2934	Ab initio study of the competing reaction channels in the reaction of HOCO radicals with NO and O ₂ . Journal of Chemical Physics, 2004, 120, 5073-5080.	1.2	25
2935	Full configuration interaction potential energy curves for the X ¹ Σ ⁺ g ⁺ , B ¹ Σ ⁺ g, and B ² Σ ⁺ g ⁺ states of C ₂ : A challenge for approximate methods. Journal of Chemical Physics, 2004, 121, 9211-9219.	1.2	127
2936	Equation of state and structural changes in diaminodinitroethylene under compression. Journal of Chemical Physics, 2004, 120, 8060-8066.	1.2	64
2937	Protonation study of peroxyntic acid and peroxyntrous acid. Journal of Chemical Physics, 2004, 121, 9498-9509.	1.2	2
2938	Density functional response theory calculations of three-photon absorption. Journal of Chemical Physics, 2004, 121, 9239-9246.	1.2	42
2939	New recurrence relations for the rapid evaluation of electron repulsion integrals based on the accompanying coordinate expansion formula. Journal of Chemical Physics, 2004, 121, 4050-4058.	1.2	13
2940	Fast vibrational self-consistent field calculations through a reduced mode-coupling scheme. Journal of Chemical Physics, 2004, 120, 562-573.	1.2	103
2941	Cycloaddition reactions of cyanogen (C ₂ N ₂) on the Si(100)-2×1 surface. Journal of Chemical Physics, 2004, 121, 5445-5450.	1.2	1
2942	Intermediate state representation approach to physical properties of electronically excited molecules. Journal of Chemical Physics, 2004, 120, 11449-11464.	1.2	213
2943	Surface reaction mechanisms of hydrazine on Si(100)-2×1 surface: NH ₃ desorption pathways. Journal of Chemical Physics, 2004, 120, 979-987.	1.2	9
2944	Ab Initio Study of H ₂ Desorption from Magnesium Hydride MgH ₂ Cluster. Journal of the Physical Society of Japan, 2004, 73, 2628-2630.	0.7	22
2945	Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2004, 120, 6346-6355.	1.2	60
2946	Docking and scoring of metallo-β-lactamases inhibitors. Journal of Computer-Aided Molecular Design, 2004, 18, 287-302.	1.3	29
2947	Experiments for correlating quaternary carbons in RNA bases. Journal of Biomolecular NMR, 2004, 29, 477-490.	1.6	26
2948	Quantum Chemical Analysis of the Chemical Bonds in Tris(8-hydroxyquinolino)aluminum as a Key Emitting Material for OLED. Journal of Physical Chemistry A, 2004, 108, 10296-10301.	1.1	69
2949	Time-Dependent Density-Functional Theory Investigation of the Fluorescence Behavior as a Function of Alkyl Chain Size for the 4-(N,N-Dimethylamino)benzotrile-like Donor-Acceptor Systems 4-(N,N-Diethylamino)benzotrile and 4-(N,N-Diisopropylamino)benzotrile. Journal of Physical Chemistry B, 2004, 108, 7132-7141.	1.2	42
2950	A Sequential Molecular Mechanics/Quantum Mechanics Study of the Electronic Spectra of Amides. Journal of the American Chemical Society, 2004, 126, 13502-13511.	6.6	68
2951	First principle calculations of ¹¹³ Cd chemical shifts for proteins and model systems. Journal of Biological Inorganic Chemistry, 2004, 9, 591-599.	1.1	35

#	ARTICLE	IF	CITATIONS
2952	A computational approach to the synthesis of dirithromycin. <i>Journal of Molecular Modeling</i> , 2004, 10, 94-101.	0.8	3
2953	FS ⁺ and FS ⁺ (OH ⁻) defect centers at the MgO(100) surface: cluster and periodic calculations. <i>Surface Science</i> , 2004, 549, 294-304.	0.8	24
2954	Interpretation of the temperature-dependent color of blue copper protein mutants. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 896-902.	1.5	21
2955	Structural impact on the methano bridge in norbornadiene, norbornene and norbornane. <i>Journal of Physics and Chemistry of Solids</i> , 2004, 65, 2041-2054.	1.9	8
2956	Theoretical studies of boron(III) complexes for the new blue luminescent material. <i>Materials Science and Engineering C</i> , 2004, 24, 269-273.	3.8	17
2957	Conformational analysis of methylphenidate: comparison of molecular orbital and molecular mechanics methods. <i>Journal of Computer-Aided Molecular Design</i> , 2004, 18, 719-738.	1.3	12
2958	Gaussian-based computations in molecular science. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 1-21.	1.5	41
2959	A molecular dynamics study of the structural stability of HIV-1 protease under physiological conditions: The role of Na ⁺ ions in stabilizing the active site. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 450-458.	1.5	25
2960	Intermolecular interaction and thermodynamic properties of N-methylacetamide and hydroxyacetonitrile dimers. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 113-117.	0.9	2
2961	The gas-phase reactivity of epichlorohydrin with hydroxide. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 241-248.	0.9	8
2962	Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 365-373.	1.0	8
2963	MCSCF study of the thermal isomerization of tricyclo[2.1.0.0 ^{2,5}]pentane to 1,3-cyclopentadiene. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 411-415.	1.0	3
2964	Conformational conversion of the boat and chair structures of bicyclo[3.2.0]hept-6-ene. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 432-435.	1.0	2
2965	Oxidative polymerization of 5-amino-1,10-phenanthroline: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2004, 97, 983-991.	1.0	6
2966	Analysis of electronic delocalization in buckminsterfullerene (C ₆₀). <i>International Journal of Quantum Chemistry</i> , 2004, 98, 361-366.	1.0	23
2967	Theory of chemical bonds in metalloenzymes I: Analytical and hybrid-DFT studies on oxo and hydroxo diiron cores. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 887-906.	1.0	49
2968	Controlling Chemoselectivity in the Lithiation of Substituted Aromatic Tertiary Amides. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 2135-2138.	7.2	26
2969	A Measureable Equilibrium between Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 3708-3711.	7.2	44

#	ARTICLE	IF	CITATIONS
2970	The Binary Group 4 Azides [Ti(N ₃) ₄], [P(C ₆ H ₅) ₄][Ti(N ₃) ₅], and [P(C ₆ H ₅) ₄] ₂ [Ti(N ₃) ₆] and on Linear Ti ₂ Ni ₂ NN Coordination. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 3148-3152.	7.2	73
2971	Polyazide Chemistry: Preparation and Characterization of As(N ₃) ₅ , Sb(N ₃) ₅ , and [P(C ₆ H ₅) ₄][Sb(N ₃) ₆]. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 6676-6680.	7.2	79
2972	Quantum-Chemical Design of Host Materials for Full-Color Triplet Emission. <i>Advanced Materials</i> , 2004, 16, 1624-1629.	11.1	96
2973	Theoretical Explorations of Enantioselective Alkylation Reactions of Pyrroles and Indoles Organocatalyzed by Chiral Imidazolidinones. <i>Advanced Synthesis and Catalysis</i> , 2004, 346, 1175-1185.	2.1	91
2978	The Electronic Structure of (Diiminopyridine)cobalt(II) Complexes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 1204-1211.	1.0	138
2979	Theoretical Investigation of Group 4 Constrained-Geometry Complexes Featuring Phosphazene and Phosphinimido Arms. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 1939-1947.	1.0	10
2980	A Molecular Tool for Measuring the Electron-Acceptor Ability of Ligands from Crystallographic Data. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 1705-1713.	1.0	31
2981	Formation of Sulfur-Sulfur Bonds in Copper Complexes. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 4430-4438.	1.0	12
2982	Kinetics and Mechanisms for the Reactions of Phenyl Radical with Ketene and its Deuterated Isotopomer: An Experimental and Theoretical Study. <i>ChemPhysChem</i> , 2004, 5, 225-232.	1.0	8
2983	Vibrational Corrections to Transition Metal NMR Shielding Constants. <i>ChemPhysChem</i> , 2004, 5, 410-414.	1.0	20
2984	On the Bond-Stretch Isomerism in the Benzo[1,2:4,5]dicyclobutadiene System—An ab initio MR-AQCC Study. <i>ChemPhysChem</i> , 2004, 5, 975-981.	1.0	18
2985	Kinetics and Mechanism of the C ₆ H ₅ + CH ₃ CHO Reaction: Experimental Measurement and Theoretical Prediction of the Reactivity toward Four Molecular Sites. <i>ChemPhysChem</i> , 2004, 5, 661-668.	1.0	13
2986	Probing the Basicity of Regular and Defect Sites of Alkaline Earth Metal Oxide Surfaces by BF ₃ Adsorption: A Theoretical Analysis. <i>ChemPhysChem</i> , 2004, 5, 642-651.	1.0	9
2987	NMR Conformational Analysis and Theoretical Calculations for 2-Aryl-1,3-dihydroxy-4,4,5,5-tetramethylimidazolidines. <i>Helvetica Chimica Acta</i> , 2004, 87, 425-438.	1.0	7
2988	Structure, Characterization, and Metal-Complexation Properties of a New Tetraazamacrocycle Containing Two Phenolic Pendant Arms. <i>Helvetica Chimica Acta</i> , 2004, 87, 2613-2628.	1.0	4
2989	Enthalpies of formation from B3LYP calculations. <i>Journal of Computational Chemistry</i> , 2004, 25, 725-733.	1.5	61
2990	Hydrogen bonding, solvation, and hydrolysis of cisplatin: A theoretical study. <i>Journal of Computational Chemistry</i> , 2004, 25, 1060-1067.	1.5	73
2991	Assessing the reliability of density functional methods in the conformational study of polypeptides: The treatment of intrasidic nonbonding interactions. <i>Journal of Computational Chemistry</i> , 2004, 25, 1333-1341.	1.5	55

#	ARTICLE	IF	CITATIONS
2992	Component-based integration of chemistry and optimization software. <i>Journal of Computational Chemistry</i> , 2004, 25, 1717-1725.	1.5	27
2993	Vibrational analysis, conformational stability, force constants, barriers to internal rotations, RHF, MP2 and DFT calculations of trans,trans-2,4-hexadiene. <i>Journal of Raman Spectroscopy</i> , 2004, 35, 869-878.	1.2	14
2994	GIAO/DFT evaluation of ^{13}C NMR chemical shifts of selected acetals based on DFT optimized geometries. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 459-466.	1.1	39
2995	Predicted signs of reduced two-bond spin-spin coupling constants ($^2h_{\text{KX}}^{\text{Y}}$) across $\text{X}^{\text{H}}\text{H}^{\text{Y}}$ hydrogen bonds. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 421-423.	1.1	33
2996	Density functional computation of ^{49}Ti NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 737-744.	1.1	25
2997	Density Functional Calculations on the Conversion of Azide and Carbon Monoxide to Isocyanate and Dinitrogen by a Nickel to Sulfur Rebound Mechanism. <i>Chemistry - A European Journal</i> , 2004, 10, 1805-1814.	1.7	13
2998	Crystal, Molecular and Electronic Structure of $\text{N,N}'$ -Diphenyl- $\text{N,N}'$ -bis(2,4-dimethylphenyl)-(1,1'-biphenyl)-4,4'-diamine and the Corresponding Radical Cation. <i>Chemistry - A European Journal</i> , 2004, 10, 83-91.		121
2999	Structure Investigation of Ti^{IV} -BODOLates Involved in the Catalytic Asymmetric Reduction of Ketones Using Catecholborane. <i>Chemistry - A European Journal</i> , 2004, 10, 182-189.	1.7	11
3000	First Investigation of Non-Classical Dihydrogen Bonding between an Early Transition-Metal Hydride and Alcohols: IR, NMR, and DFT Approach. <i>Chemistry - A European Journal</i> , 2004, 10, 661-671.	1.7	50
3001	$\text{N,N}'$ -Ethylenebis(pyridoxylideneiminato) and $\text{N,N}'$ -Ethylenebis(pyridoxylaminato): Synthesis, Characterization, Potentiometric, Spectroscopic, and DFT Studies of Their Vanadium(IV) and Vanadium(V) Complexes. <i>Chemistry - A European Journal</i> , 2004, 10, 2301-2317.	1.7	127
3002	The Diphosphate Monoanion in the Gas Phase: A Joint Mass Spectrometric and Theoretical Study. <i>Chemistry - A European Journal</i> , 2004, 10, 840-850.	1.7	5
3003	Road Maps for Nitrogen-Transfer Catalysis: The Challenge of the Osmium(VIII)-Catalyzed Diamination. <i>Chemistry - A European Journal</i> , 2004, 10, 2475-2486.	1.7	31
3004	First Structural Characterization of Binary As^{III} and Sb^{III} Azides. <i>Chemistry - A European Journal</i> , 2004, 10, 508-517.	1.7	92
3005	Mechanism of Reppe's Nickel-Catalyzed Ethyne Tetramerization to Cyclooctatetraene: A DFT Study. <i>Chemistry - A European Journal</i> , 2004, 10, 3081-3090.	1.7	36
3006	Computational Investigation of Hydrogen Abstraction from 2-Aminoethanol by the 1,5-Dideoxyribose-5-yl Radical: A Model Study of a Reaction Occurring in the Active Site of Ethanolamine Ammonia Lyase. <i>Chemistry - A European Journal</i> , 2004, 10, 2781-2788.	1.7	10
3007	The Calculation of Indirect Nuclear Spin-Spin Coupling Constants in Large Molecules. <i>Chemistry - A European Journal</i> , 2004, 10, 4627-4639.	1.7	37
3008	Low-Lying Excited States and Primary Photoproducts of $[\text{Os}_3(\text{CO})_{10}(\text{s-cis-L})]$ ($\text{L}=\text{Cyclohexa-1,3-diene}$). <i>Journal of Physical Chemistry B</i> , 2004, 108, 1078-1088.	1.7	8
3009	Electron Delocalization in Linearly π -Conjugated Systems: A Concept for Quantitative Analysis. <i>Chemistry - A European Journal</i> , 2004, 10, 5671-5680.	1.7	33

#	ARTICLE	IF	CITATIONS
3010	Vinyl Sulfoxides as Stereochemical Controllers in Intermolecular Pauson-Khand Reactions: Applications to the Enantioselective Synthesis of Natural Cyclopentanoids. <i>Chemistry - A European Journal</i> , 2004, 10, 5443-5459.	1.7	41
3011	Studies on Stereoselective [2+2] Cycloadditions between N,N-Dialkylhydrazones and Ketenes. <i>Chemistry - A European Journal</i> , 2004, 10, 6111-6129.	1.7	49
3012	Role of acidity in hydrogenation of cinnamaldehyde on platinum beta zeolite. <i>Microporous and Mesoporous Materials</i> , 2004, 75, 149-158.	2.2	26
3013	Hydrogen bonding. Part 83. The bis-troponene hydrogen cation: preparation, IR, and MO study of a proton bridged dimer of troponene with a covalent three-center OHO bond. <i>Journal of Molecular Structure</i> , 2004, 691, 211-216.	1.8	2
3014	The intramolecular hydrogen bond in ortho-hydroxy acetophenones. <i>Journal of Molecular Structure</i> , 2004, 700, 67-72.	1.8	30
3015	Characterisation of the PT-form of o-hydroxy acylaromatic Schiff bases by NMR spectroscopy and DFT calculations. <i>Journal of Molecular Structure</i> , 2004, 707, 69-75.	1.8	21
3016	Strong 1,4 P=O intramolecular interactions as a source of conformational preferences in Î±-stabilised phosphorus ylides. Part 2: metallic complexes. <i>Inorganica Chimica Acta</i> , 2004, 357, 1444-1456.	1.2	15
3017	Markedly different selectivity in the rhodium catalyzed hydroformylation of vinyl olefins containing a chiral alkoxy or alkyl group: good agreement between theory and experiment. <i>Inorganica Chimica Acta</i> , 2004, 357, 2980-2988.	1.2	17
3018	Composition and structure of activated complexes in stereoselective deprotonation of cyclohexene oxide by a mixed dimer of chiral lithium amide and lithiated imidazole. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 1607-1613.	1.8	14
3019	Application of polydentate chiral amines within magnesium-mediated asymmetric deprotonation reactions. <i>Tetrahedron Letters</i> , 2004, 45, 4175-4179.	0.7	25
3020	Rutheniumtetraoxide oxidation of alkenes—a density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 197-204.	1.5	16
3021	Theoretical study on reactivity of coordinated nitriles: structure, bonding and reactivity of [ReCl ₄ (N≡CCH ₃) ₂]. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 229-237.	1.5	35
3022	A computational study of the formation of 1,3,2-dioxaborolane from the reaction of dihydroxy borane with 1,2-ethanediol. <i>Computational and Theoretical Chemistry</i> , 2004, 673, 145-154.	1.5	15
3023	Peptide models XLII. Ab initio study on conformational changes of N-formyl-L-histidinamide caused by protonation or deprotonation of its side chain. <i>Computational and Theoretical Chemistry</i> , 2004, 675, 117-127.	1.5	4
3024	Is the charge on the nitrile carbon atom a driving force of the nucleophilic addition to coordinated nitriles?. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 33-42.	1.5	34
3025	Theoretical analysis of the NMR and electronic structure of novel Î± ⁸ -THC derivatives. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 131-138.	1.5	2
3026	Hydrogen activation and aldehyde elimination promoted by homogeneous Pt—Sn catalyst: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2004, 677, 133-143.	1.5	21
3027	Ab initio and density functional study of four-membered platina- and pallada-cycles, , X: C≡...O, C≡...NH, C≡...NH ₂ ⁺ , P(O)H, SO and SO ₂ . <i>Computational and Theoretical Chemistry</i> , 2004, 681, 191-202.	1.5	2

#	ARTICLE	IF	CITATIONS
3028	Ab initio investigation of electrophilic addition reaction of chlorine to homobenzonorbornadiene. Computational and Theoretical Chemistry, 2004, 686, 1-5.	1.5	8
3029	Theoretical study pyridine-substituted β -diketones. Computational and Theoretical Chemistry, 2004, 711, 7-11.	1.5	3
3030	The effectiveness of a primary aliphatic amino group as an internal Lewis base on the formation of a boron-oxygen-carbon linkage: a computational study. Computational and Theoretical Chemistry, 2004, 712, 9-19.	1.5	15
3031	Additivity of electron correlation energy and the ab initio MO calculation of (0 π) S1 π SO transition energies: polychlorinated dibenzofurans. Computational and Theoretical Chemistry, 2004, 710, 19-23.	1.5	4
3032	Comparative parametric method 5 (PM5) study of trans-stilbene. Computational and Theoretical Chemistry, 2004, 686, 103-108.	1.5	10
3033	The influence of the ruthenium nitrosyl complexes TM composition on the relative energies of the metastable states. Computational and Theoretical Chemistry, 2004, 712, 33-37.	1.5	4
3034	DFT calculations of the ¹ H chemical shifts and ¹³ C chemical shift tensors of retinal isomers. Computational and Theoretical Chemistry, 2004, 711, 141-147.	1.5	9
3035	Adsorption of NO and NO ₂ on terrace and step sites and on oxygen vacancies of the CaO(100) surface. Surface Science, 2004, 556, 145-158.	0.8	26
3036	Unusual reversal of regioselectivity in antibody-mediated aldol additions with unsymmetrical methyl ketones. Tetrahedron, 2004, 60, 619-632.	1.0	25
3037	The millimeter and submillimeter rotational spectrum of 1,3-dihydroxyacetone. Journal of Molecular Spectroscopy, 2004, 224, 101-106.	0.4	14
3038	Alkyl group dependence of C-Si reductive eliminations from alkyl(silyl) Pt(II) complexes: a density functional study. Journal of Organometallic Chemistry, 2004, 689, 2236-2241.	0.8	4
3039	Hybrid iodoperfluoroalkane-ferrocene supramolecular arrays: the shortest contacts iodine forms with nitrogen atoms and unsaturated moieties. Journal of Fluorine Chemistry, 2004, 125, 629-640.	0.9	29
3040	Theoretical study of the external heavy atom effect on phosphorescence of free-base porphyrin molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 3213-3224.	2.0	33
3041	A combined experimental and theoretical study of 1-phenylpropane-1,2-dione hydrogenation over heterogeneous cinchonidine-modified Pt catalyst. Journal of Catalysis, 2004, 224, 326-339.	3.1	38
3042	Theoretical study of perfluorinated oligothiophenes: electronic and structural properties. Polymer, 2004, 45, 6391-6397.	1.8	19
3043	Heteroaromatic benzyl ethers as intermediates for palladium-catalysed transfer hydrogenolysis of benzyl alcohols. Journal of Molecular Catalysis A, 2004, 215, 113-120.	4.8	31
3044	Synthesis, thermal, mass and ab initio analyses of cyclopropane-1,1,2-tricarboxylic acid. Journal of Molecular Structure, 2004, 694, 173-178.	1.8	1
3045	Deactivation in liquid-phase hydrogenation of cinnamaldehyde over aluminosilicate-supported ruthenium and platinum catalysts. Chemical Engineering Journal, 2004, 103, 35-43.	6.6	16

#	ARTICLE	IF	CITATIONS
3046	Intramolecular hydrogen bond in molecular and proton-transfer forms of Schiff bases. <i>Chemical Physics</i> , 2004, 297, 323-332.	0.9	50
3047	Correlating substituent parameter values to electron transport properties of molecules. <i>Chemical Physics</i> , 2004, 299, 89-95.	0.9	12
3048	Excited state direct dynamics of benzene with reparameterized multi-reference semiempirical configuration interaction methods. <i>Chemical Physics</i> , 2004, 304, 133-145.	0.9	60
3049	Vibrational study, crystal structure and quantum calculations of 2,2'-azobipyridine and 4,4'-dimethyl-3,3'-dinitro-2,2'-azobipyridine. <i>Chemical Physics</i> , 2004, 306, 71-92.	0.9	17
3050	A computational study on the acceleration of the Prins reaction by indium trichloride. <i>Comptes Rendus Chimie</i> , 2004, 7, 885-893.	0.2	1
3051	Tetrahydroacridin-9-ones, 9-chlorotetrahydroacridines, 9-amino-tetrahydroacridines and 9-(pyrazol-1-yl)-tetrahydroacridines derived from chiral cyclanones. <i>European Journal of Medicinal Chemistry</i> , 2004, 39, 37-48.	2.6	22
3052	The solvent effect on the aquation processes of the cis-dichloro(ethylenediamine)platinum(II) using continuum solvation models. <i>Chemical Physics Letters</i> , 2004, 387, 182-187.	1.2	43
3053	Theoretical study of tris(o-phenylenedioxy) cyclotrisphosphazene (TPP) electronic structure with ab initio and DFT methods. <i>Chemical Physics Letters</i> , 2004, 388, 422-426.	1.2	6
3054	Study on optimization of molecular structure using Hamiltonian algorithm. <i>Chemical Physics Letters</i> , 2004, 390, 84-88.	1.2	22
3055	Quantum-chemical and experimental kinetical investigation of the porphyrin diacids: role of the counterions in non-radiative deactivation of the excited electronic states. <i>Chemical Physics Letters</i> , 2004, 389, 352-358.	1.2	21
3056	A density functional study of some silver cluster hydrides. <i>Chemical Physics Letters</i> , 2004, 391, 9-15.	1.2	19
3057	The nodes of Hartree-Fock wavefunctions and their orbitals. <i>Chemical Physics Letters</i> , 2004, 392, 55-61.	1.2	24
3058	Molecular orbital engineering of single-molecular light emission. <i>Chemical Physics Letters</i> , 2004, 394, 194-197.	1.2	8
3059	Unusual hydrogen bonds in [AH ₃ H ₃ O] ⁺ radical cations (A=C, Si, Ge, Sn and Pb). <i>Chemical Physics Letters</i> , 2004, 395, 27-32.	1.2	4
3060	Theoretical study of the formation of the Î±-cyclodextrin hexahydrate. <i>Chemical Physics Letters</i> , 2004, 397, 422-428.	1.2	41
3061	Evaluation of carbohydrate molecular mechanical force fields by quantum mechanical calculations. <i>Carbohydrate Research</i> , 2004, 339, 937-948.	1.1	61
3062	Modelling Me ₅ C ₅ for reactivity studies in (Î±-5-C ₅ Me ₅) ₂ Ln ⁺ R: full DFT and QM/MM approaches. <i>New Journal of Chemistry</i> , 2004, 28, 1255-1259.	1.4	24
3063	Indium(III) hydration in aqueous solutions of perchlorate, nitrate and sulfate. Raman and infrared spectroscopic studies and ab-initio molecular orbital calculations of indium(III) water clusters. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5145-5155.	1.3	56

#	ARTICLE	IF	CITATIONS
3064	Computational QM/MM study on the structure and energetics of species involved in the activation of the C-H and C-S bonds of thiophene by Cp*RhPMe ₃ . <i>New Journal of Chemistry</i> , 2004, 28, 625-630.	1.4	24
3065	What is the nature of the long bond in the TCNE ²⁺ -dimer?. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2008-2011.	1.3	83
3066	Electrochemical and theoretical study of the redox properties of transition metal complexes with {Pt ₂ S ₂ } cores. <i>Dalton Transactions</i> , 2004, , 706-712.	1.6	10
3067	Tests of second-generation and third-generation density functionals for thermochemical kinetics Electronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 673.	1.3	242
3068	The molecular structures of pentaborane(9) with halogen substituents in apical and basal positions, determined by electron diffraction and theoretical calculations. <i>Dalton Transactions</i> , 2004, , 1719-1725.	1.6	3
3069	N-Salicylideneamino acidato complexes of oxovanadium(IV). The cysteine and penicillamine complexes. <i>Dalton Transactions</i> , 2004, , 2855.	1.6	24
3070	Structural flexibility of formally d ¹⁰ [M(biphosphinine) ₂] ^q complexes Electronic supplementary information (ESI) available: main geometrical parameters optimized for the structures whose energies are reported in Fig. 1. See http://www.rsc.org/suppdata/nj/b3/b316684h/ . <i>New Journal of Chemistry</i> , 2004, 28, 838.	1.4	10
3071	Structural properties of doped polyacetylene chains: a comparative theoretical investigation using Hartree-Fock, Møller-Plesset second-order perturbation theory, and density functional theory approaches. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3167-3174.	1.3	30
3072	Flexible N,N,N-chelates as supports for iron and cobalt chloride complexes; synthesis, structures, DFT calculations and ethylene oligomerisation studies. <i>Dalton Transactions</i> , 2004, , 3231-3240.	1.6	38
3073	Bis(iminophosphorano)methane Derivatives as Precursors of Unusual Ruthenium Carbene Complexes: A Synthetic and DFT Study. <i>Organometallics</i> , 2004, 23, 2421-2433.	1.1	40
3074	Ab Initio Modeling of the Spatial, Electronic, and Vibrational Structure of Schiff Base Models for Visual Photoreceptors. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13560-13572.	1.2	20
3075	Multielectron Atom Transfer Reactions of Perchlorate and Other Substrates Catalyzed by Rhenium Oxazoline and Thiazoline Complexes: A Reaction Kinetics, Mechanisms, and Density Functional Theory Calculations. <i>Inorganic Chemistry</i> , 2004, 43, 4036-4050.	1.9	92
3076	Molecular structure of Hf(BH ₄) ₄ investigated by quantum mechanical calculations and gas-phase electron diffraction. <i>Dalton Transactions</i> , 2004, , 967.	1.6	13
3077	Gold(I) or gold(III) as active species in AuCl ₃ -catalyzed cyclization/cycloaddition reactions? A DFT study Electronic supplementary information (ESI) available: Coordinates, energies and ball-and-stick models of the computed structures. See http://www.rsc.org/suppdata/cc/b4/b404876h/ . <i>Chemical Communications</i> , 2004, , 1726.	2.2	107
3078	Conical intersection dynamics in solution: The chromophore of Green Fluorescent Protein. <i>Faraday Discussions</i> , 2004, 127, 149-163.	1.6	222
3079	Unique 1 ⁺ 2 adduct formation of meso-tetraarylporphyrins and meso-tetraalkylporphyrins with BF ₃ : a spectroscopic and ab initio study. <i>New Journal of Chemistry</i> , 2004, 28, 1600-1607.	1.4	46
3080	B3LYP/6-31G* conformational landscape in vacuo of some pterocarpan stereoisomers with biological activity. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2849.	1.3	13
3081	Simulation of the resonance Raman spectrum of the hydrated electron in the hydrated-hydronium cluster model. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5297.	1.3	20

#	ARTICLE	IF	CITATIONS
3082	The molecular structures and electrochemical response of α -twisted-tetra(aryl)benzidenes. <i>Journal of Materials Chemistry</i> , 2004, 14, 2516-2523.	6.7	55
3083	Dynamic interaction of theory and experiment: total determination of the gas-phase molecular structure of tri-tert-butylphosphine oxide (OPBut ₃). <i>Dalton Transactions</i> , 2004, , 384-391. Molecular structure of 1,1,2,2-tetra-tert-butylidisilane: unusual structural motifs in sterically crowded disilanes Electronic supplementary information (ESI) available: Structural results from calculations at the HF level with the 3-21G* and 6-31G* basis sets (Table S1), geometric and amplitude restraints (Table S2), least-squares correlation matrix (Table S3), and experimental coordinates from the GED analysis (Table S4). See http://www.rsc.org/suppdata/dt/b3/b316701a/ . <i>Dalton Transactions</i> , 2004, , 759.	1.6	8
3084	Structures of the radical P[N(SiMe ₃) ₂](NPri ₂), its dimer, cation and chloro derivative Electronic supplementary information (ESI) available: The final Cartesian coordinates of the computed structures of the diphosphine 2 and the corresponding radical 3, a selected list of distances and associated amplitudes of vibrations and the correlation matrix from the electron diffraction least-squares refinements. See http://www.rsc.org/suppdata/dt/b4/b402926g/ . <i>Dalton Transactions</i> , 2004, , 1980.	1.6	14
3085	Molecular structure of tris(dipivaloylmethanato)lutetium(III) studied by gas electron diffraction and ab initio and DFT calculations. <i>Dalton Transactions</i> , 2004, , 1715.	1.6	29
3086	Calculations of PAH anions: When are diffuse functions necessary?. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 1113-1121.	1.6	60
3087	Size extensive modification of local multireference configuration interaction. <i>Journal of Chemical Physics</i> , 2004, 120, 1693-1704.	1.3	37
3088	Few-states models for three-photon absorption. <i>Journal of Chemical Physics</i> , 2004, 121, 2020-2029.	1.2	52
3089	Extracting dominant pair correlations from many-body wave functions. <i>Journal of Chemical Physics</i> , 2004, 121, 78.	1.2	41
3090	Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 691-698.	1.2	10
3091	Synthesis and Characterization of Pd(II) Complexes with Bis-Pyridinium and Isoquinolinium N-Ylides: Moderate CH ₂ -OC Intramolecular Hydrogen Bonds as Source of Conformational Preferences. <i>Inorganic Chemistry</i> , 2004, 43, 7622-7635.	1.1	44
3092	Factors Governing the Kinetic Competition of Nitrogen and Sulfur Ligands in Cisplatin Binding to Biological Targets. <i>Journal of the American Chemical Society</i> , 2004, 126, 5999-6004.	1.9	15
3093	Doubly Hybrid Meta DFT: A New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4786-4791.	6.6	85
3094	DFT Analysis of Fe(H ₂ O) ₆ ³⁺ and Fe(H ₂ O) ₆ ²⁺ Structure and Vibrations; Implications for Isotope Fractionation. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2726-2732.	1.1	297
3095	Quantum-Chemical Investigation of the Conformational Dynamics of Mono-meso-phenyl-Substituted Octaalkylporphyrins in the Triplet Excited State. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5684-5691.	1.1	92
3096	Calculated Volume and Energy Profiles for Water Exchange on t ₂ g ₆ Rhodium(III) and Iridium(III) Hexaquaions: A Conclusive Evidence for an Ia Mechanism. <i>Inorganic Chemistry</i> , 2004, 43, 858-864.	1.1	15
3097	A Valence Bond Description of Coordinate Covalent Bonding. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5126-5130.	1.9	22
3098	Reverse Exponential Decay of Electrical Transmission in Nanosized Graphite Sheets. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7565-7572.	1.1	30
3099		1.2	31

#	ARTICLE	IF	CITATIONS
3100	QM/MM Study of the Mononuclear Non-Heme Iron Active Site of Phenylalanine Hydroxylase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17226-17237.	1.2	14
3101	Adsorption of methanol on zeolite Y: An atomistic and quantum chemical study. <i>Studies in Surface Science and Catalysis</i> , 2004, 154, 2739-2744.	1.5	2
3102	Stabilization of Zwitterions in Solution: ^{13}C -Aminobutyric Acid (GABA). <i>Journal of Physical Chemistry A</i> , 2004, 108, 203-211.	1.1	42
3103	Molecular Prototypes for Simple SiO ₂ Potentials. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11679-11683.	1.1	7
3104	Synthesis and Properties of Compressed Dihydride Complexes of Iridium: A Theoretical and Spectroscopic Investigations. <i>Journal of the American Chemical Society</i> , 2004, 126, 8813-8822.	6.6	79
3105	Self-Consistency versus "Best-Fit" Approaches in Understanding the Structure of Metal Nitrosyl Complexes. <i>Organometallics</i> , 2004, 23, 6008-6014.	1.1	5
3106	Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartree-Fock Wave Functions with Molecular Mechanics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 632-650.	1.1	133
3107	Structure and Vibrational Spectrum of Formate and Acetate Adsorbed from Aqueous Solution onto the TiO ₂ Rutile (110) Surface. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5004-5017.	1.2	212
3108	Electronic Couplings in Organic Mixed-Valence Compounds: The Contribution of Photoelectron Spectroscopy. <i>Journal of the American Chemical Society</i> , 2004, 126, 2727-2731.	6.6	85
3109	The Field-Adapted ADMA Approach: Introducing Point Charges. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4301-4309.	1.1	94
3110	A Model for Double Asymmetric Induction in the Stereocontrolled Reduction of Glycosyl α -Ketoesters with Oxazaborolidines. <i>Journal of the American Chemical Society</i> , 2004, 126, 6996-7008.	6.6	16
3111	Copper-Mediated Peptide Radical Ions in the Gas Phase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11170-11181.	1.2	115
3112	A Homologous Series of Regioselectively Tetradepleted Group 8 Metallocenes: New Inverse Crown Ring Compounds Synthesized via a Mixed Sodium-Magnesium Tris(diisopropylamide) Synergic Base. <i>Journal of the American Chemical Society</i> , 2004, 126, 11612-11620.	6.6	110
3113	How Heme Metabolism Occurs in Heme Oxygenase: A Computational Study of Oxygen-Donation Ability of the Oxo and Hydroperoxo Species. <i>Journal of the American Chemical Society</i> , 2004, 126, 3672-3673.	6.6	38
3114	Stereoselective Conjugate Addition of Benzyl Phenylsulfonyl Carbanions to Enones Derived from d-Mannitol. <i>Journal of Organic Chemistry</i> , 2004, 69, 4013-4018.	1.7	7
3115	Gas-Phase Fragmentation Reactions of Protonated Aromatic Amino Acids: Concomitant and Consecutive Neutral Eliminations and Radical Cation Formations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3844-3853.	1.1	108
3116	Thermodynamic Properties of Biphenyl Ether in the Ideal Gas State. <i>Journal of Chemical & Engineering Data</i> , 2004, 49, 941-943.	1.0	4
3117	Electronic Structure of ScC ₆ H ₆ - and ScC ₆ H ₆ : Geometries, Electron Binding Energies, and Dyson Orbitals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2988-2992.	1.1	17

#	ARTICLE	IF	CITATIONS
3118	Dramatic Structural Effects of a Single Hydrogen Atom in HNPBut3. <i>Inorganic Chemistry</i> , 2004, 43, 5522-5528.	1.9	5
3119	Local Environment of Electrons Trapped at the MgO Surface: Spin Density on the Oxygen Ions from 17O Hyperfine Coupling Constants. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11529-11534.	1.2	28
3120	Chalcogen-Chalcogen Bonds in Edge-Sharing Square-Planar d8 Complexes. Are They Possible?. <i>Inorganic Chemistry</i> , 2004, 43, 3702-3714.	1.9	25
3121	On the Accuracy of Theoretically and Experimentally Determined Electron Densities of Polar Bonds. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9442-9452.	1.1	84
3122	Fragmentation Mechanisms of Product Ions from Protonated Tripeptides. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18743-18749.	1.2	43
3123	Direct Observation of Surface Intermediates Formed by Selective Oxidation of Alcohols on Silica-Supported Molybdenum Oxide. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3231-3239.	1.2	17
3124	External Electric Field Will Control the Selectivity of Enzymatic-Like Bond Activations. <i>Journal of the American Chemical Society</i> , 2004, 126, 11746-11749.	6.6	265
3125	One-Bond Spin-Spin Coupling Constants of X-H Proton Donors in Complexes with X-H-Y Hydrogen Bonds, for X = 13C, 15N, 17O, and 19F: Predictions, Comparisons, and Relationships among JX-H, 1KX-H, and X-H Distances. <i>Journal of the American Chemical Society</i> , 2004, 126, 15624-15631.	6.6	39
3126	Energetics and Mechanism of Organolanthanide-Mediated Aminoalkene Hydroamination/Cyclization. A Density Functional Theory Analysis. <i>Organometallics</i> , 2004, 23, 4097-4104.	1.1	109
3127	Synthesis, Structure, Theoretical Studies, and Ligand Exchange Reactions of Monomeric, T-Shaped Arylpalladium(II) Halide Complexes with an Additional, Weak Agostic Interaction. <i>Journal of the American Chemical Society</i> , 2004, 126, 1184-1194.	6.6	288
3128	Is the Enthalpy of Fusion of Tris(acetylacetonato)metal(III) Complexes Affected by Their Potential Energy in the Crystal State?. <i>Inorganic Chemistry</i> , 2004, 43, 8479-8489.	1.9	24
3129	Theoretical Study of the Low Lying Electronic States of oxoX(salen) (X = Mn, Mn-, Fe, and Cr) Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2314-2323.	1.1	31
3130	Characterization of 5-Hydroxy-8-oxo-7,8-dihydroguanosine in the Photosensitized Oxidation of 8-Oxo-7,8-dihydroguanosine and Its Rearrangement to Spiroiminodihydantoin. <i>Journal of the American Chemical Society</i> , 2004, 126, 16777-16782.	6.6	80
3131	Scanning Tunneling Microscopy and Theoretical Study of Competitive Reactions in the Dissociative Chemisorption of CCl4 on Iron Oxide Surfaces. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16753-16760.	1.2	21
3132	Structure and Nature of the Metal-Ligand Interactions in Mixed Iron(II) Phosphametalloenes. <i>Organometallics</i> , 2004, 23, 5308-5313.	1.1	20
3133	Theoretical Prediction of Partition Coefficients via Molecular Electrostatic and Electronic Properties. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 848-855.	2.8	16
3134	[2 + 2]-Photocycloaddition of 1,1-Diethoxyethylene to Chiral Polyfunctional 2-Cyclohexenones. Regioselectivity and π -Facial Discrimination. <i>Journal of Organic Chemistry</i> , 2004, 69, 1120-1125.	1.7	15
3135	Use of Computational and Synthetic Chemistry in Catalyst Design: A New Family of High-Activity Ethylene Polymerization Catalysts Based on Titanium Tris(amino)phosphinimide Complexes. <i>Organometallics</i> , 2004, 23, 5240-5251.	1.1	38

#	ARTICLE	IF	CITATIONS
3136	Catalytic Roles of Active-Site Amino Acid Residues of Coenzyme B12-Dependent Diol Dehydratase: A Protonation State of Histidine and Pull Effect of Glutamate. <i>Journal of the American Chemical Society</i> , 2004, 126, 16207-16216.	6.6	40
3137	Isomerizations of Bicyclo[2.1.0]pent-2-ene and Tricyclo[2.1.0.02,5]pentane into Cyclopenta-1,3-diene: A Computational Study by DFT and High-Level ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 507-514.	1.1	42
3138	Two-Bond Spin-Spin Coupling across a Hydrogen Bond: X-Y Coupling in the Presence and Absence of the Proton. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6820-6822.	1.1	12
3139	New Universal Solvation Model and Comparison of the Accuracy of the SM5.42R, SM5.43R, C-PCM, D-PCM, and IEF-PCM Continuum Solvation Models for Aqueous and Organic Solvation Free Energies and for Vapor Pressures. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6532-6542.	1.1	100
3140	Probing the Acid Strength of Brønsted Acidic Zeolites with Acetonitrile: A Quantum Chemical Calculation of ¹ H, ¹⁵ N, and ¹³ C NMR Shift Parameters. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7142-7151.	1.2	34
3141	Quantum Dynamical Study of ¹ H-Hydrogen Transfer in Two Selected Late-Transition-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11116-11126.	1.1	13
3142	The Resting State of P450cam: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7468-7478.	1.2	67
3143	Potential Energy Surfaces for the Reactions Si + O ₂ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 8395-8399.	1.1	8
3144	Computational Investigation of the Solvation of Nitric Acid: A Formation of the NO ₃ - and H ₃ O ⁺ Ion Pair. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10578-10585.	1.1	35
3145	Crystalline Effects on the Properties of the Dative Bond: A Computational Study of HCN-BF ₃ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 8378-8384.	1.1	16
3146	Evidence for Discrepancy between the Surface Lewis Acid Site Strength and Infrared Spectra of Adsorbed Molecules: The Case of Boric Acid-Silica. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16499-16507.	1.2	24
3147	Unusual C-H Allylic Activation in the {PtII(cod)} Fragment Bonded to a {Pt ₂ (¹ / ₄ -S) ₂ } Core. <i>Organometallics</i> , 2004, 23, 2522-2532.	1.1	16
3148	The Application of the Effective Fragment Potential Method to Molecular Anion Solvation: A Study of Ten Oxyanion-Water Clusters, A-(H ₂ O) ₁₋₄ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 833-839.	1.1	23
3149	Influence of the Cis Ligand on the H-H Separation and the Rotation Barrier of the Dihydrogen in Osmium-Elongated Dihydrogen Complexes Containing an Ortho-Metalated Ketone. <i>Organometallics</i> , 2004, 23, 3008-3015.	1.1	48
3150	Sketching a path through the hydrocarbon oxidation maze. <i>Molecular Physics</i> , 2004, 102, 289-299.	0.8	5
3151	Proton Affinity of Peroxyacetic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2930-2935.	1.1	8
3152	Predicted Signs of One-Bond Spin-Spin Coupling Constants (1hJH-Y) across X-H-Y Hydrogen Bonds for Complexes with Y = ¹⁵ N, ¹⁷ O, and ¹⁹ F. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11762-11767.	1.1	28
3153	Redox-Dependent pKa of CuBHistidine Ligand in Cytochrome c Oxidase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18383-18389.	1.2	34

#	ARTICLE	IF	CITATIONS
3154	Probing the Acid Strength of Brønsted Acidic Zeolites with Acetonitrile: An Atomistic and Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7152-7161.	1.2	58
3155	Bis(η^4 -silylene)-Bridged Dinuclear Rhodium(0) Complex and Its Palladium(0) and Platinum(0) Analogues. Theoretical Study of Their Electronic Structure, Bonding Nature, and Interconversion between η^4 -Disilene-Bridged Form and Bis(η^4 -silylene)-Bridged Form. <i>Organometallics</i> , 2004, 23, 4672-4681.	1.1	12
3156	Unexpected Influence of the Counteranion in the η^2 vs η^3 Hapticity of Polydentate N-Donor Ligands in $[\text{Rh}(\text{N-ligand})\text{L}_2]^+$ Complexes. <i>Organometallics</i> , 2004, 23, 5530-5539.	1.1	18
3157	Computational Studies on the Electrocyclizations of 1-Amino-1,3,5-hexatrienes. <i>Journal of Organic Chemistry</i> , 2004, 69, 8024-8028.	1.7	34
3158	Zipper-Featured β -Peptide Foldamers Driven by Donor-Acceptor Interaction. Design, Synthesis, and Characterization. <i>Journal of Organic Chemistry</i> , 2004, 69, 270-279.	1.7	58
3159	Computed Spin-Spin Coupling Constants ($1J_{\text{X-Y}}$) in Molecules HmX^nYHn for X and Y = ^{13}C , ^{15}N , and ^{31}P : Comparisons with Experiment and Insights into the Signs of $1J_{\text{X-Y}}$. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3662-3667.	1.1	34
3160	Metal Cation-Methyl Interactions in $\text{CB}11\text{Me}_{12}$ -Salts of Me_3Ge^+ , Me_3Sn^+ , and Me_3Pb^+ . <i>Journal of the American Chemical Society</i> , 2004, 126, 12033-12046.	6.6	62
3161	Determination of Sugar Structures in Solution from Residual Dipolar Coupling Constants: A Methodology and Application to Methyl β -D-Xylopyranoside. <i>Journal of the American Chemical Society</i> , 2004, 126, 13100-13110.	6.6	27
3162	η^2 -Palladium and Platinum(II) Complexes of a η^4 -Phosphinine Anion: Syntheses, X-ray Crystal Structures, and DFT Calculations. <i>Organometallics</i> , 2004, 23, 2870-2875.	1.1	23
3163	Adhesion of Bacterial Exopolymers to η^2 -FeOOH: Inner-Sphere Complexation of Phosphodiester Groups. <i>Langmuir</i> , 2004, 20, 11108-11114.	1.6	122
3164	Static and Dynamic Polarizabilities of Conjugated Molecules and Their Cations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11063-11072.	1.1	89
3165	Ruthenium-Catalyzed Cycloisomerization of ω -(Ethynyl)phenylalkenes to Diene Derivatives via Skeletal Rearrangement. <i>Journal of the American Chemical Society</i> , 2004, 126, 15560-15565.	6.6	77
3166	Why Is $\text{Re}^{\text{II}}\text{Re}$ Bond Formation/Cleavage in $[\text{Re}(\text{bpy})(\text{CO})_3]^{2+}$ Different from That in $[\text{Re}(\text{CO})_5]^{2+}$? Experimental and Theoretical Studies on the Dimers and Fragments. <i>Inorganic Chemistry</i> , 2004, 43, 7636-7647.	1.9	78
3167	Conformational Analysis with Both Experimental and Computational Data for Both Gaseous and Crystalline Phases: Unexpected Interactions in N-Methyldichloroacetamide. <i>Journal of Physical Chemistry A</i> , 2004, 108, 185-193.	1.1	4
3168	Synthesis of benzo-fused lactams and lactones via Ru(II)-catalyzed cycloaddition of amide- and ester-tethered η^2 -diynes with terminal alkynes: electronic directing effect of internal conjugated carbonyl group. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 1287-1294.	1.5	62
3169	B3LYP Investigation of HPO_2 , trans-HOPO , cis-HOPO , and Their Radical Anions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9390-9399.	1.1	15
3170	Adsorption of Acetylene on $\text{Si}(100)-(2 \times 1)$. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7820-7826.	1.2	24
3171	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6908-6918.	1.1	1,497

#	ARTICLE	IF	CITATIONS
3172	Density and wave function analysis of actinide complexes: What can fuzzy atom, atoms-in-molecules, Mulliken, Löwdin, and natural population analysis tell us?. <i>Journal of Chemical Physics</i> , 2004, 121, 2563.	1.2	97
3173	The Role of Fullerene Hemispheres in Determining Structural Features of Finite-Length Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11426-11434.	1.2	49
3174	A study of the reactions of molecular hydrogen with small gold clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 5169-5175.	1.2	95
3175	Ability of N-Heterocyclic Carbene Ligands to Promote Intermolecular Oxidative Addition Reactions at Unsaturated Ruthenium Centers. <i>Organometallics</i> , 2004, 23, 1857-1865.	1.1	28
3176	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. <i>Molecular Physics</i> , 2004, 102, 2563-2574.	0.8	126
3177	In-situ generation and analysis of charge transfer materials using an OTTE cell and resonance Raman scattering Electronic supplementary information (ESI) available: BPW91/6-31G(d) predicted vibrational frequencies and intensities for the neutral, radical cation and dication species of 1 and 2. See http://www.rsc.org/suppdata/cp/b4/b402015d/ . <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 3257.	1.3	15
3178	Adsorption of Water on the TiO ₂ (Rutile) (110) Surface: A Comparison of Periodic and Embedded Cluster Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7844-7853.	1.2	126
3179	Syntheses of (âˆ™)-Funebrine and (âˆ™)-Funebral, Using Sequential Transesterification and Intramolecular Cycloaddition of a Chiral Nitron. <i>Journal of Organic Chemistry</i> , 2004, 69, 1475-1480.	1.7	41
3180	Quantum Mechanical/Molecular Mechanical Investigation of the Mechanism of Câ”H Hydroxylation of Camphor by Cytochrome P450cam: A Theory Supports a Two-State Rebound Mechanism. <i>Journal of the American Chemical Society</i> , 2004, 126, 4017-4034.	6.6	269
3181	Existence of Doubly Charged Lead Monohydrate: Experimental Evidence and Theoretical Examination. <i>Journal of the American Chemical Society</i> , 2004, 126, 7975-7980.	6.6	34
3182	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. <i>Journal of Chemical Physics</i> , 2004, 120, 5027-5035.	1.2	81
3183	Theoretical Study of Thermal Isomerization of Silacyclobutene to Cyclopropene. <i>Organometallics</i> , 2004, 23, 4744-4749.	1.1	15
3184	A Computational Study of the Structure and Synthesis of Formazans. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4961-4965.	1.1	13
3185	Ground and Excited State Hydrogen Atom Transfer Reactions and Cyclization of 2-Acetylbenzoic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9331-9341.	1.1	12
3186	Global Optimization of H-Passivated Si Clusters at the Ab Initio Level via the GAM1 Semiempirical Method. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6025-6034.	1.2	12
3187	Theoretical Prediction of Benzyne-Like Species in Pyrene Diradicals. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5111-5116.	1.1	16
3188	Parametrization of 2-Bromo-2-Chloro-1,1,1-Trifluoroethane (Halothane) and Hexafluoroethane for Nonbonded Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 781-786.	1.1	31
3189	Experimental and Theoretical Study of Pentaerythritol Tetranitrate Conformers. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6216-6221.	1.1	53

#	ARTICLE	IF	CITATIONS
3190	Conformation Dependence of pKa: Ab Initio and DFT Investigation of Histidine. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6195-6205.	1.1	52
3191	Utilization of Hydrogen Bonds To Stabilize M ^{II} O(H) Units: Synthesis and Properties of Monomeric Iron and Manganese Complexes with Terminal Oxo and Hydroxo Ligands. <i>Journal of the American Chemical Society</i> , 2004, 126, 2556-2567.	6.6	173
3192	Characterization of a Kinetically Stable, Highly Ordered, Octameric Form of Lithiumtert-Butoxide and Its Implications Regarding Aggregate Formation. <i>Journal of the American Chemical Society</i> , 2004, 126, 484-485.	6.6	42
3193	Diversity of Contaminant Reduction Reactions by Zerovalent Iron: Role of the Reductate. <i>Environmental Science & Technology</i> , 2004, 38, 139-147.	4.6	175
3194	The molecular structure of tetra-tert-butyldiphosphine: an extremely distorted, sterically crowded molecule. <i>Dalton Transactions</i> , 2004, , 2469-2476.	1.6	108
3195	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 314-318.	1.3	106
3196	Study on the External Surface Acidity of MCM-22 Zeolite: Theoretical Calculation and 31P MAS NMR. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1386-1391.	1.2	41
3197	C ¹³ C Bond Cleavage of Acetonitrile by a Carbonyl Iron Complex with a Silyl Ligand. <i>Organometallics</i> , 2004, 23, 117-126.	1.1	120
3198	A long-range-corrected time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2004, 120, 8425-8433.	1.2	1,694
3199	A multimode analysis of the gas-phase photoelectron spectra in oligoacenes. <i>Journal of Chemical Physics</i> , 2004, 120, 7490-7496.	1.2	163
3200	Oxygen isotope exchange kinetics between H ₂ O and H ₄ SiO ₄ from ab initio calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2004, 68, 949-958.	1.6	13
3201	The importance of three-body terms in the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2004, 120, 6832-6840.	1.2	334
3202	¹³ C NMR Study of the Self-Association of Chloroquine, Amodiaquine, and Quinine. <i>Journal of Physical Chemistry A</i> , 2004, 108, 8505-8513.	1.1	25
3203	Mechanisms of Staudinger Reactions within Density Functional Theory. <i>Journal of Organic Chemistry</i> , 2004, 69, 4299-4308.	1.7	96
3204	Binding of Benzylpenicillin to Metallo-β-lactamase: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17639-17648.	1.2	25
3205	Toluene Model for Molecular Dynamics Simulations in the Ranges 298 < T (K) < 350 and 0.1 < P (MPa) < 10. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11774-11781.	1.2	23
3206	Kinetics of the CCO + NO and CCO + NO ₂ Reactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 74-79.	1.1	20
3207	Variable Electronic Coupling in Phenylacetylene Dendrimers: The Role of Förster, Dexter, and Charge-Transfer Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 671-682.	1.1	111

#	ARTICLE	IF	CITATIONS
3208	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2715-2719.	1.1	639
3209	A Synthesis and Luminescence Study of Ir(ppz) ₃ for Organic Light-Emitting Devices. <i>Bulletin of the Chemical Society of Japan</i> , 2004, 77, 751-755.	2.0	34
3210	Mutational analysis of the catalytic centre of the <i>Citrobacter freundii</i> AmpD N-acetylmuramyl-l-alanine amidase. <i>Biochemical Journal</i> , 2004, 377, 111-120.	1.7	25
3211	Vertical Ionization Energies of L-Amino Acids as a Function of Their Conformation: an Ab Initio Study. <i>International Journal of Molecular Sciences</i> , 2004, 5, 301-332.	1.8	66
3212	Tautomerization in the ground and first excited singlet states of phenyl-lapimidazole. <i>Journal of Luminescence</i> , 2004, 109, 207-214.	1.5	2
3213	n-Body Decomposition Approach to the Calculation of Interaction Energies of Water Clusters. , 0, , 27-41.		23
3214	End-Cap Effects on Vibrational Structures of Finite-Length Carbon Nanotubes. <i>Journal of the American Chemical Society</i> , 2005, 127, 11769-11776.	6.6	59
3215	Terahertz molecular electronics devices and systems. , 2005, , .		2
3216	Theoretical modeling of the isopropylum cation: Exploring nonclassical carbonyl behavior. <i>Journal of Coordination Chemistry</i> , 2005, 58, 595-603.	0.8	0
3217	Theoretical Study on the Transformation of Bis(acetylene)cobalt to Cobaltacyclopentadiene and the Regioselectivity in this Transformation. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 781-791.	2.0	55
3218	Generalization of the Projection Space Improves the SAC-SD (symmetry-adapted cluster-singles and) Tj ETQq 0 0 0 r gBT /Overlock 10 Tf 5	0.7	3
3219	Theoretical Study of the Formation of a Benzene Cobalt Complex from Cobaltacyclopentadiene and Acetylene. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 792-803.	2.0	61
3220	Ab Initio Study of DNA Double-Strand Breaks by Hydroxyl Radical. <i>JSME International Journal Series B</i> , 2005, 48, 196-201.	0.3	10
3221	Vibrational spectra and chemical quantum calculations for 2-adamantylamino-5-nitropyridine crystals a novel material for laser Raman converters. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 685-695.	2.0	7
3222	Steric and electronic effects on the conformations of n-butane derivatives with trichlorosilyl, silyl and trichloromethyl groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 1411-1417.	2.0	1
3223	Matrix-isolation FT-IR spectra and theoretical study of dimethyl sulfate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 1461-1470.	2.0	28
3224	Theoretical study on interaction of different coordination modes of BH ₄ ligand with transition metal in [TM(BH ₄)(CO) ₄] ⁺ (TM=Cr, Mo). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 84-95.	0.8	8
3225	The cocondensation reaction of lithium atoms and anisole: an experimental and theoretical study of the reaction pathway. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 1511-1522.	0.8	3

#	ARTICLE	IF	CITATIONS
3226	Oxidative addition to dimethylplatinum (II) compounds containing bulky nitrogen ligands: crystal structures of compounds [PtMe ₂ {(Me ₂ NCH ₂ CH ₂ NCH)Ar}] (Ar= phenanthryl or anthryl). <i>Journal of Organometallic Chemistry</i> , 2005, 690, 2062-2070.	0.8	7
3227	Synthesis, structure and optical limiting properties of organoruthenium chalcogenide clusters. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 1487-1497.	0.8	19
3228	Alkyl-rhodium transition state stabilities as a tool to predict regio- and stereoselectivity in the hydroformylation of chiral substrates. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 2339-2350.	0.8	15
3229	Synthesis, characterization, and in vitro antimicrobial activity of organotin(IV) complexes with triazolo-pyrimidine ligands containing exocyclic oxygen atoms. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 4773-4783.	0.8	39
3230	On the ligand properties of the P- versus the N-heterocyclic carbene for a Grubbs catalyst in olefin metathesis. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 6079-6088.	0.8	19
3231	An extremely stable Ni(II) complex derived from the hydrolytic cleavage of the C-terminal tail of histone H2A. <i>Journal of Inorganic Biochemistry</i> , 2005, 99, 637-643.	1.5	16
3232	Sorption of the antibiotic ofloxacin to mesoporous and nonporous alumina and silica. <i>Journal of Colloid and Interface Science</i> , 2005, 283, 160-170.	5.0	173
3233	Cation templation of Mn ²⁺ /[Mo(CN) ₇] ⁴⁻ system: Formation of pseudo-dimorphs (NH ₄) ₂ Mn ₃ (H ₂ O) ₄ [Mo(CN) ₇] ₂ ·nH ₂ O (n=4, 5). <i>Polyhedron</i> , 2005, 24, 1033-1046.	1.0	5
3234	A theoretical study of zero-field splitting of organic biradicals. <i>Polyhedron</i> , 2005, 24, 2708-2715.	1.0	37
3235	Theoretical study on the magnetic interactions of active site in hemerythrin. <i>Polyhedron</i> , 2005, 24, 2701-2707.	1.0	14
3236	Highly selective isomerization of N-allylamines catalyzed by ruthenium and rhodium complexes. <i>Journal of Molecular Catalysis A</i> , 2005, 237, 17-25.	4.8	22
3237	Crystal structure, vibrational and NMR studies and chemical quantum calculations of 2-phenylazo-5-nitro-6-methyl-pyridine (C ₁₂ H ₁₀ N ₄ O ₂). <i>Journal of Molecular Structure</i> , 2005, 744-747, 377-392.	1.8	17
3238	The molecular structure of Sc(hfa) ₃ (hfa=1,1,1,5,5,5-hexafluoropentane-2,4-dionato) studied by gas electron diffraction and ab initio and DFT calculations. <i>Journal of Molecular Structure</i> , 2005, 779, 23-29.	1.8	8
3239	An ab initio study of CO adsorption on ceria(110). <i>Chemical Physics</i> , 2005, 318, 180-190.	0.9	27
3240	A priori evaluation of the solvent contribution to the reorganization energy accompanying intramolecular electron transfer: Predicting the nature of the Creutz-Taube ion. <i>Chemical Physics</i> , 2005, 319, 39-51.	0.9	24
3241	Vibrational spectra, DFT chemical quantum calculations and conformation of the hydrazo-bond in 2,2'-hydrazobipyridine with relation to 2,2'-azobipyridine. <i>Vibrational Spectroscopy</i> , 2005, 39, 1-14.	1.2	16
3242	Temperature-dependent Raman, IR and X-ray studies of 2-ethylimino-4-nitropyridine N-oxide. <i>Vibrational Spectroscopy</i> , 2005, 37, 195-207.	1.2	15
3243	Diastereoselective synthesis of 3,4-disubstituted 5-(p-tolylsulfinyl)-5,6-dehydropiperidin-2-ones: chirality transfer in the enantioselective synthesis of ethyl (+)-(3S,4aS,7aS)-1-oxo-octahydro-1H-cyclopenta[c]pyridine-3-carboxylate. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 4034-4044.	1.8	4

#	ARTICLE	IF	CITATIONS
3244	Computational experiment on hydroformylation and hydrogenation of propenal catalyzed by Rh complex: a competitive study. <i>Computational and Theoretical Chemistry</i> , 2005, 714, 61-72.	1.5	5
3245	Computational experiment on hydroformylation and hydrogenation of ethyne catalyzed by Rh complex: a competitive study. <i>Computational and Theoretical Chemistry</i> , 2005, 714, 179-188.	1.5	4
3246	Liu's Parr's Nagy analysis on density functional theory calculations of spin densities in first-row atoms and diatomic hydrides. <i>Computational and Theoretical Chemistry</i> , 2005, 722, 169-183.	1.5	3
3247	Common binding mode for structurally and chemically diverse non-nucleosidic HIV-1RT inhibitors. <i>Computational and Theoretical Chemistry</i> , 2005, 723, 205-209.	1.5	3
3248	First principles determination of 99Ru chemical shifts using moderately sized basis sets. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 45-52.	1.5	6
3249	Intramolecular dative bonds involving boron with oxygen and nitrogen in boronic acids and esters: a computational study. <i>Computational and Theoretical Chemistry</i> , 2005, 723, 147-157.	1.5	29
3250	An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Diels-Alder reaction. Exploring the validity of different indicators of aromaticity. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 165-171.	1.5	59
3251	Role of solvent effects on nucleophilic substitution of 4H-pyran-4-one and its 2,6-dimethyl derivative with hydroxide ion in aqueous solution: ab initio and density functional theory studies on a supermolecular reaction model. <i>Computational and Theoretical Chemistry</i> , 2005, 728, 117-122.	1.5	2
3252	DFT study of the fixation of CO by SPS-based pincer Rh(I) and Ir(I) complexes: Regioselectivity and reactivity. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 73-79.	1.5	11
3253	Theoretical study of adsorption on Ni(111) and Cu(111) surfaces. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 81-86.	1.5	4
3254	Density functional theory study of conformational and opto-electronic properties of oligo-para-phenylenes. <i>Computational and Theoretical Chemistry</i> , 2005, 725, 39-44.	1.5	29
3255	A theoretical study of 18+ complexes. <i>Computational and Theoretical Chemistry</i> , 2005, 726, 149-154.	1.5	1
3256	A comparative theoretical study on CO insertion into Rh-C bond. <i>Computational and Theoretical Chemistry</i> , 2005, 730, 177-183.	1.5	4
3257	Ab initio study of the thermal isomerization of quadricyclane to norbornadiene. <i>Computational and Theoretical Chemistry</i> , 2005, 728, 67-70.	1.5	12
3258	An ab initio and DFT study on the hydrolysis of carbonyl dichloride. <i>Computational and Theoretical Chemistry</i> , 2005, 730, 155-160.	1.5	1
3259	Conformational features of calix[4]arenes with alkali metal cations: A quantum chemical investigation with density functional theory. <i>Computational and Theoretical Chemistry</i> , 2005, 732, 7-20.	1.5	24
3260	Reactivity of low-coordinated MgO anions towards CO: A DFT study of (CnOn+1)2 polymeric species. <i>Surface Science</i> , 2005, 591, 70-89.	0.8	7
3261	Structural analyses of 4-benzoylpyridine thiosemicarbazone using NMR techniques and theoretical calculations. <i>Tetrahedron</i> , 2005, 61, 7045-7053.	1.0	18

#	ARTICLE	IF	CITATIONS
3262	Towards the rational design of palladium-N-heterocyclic carbene catalysts by a combined experimental and computational approach. <i>Tetrahedron</i> , 2005, 61, 9723-9735.	1.0	116
3263	Wurster's crownophanes: an alternate topology for para-phenylenediamine-based macrocycles. <i>Tetrahedron</i> , 2005, 61, 12350-12357.	1.0	14
3264	Pharmacophoric features and Ca ²⁺ ion holding capacity of verapamil. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 5412-5415.	1.0	3
3265	Theoretical studies of cyclometalated phenylpyrazol Ir(III) complex using density functional theory. <i>Current Applied Physics</i> , 2005, 5, 79-84.	1.1	22
3266	Topological analysis of the electron density and of the electron localization function of pyrene and its radicals. <i>Chemical Physics</i> , 2005, 308, 181-192.	0.9	21
3267	Electronic structures and band gaps of chains and sheets based on phenylacetylene units. <i>Chemical Physics</i> , 2005, 312, 289-297.	0.9	43
3268	Theoretical/experimental study of the solvation enthalpy of acetone in dilute aqueous solution. <i>Chemical Physics</i> , 2005, 315, 76-80.	0.9	12
3269	Theoretical DFT study of phosphorescence from porphyrins. <i>Chemical Physics</i> , 2005, 315, 215-239.	0.9	94
3270	The 17O hyperfine structure of trapped holes photo generated at the surface of polycrystalline MgO. <i>Chemical Physics Letters</i> , 2005, 403, 124-128.	1.2	32
3271	Ionization energies and electron distributions of one-end open sandwich clusters: Eun(C ₈ H ₈) _n (n=1-4). <i>Chemical Physics Letters</i> , 2005, 403, 169-174.	1.2	29
3272	Ab initio QM/MM dynamics of anion/water hydrogen bonds in aqueous solution. <i>Chemical Physics Letters</i> , 2005, 403, 314-319.	1.2	31
3273	Structural characterization of Y@C ₈₂ . <i>Chemical Physics Letters</i> , 2005, 405, 274-277.	1.2	43
3274	On the influence of non-additive interactions on the optical properties of the selected subsystems of crystalline urea. <i>Chemical Physics Letters</i> , 2005, 406, 29-37.	1.2	19
3275	Conformational analysis of the 1- and 2-propyl peroxy radicals. <i>Chemical Physics Letters</i> , 2005, 406, 81-89.	1.2	29
3276	Ab initio study of nucleation on the diamond (100) surface during chemical vapor deposition with methyl and H radicals. <i>Chemical Physics Letters</i> , 2005, 406, 197-201.	1.2	18
3277	Magnetic exchange of trinuclear spin frustration system: CASPT2 and density functional theory study on hydroxo-bridged chromium complex [Cr ₃ (NH ₃) ₁₀ (OH) ₄] ⁺ Br ₅ ⁻ . <i>Chemical Physics Letters</i> , 2005, 407, 147-152.	1.2	13
3278	Parity violation energy of biomolecules II: DNA. <i>Chemical Physics Letters</i> , 2005, 407, 522-526.	1.2	19
3279	Are resonance-assisted hydrogen bonds resonance assisted? A theoretical NMR study. <i>Chemical Physics Letters</i> , 2005, 411, 411-415.	1.2	106

#	ARTICLE	IF	CITATIONS
3280	A theoretical investigation of Nâ€“Hâ€“OP hydrogen bonds through ¹⁵ Nâ€“ ³¹ P and ¹ Hâ€“ ³¹ P coupling constants. <i>Chemical Physics Letters</i> , 2005, 412, 97-100.	1.2	11
3281	The binding of the noble metal cations Au ⁺ and Ag ⁺ to propene. <i>Chemical Physics Letters</i> , 2005, 412, 416-419.	1.2	8
3282	Response theory calculations of two-photon circular dichroism. <i>Chemical Physics Letters</i> , 2005, 414, 461-467.	1.2	40
3283	Role of differential correlation energy in core ionization of pyrrole and pyridine. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2005, 142, 163-171.	0.8	15
3284	Ferrocenyl-Based π -Conjugated Complexes: Modulation of Electronic Properties by Symmetric/Asymmetric Cyclopentadienyl Substitution. <i>Organometallics</i> , 2005, 24, 1198-1203.	1.1	18
3285	Carbon Nanotube Inner Phase Chemistry: The Cl-Exchange S _N 2 Reaction. <i>Nano Letters</i> , 2005, 5, 1861-1866.	4.5	31
3286	Local Aromaticity of [n]Acenes, [n]Phenacenes, and [n]Helicenes (n = 1â€“9). <i>Journal of Organic Chemistry</i> , 2005, 70, 2509-2521.	1.7	195
3287	Behaviour of density functionals with respect to basis set: II. Polarization consistent basis sets. <i>Molecular Physics</i> , 2005, 103, 345-358.	0.8	32
3288	Newly developed basis sets for density functional calculations. <i>Journal of Computational Chemistry</i> , 2005, 26, 175-184.	1.5	58
3289	Charge distribution in the water molecule? A comparison of methods. <i>Journal of Computational Chemistry</i> , 2005, 26, 97-105.	1.5	287
3290	Short-time Fourier transform analysis of ab initio molecular dynamics simulation: Collision reaction between CN and C ₄ H ₆ . <i>Journal of Computational Chemistry</i> , 2005, 26, 436-442.	1.5	11
3291	The behavior of transition metal nitrido bonds towards protonation rationalized by means of localized bonding schemes and their weights. <i>Journal of Computational Chemistry</i> , 2005, 26, 532-551.	1.5	11
3292	A CSOV study of the difference between HF and DFT intermolecular interaction energy values: The importance of the charge transfer contribution. <i>Journal of Computational Chemistry</i> , 2005, 26, 1052-1062.	1.5	99
3293	Effect of the axial cysteine ligand on the electronic structure and reactivity of high-valent iron(IV) oxo-porphyrins (Compound I): A theoretical study. <i>Journal of Computational Chemistry</i> , 2005, 26, 1600-1611.	1.5	15
3294	1,1'-Bis(oxazolin-2-yl)ferrocenes: An Investigation of Their Complexation Behavior toward [Pd(η -3-allyl)Cl] ₂ . <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 1589-1600.	1.0	14
3295	A Theoretical Assessment of the Thermodynamic Preferences in the Cyclopalladation of Amines. <i>European Journal of Inorganic Chemistry</i> , 2005, 2005, 4040-4047.	1.0	10
3296	Theoretical Study on the Reactivity and Regioselectivity of the Ene Reaction of η^2 -O ₂ with η^2 -Unsaturated Carbonyl Compounds. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3643-3649.	1.2	22
3297	Through versus Cross Electron Delocalization in Polytriacetylene Oligomers: A Computational Analysis. <i>ChemPhysChem</i> , 2005, 6, 511-519.	1.0	16

#	ARTICLE	IF	CITATIONS
3298	Aromaticity Analysis of Lithium Cation/ π Complexes of Aromatic Systems. <i>ChemPhysChem</i> , 2005, 6, 2552-2561.	1.0	46
3299	MOCVD of Sr-Containing Oxides: Transport Properties and Deposition Mechanisms of the Sr(tmhd) ₂ -pmdeta Precursor. <i>Chemical Vapor Deposition</i> , 2005, 11, 269-275.	1.4	9
3300	Structures of Nonheme Oxoiron(IV) Complexes from X-ray Crystallography, NMR Spectroscopy, and DFT Calculations. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3690-3694.	7.2	247
3301	Origin of the High Activity of Second-Generation Grubbs Catalysts. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 5974-5978.	7.2	148
3302	The Aromaticity of the Stannole Dianion. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6553-6556.	7.2	90
3306	The Direct, Enantioselective, One-Pot, Three-Component, Cross-Mannich Reaction of Aldehydes: The Reason for the Higher Reactivity of Aldimine versus Aldehyde in Proline-Mediated Mannich and Aldol Reactions. <i>Advanced Synthesis and Catalysis</i> , 2005, 347, 1595-1604.	2.1	44
3307	Kinetics and mechanisms for reactions of HNO with CH ₃ and C ₆ H ₅ studied by quantum-chemical and statistical-theory calculations. <i>International Journal of Chemical Kinetics</i> , 2005, 37, 261-274.	1.0	23
3308	A QM/MM Study of the Asymmetric Dihydroxylation of Terminal Aliphatic Alkenes with OsO ₄ ·(DHQD)2PYDZ: Enantioselectivity as a Function of Chain Length. <i>Chemistry - A European Journal</i> , 2005, 11, 1017-1029.	1.7	24
3309	Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to [Cp*Fe(dppe)H]. <i>Chemistry - A European Journal</i> , 2005, 11, 873-888.	1.7	58
3310	Ring-Closing Olefin Metathesis on Ruthenium Carbene Complexes: Model DFT Study of Stereochemistry. <i>Chemistry - A European Journal</i> , 2005, 11, 3921-3935.	1.7	51
3311	Multistate Reactivity in Styrene Epoxidation by Compound I of Cytochrome P450: Mechanisms of Products and Side Products Formation. <i>Chemistry - A European Journal</i> , 2005, 11, 2825-2835.	1.7	108
3312	Loss of Ammine from Platinum(II) Complexes: Implications for Cisplatin Inactivation, Storage, and Resistance. <i>Chemistry - A European Journal</i> , 2005, 11, 2849-2855.	1.7	89
3313	Computational Study of Structures and Properties of Metallaboranes: Cobalt Bis(dicarbollide). <i>Chemistry - A European Journal</i> , 2005, 11, 4109-4120.	1.7	65
3314	Zirconium Bis(indenyl) Sandwich Complexes with an Unprecedented Indenyl Coordination Mode and Their Role in the Reactivity of the Parent Bent-Metallocenes: A Detailed DFT Mechanistic Study. <i>Chemistry - A European Journal</i> , 2005, 11, 2505-2518.	1.7	33
3315	Binolam-AlCl: A Two-Centre Catalyst for the Synthesis of Enantioenriched Cyanohydrin O-Phosphates. <i>Chemistry - A European Journal</i> , 2005, 11, 3849-3862.	1.7	53
3316	Elongated Dihydrogen Versus Compressed Dihydride Complexes: The Temperature Dependence of the H-D Spin-Spin Coupling Constant as a Criterion To Distinguish between Them. <i>Chemistry - A European Journal</i> , 2005, 11, 6315-6325.	1.7	20
3317	The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. <i>Chemistry - A European Journal</i> , 2005, 11, 6743-6753.	1.7	90
3318	Metal Ion Coordination to Azole Nucleosides. <i>Chemistry - A European Journal</i> , 2005, 11, 6246-6253.	1.7	69

#	ARTICLE	IF	CITATIONS
3319	Theoretical search for atomic-like states of silicon at the surface of thermally grown SiO ₂ films on silicon surfaces. <i>Applied Physics A: Materials Science and Processing</i> , 2005, 80, 1617-1623.	1.1	3
3320	Multipole electrostatic model for MNDO-like techniques with minimal valence spd-basis sets. <i>Theoretical Chemistry Accounts</i> , 2005, 114, 159-168.	0.5	16
3321	The effects of solvation in the theoretical spectra of cationic dyes. <i>Theoretical Chemistry Accounts</i> , 2005, 113, 274-280.	0.5	74
3322	On the coordination chemistry of corannulene, the smallest "buckybowl". <i>Journal of Organometallic Chemistry</i> , 2005, 690, 3440-3450.	0.8	33
3323	Oxidative addition of aryl chlorides to palladium N-heterocyclic carbene complexes and their role in catalytic arylamination. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 6054-6067.	0.8	54
3324	Bonding and fluxionality in group-4 metal complexes with pyrrolyl ligands. <i>Comptes Rendus Chimie</i> , 2005, 8, 1444-1452.	0.2	10
3325	Thermochemistry and structures of solvated S _N 2 complexes and transition states in the gas phase: experiment and theory. <i>International Journal of Mass Spectrometry</i> , 2005, 241, 205-223.	0.7	33
3326	Behavior of hydrogen atom at Nafion®/Pt interface. <i>Solid State Communications</i> , 2005, 134, 601-605.	0.9	12
3327	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 181-189.	1.1	60
3328	Binding of transition metal complexes to guanine and guanine-cytosine: hydrogen bonding and covalent effects. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 854-866.	1.1	37
3329	Computational study on the difference between the Co-C bond dissociation energy in methylcobalamin and adenosylcobalamin. <i>Journal of Biological Inorganic Chemistry</i> , 2005, 10, 509-517.	1.1	47
3330	Regression formulae for ab initio and density functional calculated chemical shifts. <i>Journal of Molecular Modeling</i> , 2005, 11, 175-185.	0.8	70
3331	AM1* parameters for aluminum, silicon, titanium and zirconium. <i>Journal of Molecular Modeling</i> , 2005, 11, 439-456.	0.8	40
3332	Preparation, Structural Characterization and the Molecular Structure of 2,3,5-Trinitro-p-xylene. <i>Structural Chemistry</i> , 2005, 16, 475-483.	1.0	9
3333	A Theoretical Study on the Tautomerism of C-Carboxylic and Methoxycarbonyl Substituted Azoles. <i>Structural Chemistry</i> , 2005, 16, 507-514.	1.0	28
3334	Ab Initio Study and Its Comparison with X-ray Crystal Structure of 4-[1-(4-Chloro-phenylamino)-ethyl] 5-methyl-2-p-tolyl-2,4-dihydro-pyrazol-3-one. <i>Structural Chemistry</i> , 2005, 16, 515-520.	1.0	11
3335	Correlation between structure and spectral characteristics of rhodium(I) chelate dicarbonyl complexes and their electron. <i>Journal of Structural Chemistry</i> , 2005, 46, 220-229.	0.3	15
3336	Parity Violation Energy Of Biomolecules "I: Polypeptides. <i>Origins of Life and Evolution of Biospheres</i> , 2005, 35, 461-475.	0.8	26

#	ARTICLE	IF	CITATIONS
3337	Mechanism of asymmetric hydrogenation of enamides with [Rh(BisP*)] ⁺ catalyst: Model DFT study. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 53-63.	1.0	17
3338	Simulation of UV/visible absorption spectra of (±-diimine)nickel(II) catalysts by time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 840-848.	1.0	9
3339	B3LYP, BLYP and PBE DFT band structures of the nucleotide base stacks. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 422-426.	1.0	18
3340	Elongation method with cutoff technique for linear SCF scaling. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 785-794.	1.0	46
3341	Local HSAB principle in the conjugate addition of p-substituted thiophenols to cyclohexenone. <i>International Journal of Quantum Chemistry</i> , 2005, 104, 29-37.	1.0	10
3342	Elongation method at restricted open-shell Hartree-Fock level of theory. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 875-882.	1.0	41
3343	Computational investigation of enantio- and regioselectivity of rhodium-catalyzed asymmetric hydroformylation of vinyl formate with CHIRAPHOS-type ligand. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 108-123.	1.0	11
3344	Non-linear absorption of 2,5-dialkynyl thiophenes. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 426-433.	0.9	9
3345	Assessment of Clar's aromatic 6π-sextet rule by means of PDI, NICS and HOMA indicators of local aromaticity. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 785-791.	0.9	147
3346	Locating the charge site in isomeric pyrrolyl ions by Eberlin ion/molecule reactions. <i>Rapid Communications in Mass Spectrometry</i> , 2005, 19, 1775-1778.	0.7	6
3347	Comparative analysis of the trypanocidal activity and chemical properties of E-lychnophoric acid and its derivatives using theoretical calculations. <i>Ecletica Quimica</i> , 2005, 30, 37-45.	0.2	7
3348	Ab Initio Study of Cyclohexane Dehydrogenation on Pt(111). <i>Shinku/Journal of the Vacuum Society of Japan</i> , 2005, 48, 208-210.	0.2	0
3349	Theoretical and Computational Studies of Energetic Salts. , 2005, , 431-471.		5
3350	Combination of computational prescreening and experimental library construction can accelerate enzyme optimization by directed evolution. <i>Protein Engineering, Design and Selection</i> , 2005, 18, 509-514.	1.0	32
3351	Monte Carlo simulations of the finite temperature properties of (H ₂ O) ₆ . , 2005, , 995-1009.		2
3352	Degradation of Assembled Silicon Nanostructured Thin Films: a Theoretical and Experimental Study. <i>Materials Research Society Symposia Proceedings</i> , 2005, 887, 1.	0.1	0
3353	Computational chemistry applied to studies of organic contaminants in the environment: Examples based on benzo[a]pyrene. <i>Numerische Mathematik</i> , 2005, 305, 621-644.	0.7	11
3354	Inelastic Neutron Scattering Spectra of Free Base and Zinc Porphines: A Comparison with DFT-Based Vibrational Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5724-5733.	1.1	20

#	ARTICLE	IF	CITATIONS
3355	Using ONETEP for accurate and efficient density functional calculations. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 5757-5769.	0.7	44
3356	Application of variational reduced-density-matrix theory to the potential energy surfaces of the nitrogen and carbon dimers. <i>Journal of Chemical Physics</i> , 2005, 122, 194104.	1.2	31
3357	Orbital-dependent correlation energy in density-functional theory based on a second-order perturbation approach: Success and failure. <i>Journal of Chemical Physics</i> , 2005, 123, 062204.	1.2	99
3358	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. <i>Journal of Chemical Physics</i> , 2005, 123, 084107.	1.2	107
3359	Extension of renormalized coupled-cluster methods including triple excitations to excited electronic states of open-shell molecules. <i>Journal of Chemical Physics</i> , 2005, 122, 214107.	1.2	113
3360	Active-space equation-of-motion coupled-cluster methods for excited states of radicals and other open-shell systems: EA-EOMCCSDt and IP-EOMCCSDt. <i>Journal of Chemical Physics</i> , 2005, 123, 134113.	1.2	103
3361	Electronic conductance through organic nanowires. <i>Physical Review B</i> , 2005, 71, .	1.1	29
3362	Mid-infrared characterization of the $\text{NH}_4^+(\text{H}_2\text{O})_n$ clusters in the neighborhood of the $n=20$ magic number. <i>Journal of Chemical Physics</i> , 2005, 123, 164309.	1.2	47
3363	Nuclear-electronic orbital nonorthogonal configuration interaction approach. <i>Journal of Chemical Physics</i> , 2005, 123, 134108.	1.2	51
3364	Magnetized/charged MgH_2 -based hydrogen storage materials. <i>Applied Physics Letters</i> , 2005, 86, 213109.	1.5	17
3365	Theoretical study of the electronic spectroscopy of CO adsorbed on Pt(111). <i>Journal of Chemical Physics</i> , 2005, 122, 184706.	1.2	19
3366	Analysis of the nuclear-electronic orbital method for model hydrogen transfer systems. <i>Journal of Chemical Physics</i> , 2005, 123, 014303.	1.2	25
3367	Comparison of low-order multireference many-body perturbation theories. <i>Journal of Chemical Physics</i> , 2005, 122, 134105.	1.2	62
3368	Exploring electron density distributions for the complete valence shell of cyclopentene using a binary(e,2e)spectrometer. <i>Physical Review A</i> , 2005, 72, .	1.0	2
3369	Complex polarization propagator method for calculation of dispersion coefficients of extended π -conjugated systems: The C6 coefficients of polyacenes and C60. <i>Journal of Chemical Physics</i> , 2005, 123, 124312.	1.2	32
3370	Density-functional study of the mechanical and electronic properties of narrow carbon nanotubes under axial stress. <i>Physical Review B</i> , 2005, 72, .	1.1	31
3371	The structure and spin-states of some Fe(III) mimics of nitrile hydratase, studied by DFT and ONIOM(DFT:PM3) calculations. <i>Molecular Physics</i> , 2005, 103, 905-923.	0.8	12
3372	Laser control of vibrational excitation in carboxyhemoglobin: A quantum wave packet study. <i>Journal of Chemical Physics</i> , 2005, 123, 044504.	1.2	35

#	ARTICLE	IF	CITATIONS
3373	Multireference second-order perturbation theory: How size consistent is \hat{e} almost size consistent \hat{e} . Journal of Chemical Physics, 2005, 122, 044105.	1.2	70
3374	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	1.2	396
3375	Equation-of-motion coupled-cluster study on exciton states of polyethylene with periodic boundary condition. Journal of Chemical Physics, 2005, 122, 224901.	1.2	33
3376	A phase-space approach to the T1 \rightarrow S0 radiationless decay in benzene: The effect of deuteration. Journal of Chemical Physics, 2005, 123, 074304.	1.2	10
3377	Time-dependent density-functional theory calculations of triplet-triplet absorption. Journal of Chemical Physics, 2005, 122, 224104.	1.2	12
3378	METAL ATOM ENDOHEDRALLY DOPED C20 CAGE STRUCTURE: (X@C20; X =Ni, Fe, Co). International Journal of Modern Physics C, 2005, 16, 1553-1560.	0.8	2
3379	Aza-substitution effect on the Q-band excitations of free-base porphin, chlorin, and bacteriochlorin: SAC-CI theoretical study. Journal of Porphyrins and Phthalocyanines, 2005, 09, 305-315.	0.4	9
3380	STRUCTURAL AND ELECTRONIC PROPERTIES OF (CnLi)+ CLUSTER IONS. International Journal of Modern Physics C, 2005, 16, 271-280.	0.8	1
3381	Two-Bond Spin \rightarrow Spin Coupling Constants (2hJXY) Across XHY Hydrogen Bonds: Some Fundamental Questions. Advances in Quantum Chemistry, 2005, , 23-35.	0.4	4
3382	Enhanced triplet exciton generation in polyfluorene blends. Physical Review B, 2005, 71, .	1.1	96
3383	Computational Characterization of the Role of the Base in the Suzuki \rightarrow Miyaura Cross-Coupling Reaction. Journal of the American Chemical Society, 2005, 127, 9298-9307.	6.6	317
3384	Renormalized coupled-cluster methods exploiting left eigenstates of the similarity-transformed Hamiltonian. Journal of Chemical Physics, 2005, 123, 224105.	1.2	391
3385	Theoretical Study of the Solvation of Fluorine and Chlorine Anions by Water. Journal of Physical Chemistry A, 2005, 109, 7688-7699.	1.1	82
3386	Energetic Aspects of Cyclic Pi-Electron Delocalization: A Evaluation of the Methods of Estimating Aromatic Stabilization Energies. Chemical Reviews, 2005, 105, 3773-3811.	23.0	559
3387	Intermolecular Proton Transfer in Anionic Complexes of Uracil with Alcohols. Journal of Physical Chemistry B, 2005, 109, 13383-13391.	1.2	55
3388	Mechanism of Enyne Metathesis Catalyzed by Grubbs Ruthenium \rightarrow Carbene Complexes: A DFT Study. Journal of the American Chemical Society, 2005, 127, 7444-7457.	6.6	139
3389	Application of the Palladium(0)-Catalyzed Ullmann Cross-Coupling Reaction in a Total Synthesis of (A \pm)-Aspidospermidine and thus Representing an Approach to the Lower Hemisphere of the Binary Indole - Indoline Alkaloid Vinblastine. Australian Journal of Chemistry, 2005, 58, 722.	0.5	40
3390	A computational study of the 1,3-dipolar cycloaddition reaction mechanism for nitrilimines. Canadian Journal of Chemistry, 2005, 83, 1615-1625.	0.6	17

#	ARTICLE	IF	CITATIONS
3391	Exploring the Mechanism for the Synthesis of Silsesquioxanes. 4. The Synthesis of T8. Journal of Physical Chemistry A, 2005, 109, 5424-5429.	1.1	29
3392	Ground- and excited-state electronic structure of an iron-containing molecular spin photoswitch. Journal of Chemical Physics, 2005, 123, 094709.	1.2	9
3393	An ab initio study of 1,5-suprafacial shifts in 5-substituted 1,3-cyclopentadienes. Canadian Journal of Chemistry, 2005, 83, 1299-1305.	0.6	6
3394	Successes and failures of time-dependent density functional theory for the low-lying excited states of chlorophylls. Molecular Physics, 2005, 103, 1057-1065.	0.8	37
3395	Towards an understanding of structure-property relationships in hole-transport materials: The influence of molecular conformation on oxidation potential in poly(aryl)amines. Journal of Materials Chemistry, 2005, 15, 2304.	6.7	115
3396	Evaluation of the field-adapted ADMA approach: absolute and relative energies of crambin and derivatives. Physical Chemistry Chemical Physics, 2005, 7, 4061.	1.3	45
3397	Unusual structural and energetic features of homolytic bond dissociation: from tetrakis(disilyl)diphosphine to tetrakis(di-tert-butylsilyl)hydrazine. Dalton Transactions, 2005, , 2382.	1.6	3
3398	The molecular structure of [Sn(P2C2But2)] using gas-phase electron diffraction and DFT calculations. Dalton Transactions, 2005, , 1972.	1.6	11
3399	Use of tetrameric cubane aggregates of lithium aryloxides as secondary building units in controlling network assembly. Chemical Communications, 2005, , 456.	2.2	52
3400	Can weak interactions modify the binding properties of a strong nitrogen donor? Unusual N-coordination of a phosphoranylidene-substituted pyrazolone unit towards palladium(ii) centres: an experimental and theoretical study. Dalton Transactions, 2005, , 3155.	1.6	7
3401	The role of multiple parallel and antiparallel local dipoles for molecular structure and intermolecular interactions of oxalamides. CrystEngComm, 2005, 7, 260-265.	1.3	14
3402	Linear Response Properties Required to Simulate Vibrational Spectra of Biomolecules in Various Media: (R)-Phenyloxirane (A Comparative Theoretical and Spectroscopic Vibrational Study). Advances in Quantum Chemistry, 2005, , 91-124.	0.4	13
3403	Theoretical Study of the Antioxidant Activity of Vitamin E: Reactions of α -Tocopherol with the Hydroperoxy Radical. Journal of Chemical Theory and Computation, 2005, 1, 337-344.	2.3	32
3404	Anharmonic Vibrational Properties of Explosives from Temperature-Dependent Raman. Journal of Physical Chemistry A, 2005, 109, 9919-9927.	1.1	46
3405	A New Algorithm for Efficient Direct Dynamics Calculations of Large-Curvature Tunneling and Its Application to Radical Reactions with 9×15 Atoms. Journal of Chemical Theory and Computation, 2005, 1, 1063-1078.	2.3	33
3406	Balancing Dynamic and Nondynamic Correlation for Diradical and Aromatic Transition States: A Renormalized Coupled-Cluster Study of the Cope Rearrangement of 1,5-Hexadiene. Journal of the American Chemical Society, 2005, 127, 2608-2614.	6.6	56
3407	Gas-phase structures of aminodifluorophosphines determined using electron diffraction data and computational techniques. Dalton Transactions, 2005, , 2572.	1.6	2
3408	The experimental gas-phase structures of 1,3,5-trisilylbenzene and hexasilylbenzene and the theoretical structures of all benzenes with three or more silyl substituents. Dalton Transactions, 2005, , 2292.	1.6	6

#	ARTICLE	IF	CITATIONS
3409	The electron transfer rate of large TPA based compounds: a joint theoretical and electrochemical approach. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3738.	1.3	17
3410	Influence of the terminal ligands on the redox properties of the $\{Pt_2(\mu-S)_2\}$ core in $[Pt_2(Ph_2X(CH_2)_2XPh_2)_2(\mu-S)_2]$ (X = P or As) complexes and on their reactivity towards metal centres, protic acids and organic electrophiles. <i>Dalton Transactions</i> , 2005, , 2742.	1.6	28
3411	Ruthenium trihydrides with N-heterocyclic carbene ligands: effects on quantum mechanical exchange coupling. <i>Chemical Communications</i> , 2005, , 5994.	2.2	10
3412	Preparation and characterization of diarylphosphazene and diarylphosphinohydrazide complexes of titanium, tungsten and ruthenium and phosphorylketimido complexes of rhenium. <i>Dalton Transactions</i> , 2005, , 680.	1.6	12
3413	Ti ₂ C ₈₀ is more likely a titanium carbide endohedral metallofullerene (Ti ₂ C ₂)@C ₇₈ . <i>Chemical Communications</i> , 2005, , 4444.	2.2	68
3414	Carbonate, carbamate, urea, and guanidine as model species for functional groups in biological molecules— A combined density functional theory and mass spectrometry examination of polysodiation and gas-phase dissociation. <i>Canadian Journal of Chemistry</i> , 2005, 83, 1941-1952.	0.6	7
3415	First Singlet (n, π^*) Excited State of Hydrogen-Bonded Complexes between Water and Pyrimidine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1576-1586.	1.1	13
3416	New Type of Bonding Formed from an Overlap between π Aromatic and π^* CO Molecular Orbitals Stabilizes the Coexistence in One Molecule of the Ionic and Neutral meso-ionic Forms of Imidazopyridine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4568-4574.	1.1	12
3417	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 43.	1.3	393
3418	Theory of Nanoscale Atomic Lithography. An ab Initio Study of the Interaction of Xe Cs Atoms with Organthiols Self-assembled Monolayers on Au(111). <i>Journal of Physical Chemistry B</i> , 2005, 109, 1815-1821.	1.2	5
3419	Regioselectivity of the Addition of O ₂ on SPS-Based Rhodium(I) and Iridium(I) Complexes. <i>Organometallics</i> , 2005, 24, 1608-1613.	1.1	18
3420	Theoretical Investigation of Uranyl Dihydroxide: μ -Oxo Ligand Exchange, Water Catalysis, and Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8579-8586.	1.1	35
3421	⁴ JCOCH and ⁴ JCCCCH as Probes of Exocyclic Hydroxymethyl Group Conformation in Saccharides. <i>Journal of Organic Chemistry</i> , 2005, 70, 7542-7549.	1.7	22
3422	Ab Initio Study of Complexes with Two Cations as N-H Donors to F- Structures and Spin-Spin Coupling Constants across N-H...F Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10753-10758.	1.1	11
3423	Combined Quantum Mechanical/Molecular Mechanical Study on the Pentacoordinated Ferric and Ferrous Cytochrome P450cam Complexes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1268-1280.	1.2	60
3424	Density Functional Theory Predicts the Barriers for Radical Fragmentation in Solution. <i>Journal of Organic Chemistry</i> , 2005, 70, 2014-2020.	1.7	19
3425	Hydrogen Bonding and Covalent Effects in Binding of Cisplatin to Purine Bases: An Ab Initio and Atoms in Molecules Studies. <i>Inorganic Chemistry</i> , 2005, 44, 267-274.	1.9	52
3426	Hydrogen Elimination from a Hydroxycyclopentadienyl Ruthenium(II) Hydride: A Study of Hydrogen Activation in a Ligand-Metal Bifunctional Hydrogenation Catalyst. <i>Journal of the American Chemical Society</i> , 2005, 127, 3100-3109.	6.6	160

#	ARTICLE	IF	CITATIONS
3427	Characterization of the Conformational Probability of N-Acetyl-Phenylalanyl-NH ₂ by RHF, DFT, and MP2 Computation and AIM Analyses, Confirmed by Jet-Cooled Infrared Data. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5289-5302.	1.1	32
3428	Theoretical Study of the $\hat{\pm}$ -Cyclodextrin Dimer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3209-3219.	1.1	43
3429	B3LYP and MP2 Calculations of the Enthalpies of Hydrogen-Bonded Complexes of Methanol with Neutral Bases and Anions: Comparison with Experimental Data. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11907-11913.	1.1	75
3430	Characterizing Hydrogen Bonding and Proton Transfer in 2:1 FH:NH ₃ and FH:Collidine Complexes through One- and Two-Bond Spin-Spin Coupling Constants across Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10759-10769.	1.1	30
3431	Hydrogen Bond vs Proton Transfer in HZSM5 Zeolite. A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19301-19308.	1.2	22
3432	Computational Rationalization of the Dependence of the Enantioselectivity on the Nature of the Catalyst in the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. <i>Journal of the American Chemical Society</i> , 2005, 127, 3624-3634.	6.6	73
3433	The Electronic Structure of Inorganic Benzenes: Valence Bond and Ring-Current Descriptions. <i>Inorganic Chemistry</i> , 2005, 44, 5266-5272.	1.9	71
3434	Cyclocarbopalladation Involving an Unusual 1,5-Palladium Vinyl to Aryl Shift as Termination Step: Theoretical Study of the Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 7171-7182.	6.6	147
3435	Proximity Effects in the Palladium-Catalyzed Substitution of Aryl Fluorides. <i>Organic Letters</i> , 2005, 7, 1011-1014.	2.4	43
3436	Silicon-Nitrogen Bonding in Silatranes: Assignment of Photoelectron Spectra. <i>Journal of the American Chemical Society</i> , 2005, 127, 986-995.	6.6	46
3437	Potential Energy Surfaces of SimOnCluster Formation and Isomerization. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6294-6302.	1.1	37
3438	Surface SN ₂ Reaction by H ₂ O on Chlorinated Si(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10909-10914.	1.2	7
3439	Multireference calculations of the fluorescence, phosphorescence and photodissociation of p-chlorotoluene. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3938.	1.3	8
3440	Photodissociation of Azulene at 193 nm: Ab Initio and RRKM Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8774-8784.	1.1	27
3441	Analytical gradients for LEDO-DFT. <i>Molecular Physics</i> , 2005, 103, 175-182.	0.8	3
3442	Determination of the Temperature Dependence of the H $\hat{\pm}$ D Spin-Spin Coupling Constant and the Isotope Effect on the Proton Chemical Shift for the Compressed Dihydride Complex [Cp*Ir(P $\hat{\pm}$ P)H ₂] ²⁺ . <i>Journal of the American Chemical Society</i> , 2005, 127, 5632-5640.	6.6	37
3443	Mechanisms of Methane Activation and Transformation on Molybdenum Oxide Based Catalysts. <i>Journal of the American Chemical Society</i> , 2005, 127, 3989-3996.	6.6	134
3444	Geometric and Electronic Structures of Multiple-Decker One-End Open Sandwich Clusters: Eun(C ₈ H ₈) _n (n = 1-4). <i>Journal of Physical Chemistry A</i> , 2005, 109, 2476-2486.	1.1	35

#	ARTICLE	IF	CITATIONS
3445	Experimental and Theoretical Studies of Carbodiphosphorane π CX ₂ Adducts with Unusual Bonding Situations: A Preparation, Crystal Structures, and Bonding Analyses of S ₂ CC(PPh ₃) ₂ , O ₂ CC(PPh ₃) ₂ , and [(CO) ₄ MS ₂ CC(PPh ₃) ₂] (M = Cr, Mo, W). <i>Inorganic Chemistry</i> , 2005, 44, 1263-1274.	1.9	90
3446	Mechanisms of Initial Propane Activation on Molybdenum Oxides: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6416-6421.	1.2	63
3447	Generalized Anomeric Interpretation of the σ -High-Energy σ N π P Bond in N-Methyl-N π -phosphorylguanidine: Importance of Reinforcing Stereoelectronic Effects in σ -High-Energy σ Phosphoester Bonds. <i>Journal of the American Chemical Society</i> , 2005, 127, 17789-17798.	6.6	20
3448	Calculation of Vibrational Spectra of Linear Tetrapyrroles. 3. Hydrogen-Bonded Hexamethylpyromethene Dimers. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2139-2150.	1.1	20
3449	Condensed-Phase Effects on the Structural Properties of C ₆ H ₅ CN π BF ₃ and (CH ₃) ₃ CCN π BF ₃ : IR Spectra, Crystallography, and Computations. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8199-8208.	1.1	35
3450	Structural and Thermodynamic Features of Spiroiminodihydantoin Damaged DNA Duplexes. <i>Biochemistry</i> , 2005, 44, 13342-13353.	1.2	47
3451	Chemical Reactivities of the Cation and Anion of M@C ₈₂ (M = Y, La, and Ce). <i>Journal of the American Chemical Society</i> , 2005, 127, 2143-2146.	6.6	54
3452	PGSE NMR Diffusion, Overhauser, and DFT Studies on the Salts [Pd(π -3-CH ₃ CHCHCHPh)(dppe)](anion). <i>Organometallics</i> , 2005, 24, 5710-5717.	1.1	18
3453	Comparative Study of Surface Cycloadditions of Ethylene and 2-Butene on the Si(100)-2 \times 1 Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5067-5072.	1.2	23
3454	Energetics of the N π O Bonds in 2-Hydroxyphenazine-di-N-oxide. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16188-16195.	1.2	16
3455	Properties of Ternary Insulating Systems: The Electronic Structure of MgSO ₄ \cdot H ₂ O. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4118-4124.	1.1	16
3456	Quantum Mechanics/Molecular Mechanics Calculations of the Vanadium Dependent Chloroperoxidase. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1265-1274.	2.3	53
3457	Factors Controlling Metal-Ion Selectivity in the Binding Sites of Calcium-Binding Proteins. The Metal-Binding Properties of Amide Donors. A Crystallographic and Thermodynamic Study. <i>Inorganic Chemistry</i> , 2005, 44, 8495-8502.	1.9	39
3458	Quantum Chemical and Master Equation Simulations of the Oxidation and Isomerization of Vinyloxy Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2514-2524.	1.1	43
3459	Ultrafast Infrared Mechanistic Studies of the Interaction of 1-Hexyne with Group 6 Hexacarbonyl Complexes. <i>Organometallics</i> , 2005, 24, 1852-1859.	1.1	28
3460	Performance of Molecular Orbital Methods and Density Functional Theory in the Computation of Geometries and Energies of Metal Aqua Ions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1510-1527.	1.2	102
3461	Helix Switching of a Key Active-Site Residue in the Cytochrome _{bb3} Oxidases. <i>Biochemistry</i> , 2005, 44, 10766-10775.	1.2	56
3462	Intrinsic Carbon π Carbon Bond Reactivity at the Manganese Center of Oxalate Decarboxylase from Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 994-1007.	2.3	11

#	ARTICLE	IF	CITATIONS
3463	The Nature of Interactions in the Ionic Crystal of 3-Pentenenitrile, 2-Nitro-5-oxo, Ion ($\hat{\sim}1$), Sodium. Journal of Physical Chemistry B, 2005, 109, 2027-2033.	1.2	38
3464	Electronic Structure, Excited States, and Photoelectron Spectra of Uranium, Thorium, and Zirconium Bis(Ketimido) Complexes $(C_5R_5)_2M[\hat{\sim}NCP_2]_2$ ($M = Th, U, Zr$; $R = H, CH_3$). Journal of Physical Chemistry A, 2005, 109, 5481-5491.	1.1	40
3465	DFT/Electrostatic Calculations of pKaValues in CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 3616-3626.	1.2	54
3466	Theoretical Group 14 Chemistry. 4. Cyclotriplumbanes: Relativistic and Substituents Effects. Journal of Chemical Theory and Computation, 2005, 1, 1298-1303.	2.3	5
3467	Chemical Reactivity of $Sc_3N@C_{80}$ and $La_2@C_{80}$. Journal of the American Chemical Society, 2005, 127, 9956-9957.	6.6	134
3468	Understanding Structural and Dynamic Properties of Well-Defined Rhenium-Based Olefin Metathesis Catalysts, $Re(\hat{\sim}CR)(CHR)(X)(Y)$, from DFT and QM/MM Calculations. Organometallics, 2005, 24, 1586-1597.	1.1	59
3469	Theoretical Study of $C\hat{\sim}H$ and $C\hat{\sim}F$ Activation in CH_4-nFn ($n = 1\hat{\sim}4$) Molecules by Platinum. Journal of Physical Chemistry A, 2005, 109, 10587-10593.	1.1	12
3470	Modeling Water Exchange on an Aluminum Polyoxocation. Journal of Physical Chemistry B, 2005, 109, 23771-23775.	1.2	20
3471	Which Do Endohedral Ti_2C_{80} Metallofullerenes Prefer Energetically: $Ti_2@C_{80}$ or $Ti_2C_2@C_{78}$? A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 20251-20255.	1.2	78
3472	Mechanism of Ligand Exchange Studied Using Transition Path Sampling. Journal of the American Chemical Society, 2005, 127, 1286-1290.	6.6	22
3473	Cycloaddition of Benzene on Si(100) and Its Surface Conversions. Journal of the American Chemical Society, 2005, 127, 3131-3139.	6.6	48
3474	Photostability via a Sloped Conical Intersection: A CASSCF and RASSCF Study of Pyracylene. Journal of Physical Chemistry A, 2005, 109, 8849-8856.	1.1	22
3475	Computational Exploration of the Catalytic Mechanism of Dopamine $\hat{2}$ -Monoxygenase: Modeling of Its Mononuclear Copper Active Sites. Inorganic Chemistry, 2005, 44, 4226-4236.	1.9	82
3476	Reversible and Regioselective Reaction of $La@C_{82}$ with Cyclopentadiene. Journal of the American Chemical Society, 2005, 127, 12190-12191.	6.6	61
3477	Stabilization of Zwitterions in Solution: GABA Analogues. Journal of Physical Chemistry A, 2005, 109, 4195-4201.	1.1	21
3478	Intramolecular Hydrogen Bonding in Disubstituted Ethanes. A Comparison of $NH\hat{\sim}O$ - and $OH\hat{\sim}O$ -Hydrogen Bonding through Conformational Analysis of 4-Amino-4-oxobutanoate (succinamate) and Monohydrogen 1,4-Butanoate (monohydrogen succinate) Anions. Journal of Physical Chemistry A, 2005, 109, 9076-9082.	1.1	33
3479	Theoretical UV Circular Dichroism of Aliphatic Cyclic Dipeptides. Journal of Physical Chemistry A, 2005, 109, 5463-5470.	1.1	19
3480	New Effective Core Method (Effective Core Potential and Valence Basis Set) for Al Clusters and Nanoparticles and Heteronuclear Al-Containing Molecules. Journal of Chemical Theory and Computation, 2005, 1, 41-53.	2.3	21

#	ARTICLE	IF	CITATIONS
3481	Reactions of Neutral and Cationic Diamide-Supported Imido Complexes with CO ₂ and Other Heterocumulenes: Issues of Site Selectivity. <i>Organometallics</i> , 2005, 24, 2368-2385.	1.1	35
3482	Cycloaddition Isomerizations of Adsorbed 1,3-Cyclohexadiene on Si(100)-2 \times 1 Surface: First Neighbor Interactions. <i>Journal of the American Chemical Society</i> , 2005, 127, 8485-8491.	6.6	17
3483	The Band 12 Issue in the Electron Momentum Spectra of Norbornane: A Comparison with Additional Green's Function Calculations and Ultraviolet Photoemission Measurements. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4267-4273.	1.1	19
3484	Modeling the Absorption Spectrum of Tryptophan in Proteins. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23061-23069.	1.2	46
3485	Formation of Abundant [Pb(H ₂ O)] ²⁺ by Ligand-Exchange Reaction between [Pb(N ₂) _n] ²⁺ (n = 1-3) and H ₂ O. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10590-10593.	1.2	16
3486	Probing Occupied States of the Molecular Layer in Au-Alkanedithiol-GaAs Diodes. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5719-5723.	1.2	24
3487	8-Endo versus 7-Exo Cyclization of $\hat{\pm}$ -Carbamoyl Radicals. A Combination of Experimental and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2005, 70, 1539-1544.	1.7	37
3488	Study on Conformation Interconversion of 3-Alkyl-4-acetyl-3,4-dihydro-2H-1,4-benzoxazines from Dynamic NMR Experiments and ab Initio Density Functional Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18690-18698.	1.2	12
3489	Mechanism of the Aminolysis of Methyl Benzoate: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11470-11474.	1.1	41
3490	Trapping of the OH Radical by $\hat{\pm}$ -Tocopherol: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4777-4784.	1.1	39
3491	Surface-Stabilized Amorphous Germanium Nanoparticles for Lithium-Storage Material. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20719-20723.	1.2	112
3492	Reversal of Reactivity in Diene-Complexed Quinone Methide Complexes: Insights and Explanations from ab Initio Density Functional Theory Calculations. <i>Organometallics</i> , 2005, 24, 4232-4240.	1.1	14
3493	Aminoimidazolymethyluracil Analogues as Potent Inhibitors of Thymidine Phosphorylase and Their Bioreductive Nitroimidazolyl Prodrugs. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 392-402.	2.9	43
3494	AB INITIO QUANTUM CHEMICAL AND MIXED QUANTUM MECHANICS/MOLECULAR MECHANICS (QM/MM) METHODS FOR STUDYING ENZYMATIC CATALYSIS. <i>Annual Review of Physical Chemistry</i> , 2005, 56, 389-427.	4.8	493
3495	Using Hessian Updating To Increase the Efficiency of a Hessian Based Predictor-Corrector Reaction Path Following Method. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 61-69.	2.3	810
3496	Multilayer Formulation of the Fragment Molecular Orbital Method (FMO). <i>Journal of Physical Chemistry A</i> , 2005, 109, 2638-2646.	1.1	125
3497	Multiconfiguration self-consistent-field theory based upon the fragment molecular orbital method. <i>Journal of Chemical Physics</i> , 2005, 122, 054108.	1.2	115
3498	The 2.1 \AA ... Crystal Structure of the Far-red Fluorescent Protein HcRed: Inherent Conformational Flexibility of the Chromophore. <i>Journal of Molecular Biology</i> , 2005, 349, 223-237.	2.0	79

#	ARTICLE	IF	CITATIONS
3499	A structural model of $\text{La}_2\text{O}_3\text{-Nb}_2\text{O}_5\text{-B}_2\text{O}_3$ glasses based upon infrared and luminescence spectroscopy and quantum chemical calculations. <i>Journal of Non-Crystalline Solids</i> , 2005, 351, 3121-3126.	1.5	35
3500	Theoretical investigation of iron isotope fractionation between $\text{Fe}(\text{H}_2\text{O})_6^{3+}$ and $\text{Fe}(\text{H}_2\text{O})_6^{2+}$: Implications for iron stable isotope geochemistry. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 825-837.	1.6	219
3501	Sorption of naphthalene derivatives to soils from a long-term field experiment. <i>Chemosphere</i> , 2005, 59, 639-647.	4.2	23
3502	An Experimental and Theoretical Study of Stereoselectivity of Furan \rightarrow Maleic Anhydride and Furan \rightarrow Maleimide Diels \rightarrow Alder Reactions. <i>Journal of Organic Chemistry</i> , 2005, 70, 6295-6302.	1.7	107
3503	Electronic and magnetic properties of a hexanuclear ferric wheel. <i>European Physical Journal B</i> , 2005, 44, 209-215.	0.6	4
3504	Time-resolved gas-phase kinetic and quantum chemical studies of the reaction of silylene with oxygen. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2900.	1.3	30
3505	$[(\text{Triphos})\text{Ni}(\eta^2\text{-BH}_4)]$: An Unusual Nickel(I) Borohydride Complex. <i>Inorganic Chemistry</i> , 2005, 44, 8650-8652.	1.9	46
3506	Evaluation of Functionals O3LYP, KMLYP, and MPW1K in Comparison to B3LYP for Selected Transition-Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 848-855.	2.3	54
3507	Theoretical study of the o-OH participation in catechol ester ammonolysis. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 737.	1.5	16
3508	O-Atom Transport Catalysis by Atomic Cations in the Gas Phase: O^+ Reduction of N_2O by CO . <i>Journal of the American Chemical Society</i> , 2005, 127, 3545-3555.	6.6	136
3509	The structure, energetics, and nature of the chemical bonding of phenylthiol adsorbed on the Au(111) surface: Implications for density-functional calculations of molecular-electronic conduction. <i>Journal of Chemical Physics</i> , 2005, 122, 094708.	1.2	150
3510	Matrix Isolation FTIR Spectroscopic and Theoretical Study of Dimethyl Sulfite. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3578-3586.	1.1	34
3511	Theoretical and Experimental Evaluation of Homo- and Heterodimeric Hydrogen-Bonded Motifs Containing Boronic Acids, Carboxylic Acids, and Carboxylate Anions: Application for the Generation of Highly Stable Hydrogen-Bonded Supramolecular Systems. <i>Crystal Growth and Design</i> , 2005, 5, 167-175.	1.4	80
3512	d ORe -Based Olefin Metathesis Catalysts, $\text{Re}(\text{CHR})(\text{X})(\text{Y})$: The Key Role of X and Y Ligands for Efficient Active Sites. <i>Journal of the American Chemical Society</i> , 2005, 127, 14015-14025.	6.6	158
3513	Adsorption of NH_3 and H_2O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3539-3545.	1.2	96
3514	Synthesis and structural study of new highly lipophilic 1,4-dihydropyridines. <i>New Journal of Chemistry</i> , 2005, 29, 1567.	1.4	17
3515	Ab Initio Study of the Influence of Trimer Formation on One- and Two-Bond Spin \rightarrow Spin Coupling Constants Across an $\text{X}^{\text{A}}\text{-H}^{\text{B}}\text{-Y}$ Hydrogen Bond: $\text{AH}:\text{XH}:\text{YH}_3$ Complexes for A, X = 19F, 35Cl and Y = 15N, 31P. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2350-2355.	1.1	10
3516	Excited electronic states of small water clusters. <i>Journal of Chemical Physics</i> , 2005, 122, 044111.	1.2	69

#	ARTICLE	IF	CITATIONS
3517	Computational estimates of the gas-phase basicities, proton affinities and ionization potentials of the six isomers of dihydroxybenzoic acid. <i>Molecular Physics</i> , 2005, 103, 183-189.	0.8	24
3518	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Real Catalyst, Ligand Effects, and Solvation Effects. <i>Journal of the American Chemical Society</i> , 2005, 127, 4021-4032.	6.6	183
3519	Principal Active Species of Horseradish Peroxidase, Compound I: A Hybrid Quantum Mechanical/Molecular Mechanical Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 13611-13621.	6.6	77
3520	Treatment of Substitution and Rearrangement Mechanisms of Transition Metal Complexes with Quantum Chemical Methods. <i>Chemical Reviews</i> , 2005, 105, 2003-2038.	23.0	167
3521	An ab initio study of the structure, torsional potential energy function, and electric properties of disilane, ethane, and their deuterated isotopomers. <i>Journal of Chemical Physics</i> , 2005, 122, 054315.	1.2	34
3522	Excited States of Porphyrin Isomers and Porphycene Derivatives: A SAC-CI Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3187-3200.	1.1	46
3523	PRACTICAL PERFORMANCE ASSESSMENT OF ACCOMPANYING COORDINATE EXPANSION RECURRENCE RELATION ALGORITHM FOR COMPUTATION OF ELECTRON REPULSION INTEGRALS. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 139-149.	1.8	8
3524	Vibrational Raman optical activity as a mean for revealing the helicity of oligosilanes: A quantum chemical investigation. <i>Journal of Chemical Physics</i> , 2005, 122, 214304.	1.2	23
3525	Density Functional Theory Predictions of Isotropic Hyperfine Coupling Constants. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1114-1124.	1.1	102
3526	Single Electron Traps at the Surface of Polycrystalline MgO: Assignment of the Main Trapping Sites. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7314-7322.	1.2	74
3527	When Light Falls in LOV: A Quantum Mechanical/Molecular Mechanical Study of Photoexcitation in Phot-LOV1 of <i>Chlamydomonas reinhardtii</i> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 13006-13013.	1.2	65
3528	Quantum Chemical and Master Equation Studies of the Methyl Vinyl Carbonyl Oxides Formed in Isoprene Ozonolysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10710-10725.	1.1	56
3529	Ligand-Assisted Reduction of Osmium Tetroxide with Molecular Hydrogen via a [3+2] Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 3423-3432.	6.6	37
3530	Can Steric Effects Induce the Mechanism Switch in the Rhodium-Catalyzed Imine Boration Reaction? A Density Functional and ONIOM Study. <i>Organometallics</i> , 2005, 24, 1938-1946.	1.1	34
3531	The (010) surface of $\text{H}_2\text{-MoO}_3$, a DFT + U study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3819.	1.3	146
3532	Simulation of Fullerite C60 Polymerization Under Particle Beam Irradiation. <i>Molecular Crystals and Liquid Crystals</i> , 2005, 426, 171-178.	0.4	4
3533	Amphoteric doping of carbon nanotubes by encapsulation of organic molecules: Electronic properties and quantum conductance. <i>Journal of Chemical Physics</i> , 2005, 123, 024705.	1.2	62
3534	Investigation of isotope effects with the nuclear-electronic orbital approach. <i>Journal of Chemical Physics</i> , 2005, 123, 064104.	1.2	65

#	ARTICLE	IF	CITATIONS
3535	TDDFT Study of One- and Two-Photon Absorption Properties: A Donor-Acceptor Chromophores. <i>Journal of Physical Chemistry B</i> , 2005, 109, 1803-1814.	1.2	101
3536	The structures of higher boron halides B ₈ X ₁₂ (X = F, Cl, Br and I) by gas-phase electron diffraction and ab initio calculations. <i>Dalton Transactions</i> , 2005, , 607.	1.6	13
3537	Inorganic-Metalorganic Hybrids Based on Copper(II)-Monosubstituted Keggin Polyanions and Dinuclear Copper(II)-Oxalate Complexes. Synthesis, X-ray Structural Characterization, and Magnetic Properties. <i>Inorganic Chemistry</i> , 2005, 44, 9731-9742.	1.9	132
3538	Solid-State Modeling of the Terahertz Spectrum of the High Explosive HMX. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1951-1959.	1.1	166
3539	Mechanism of the Aerobic Oxidation of Alcohols by Palladium Complexes of N-Heterocyclic Carbenes. <i>Journal of the American Chemical Society</i> , 2006, 128, 9651-9660.	6.6	77
3540	Dependence of the Intermolecular Electrostatic Interaction Energy on the Level of Theory and the Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 81-89.	2.3	36
3541	A fragment molecular-orbital-multicomponent molecular-orbital method for analyzing H/D isotope effects in large molecules. <i>Journal of Chemical Physics</i> , 2006, 124, 014112.	1.2	29
3542	A theoretical anharmonic study of the infrared absorption spectra of FHF ⁻ , FDF ⁻ , OHF ⁻ , and ODF ⁻ anions. <i>Journal of Chemical Physics</i> , 2006, 124, 174308.	1.2	29
3543	Adsorption of Benzene on Copper, Silver, and Gold Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1093-1105.	2.3	141
3544	Kinetics, Mechanism, and Computational Studies of Rhenium-Catalyzed Desulfurization Reactions of Thiiranes (Thioepoxides). <i>Inorganic Chemistry</i> , 2006, 45, 5351-5357.	1.9	16
3545	H-X Bond Activation via Hydrogen Transfer to Hydride in Ruthenium N-Heterocyclic Carbene Complexes: A Density Functional and Synthetic Studies. <i>Organometallics</i> , 2006, 25, 99-110.	1.1	44
3546	Aminophosphonates as organocatalysts in the direct asymmetric aldol reaction: towards syn selectivity in the presence of Lewis bases. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 2091-2096.	1.5	74
3547	A Theoretical Study on the Third-Order Nonlinear Optical Properties of π -Conjugated Linear Porphyrin Arrays. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4888-4899.	1.1	32
3548	Mono- and Bimetallic (NacNac)Ni Cyclopentadienyl Complexes. <i>Organometallics</i> , 2006, 25, 5870-5878.	1.1	21
3549	Resonance Raman Spectrum of the Solvated Electron in Methanol: A Simulation within a Cluster Model. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5613-5619.	1.1	6
3550	Mono- vs. bi-metallic assembly on a bulky bis(imino)terpyridine framework: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2006, , 2350-2361.	1.6	29
3551	Second-order Møller-Plesset perturbation energy obtained from divide-and-conquer Hartree-Fock density matrix. <i>Journal of Chemical Physics</i> , 2006, 125, 204106.	1.2	72
3552	Enantioselective Synthesis of Vinylcyclopropanes and Vinylepoxides Mediated by Camphor-Derived Sulfur Ylides: A Rationale of Enantioselectivity, Scope, and Limitation. <i>Journal of the American Chemical Society</i> , 2006, 128, 9730-9740.	6.6	181

#	ARTICLE	IF	CITATIONS
3553	[13C,15N]2-Acetamido-2-deoxy-d-aldohexoses and Their Methyl Glycosides: Synthesis and NMR Investigations of J-Couplings Involving 1H, 13C, and 15N. <i>Journal of Organic Chemistry</i> , 2006, 71, 466-479.	1.7	22
3554	Phosphorous oxygen hole centers in phosphosilicate glass films. <i>Physical Review B</i> , 2006, 74, .	1.1	12
3555	Ruthenium Tetraoxide Oxidations of Alkanes: DFT Calculations of Barrier Heights and Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2006, 71, 1755-1760.	1.7	38
3556	Diels Alder Reactions of Cyclopentadiene and 9,10-Dimethylanthracene with Cyanoalkenes: The Performance of Density Functional Theory and Hartree Fock Calculations for the Prediction of Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1216-1224.	1.1	67
3557	Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, [(SiO)Re(CR)(CHR)(CH ₂ R)], through DFT periodic calculations: silica is just a large siloxy ligand. <i>New Journal of Chemistry</i> , 2006, 30, 842-850.	1.4	77
3558	Synthesis, Reactivity, and DFT Studies of Tantalum Complexes Incorporating Diamido-N-heterocyclic Carbene Ligands. Facile Endocyclic C-H Bond Activation. <i>Journal of the American Chemical Society</i> , 2006, 128, 12531-12543.	6.6	87
3559	Structure and bonding in a cyclobutyl tris(pyrazolyl)boratoniobium complex and the variation in agostic behaviour with ring size in the series TpMe ₂ NbCl(c-C _n H _{2n-1})(MeCMe), n = 3-6. <i>Dalton Transactions</i> , 2006, , 2362-2367.	1.6	11
3560	4-Methoxy- and 4-cyano-substituted lithium aryloxides: electronic effects of substituents on aggregation. <i>Dalton Transactions</i> , 2006, , 1875.	1.6	25
3561	On the evaluation of quadratic response functions at the four-component Hartree-Fock level: Nonlinear polarization and two-photon absorption in bromo- and iodobenzene. <i>Journal of Chemical Physics</i> , 2006, 124, 214311.	1.2	8
3562	The nonadiabatic deactivation paths of pyrrole. <i>Journal of Chemical Physics</i> , 2006, 125, 164323.	1.2	101
3563	Distributed memory parallel implementation of energies and gradients for second-order Moller-Plesset perturbation theory with the resolution-of-the-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1159.	1.3	223
3564	An experimental and theoretical study of the molecular structure and vibrational spectra of iodotrimethylsilane (SiI ₃ Me ₃). <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 477-485.	1.3	9
3565	A new and convenient approach towards bis(iminophosphoranyl)methane ligands and their dicationic, cationic, anionic and dianionic derivatives. <i>New Journal of Chemistry</i> , 2006, 30, 1745-1754.	1.4	65
3566	Molecular structures of the 1,6-disubstituted triptycenes Sb ₂ (C ₆ F ₄) ₃ and Bi ₂ (C ₆ F ₄) ₃ using gas-phase electron diffraction and ab initio and DFT calculations. <i>Dalton Transactions</i> , 2006, , 1654-1659.	1.6	5
3567	Model studies of the CuB site of cytochrome c oxidase utilizing a Zn(ii) complex containing an imidazole phenol cross-linked ligand. <i>Dalton Transactions</i> , 2006, , 3326-3337.	1.6	9
3568	Catalysed low temperature H ₂ release from nitrogen heterocycles. <i>New Journal of Chemistry</i> , 2006, 30, 1675.	1.4	121
3569	An ab initio investigation of zinc chloro complexes. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 5428.	1.3	29
3570	Two conformational states of Glu242 and pK _a s in bovine cytochrome c oxidase. <i>Photochemical and Photobiological Sciences</i> , 2006, 5, 611.	1.6	19

#	ARTICLE	IF	CITATIONS
3571	Structural, spectroscopic, and electrochemical behavior of trans-phenolato cobalt(III) complexes of asymmetric NN \rightarrow O ligands as archetypes for metallomesogens. <i>Dalton Transactions</i> , 2006, , 2517-2525.	1.6	55
3572	Electronic properties and reactivity of Pt-doped carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3528.	1.3	28
3573	On the stereoselectivity of 4-penten-1-oxyl radical 5-exo-trig cyclizations. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 4089.	1.5	25
3574	Auolysis of $\hat{\text{I}}\pm$ -C-deprotonated group 6 aminocarbene and thiocarbene complexes with Ph ₃ PAu ⁺ . <i>Dalton Transactions</i> , 2006, , 4580-4589.	1.6	14
3575	Ab Initio Optical Rotatory Dispersion and Electronic Circular Dichroism Spectra of (S)-2-Chloropropionitrile. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7649-7654.	1.1	39
3576	Models for Solvation of Zirconocene Cations: $\hat{\text{A}}$ Synthesis, Reactivity, and Computational Studies of Cationic Zirconocene Benzyl Compounds. <i>Organometallics</i> , 2006, 25, 4427-4432.	1.1	15
3577	Functionalizing Titanium $\hat{\text{V}}$ Phosphinimide Complexes. <i>Organometallics</i> , 2006, 25, 4779-4786.	1.1	7
3578	Water Vibrational Bands as a Polarity Indicator in Ionic Liquids. <i>Zeitschrift Fur Physikalische Chemie</i> , 2006, 220, 1361-1376.	1.4	28
3579	Theoretical Studies of Borazines and Azaborines. <i>Inorganic Chemistry</i> , 2006, 45, 2494-2500.	1.9	26
3580	Probing the mechanism of hypoxia selectivity of copper bis(thiosemicarbazonato) complexes: DFT calculation of redox potentials and absolute acidities in solution. <i>Dalton Transactions</i> , 2006, , 783-794.	1.6	101
3581	Tryptophan $\hat{\text{B}}$ BODIPY: A versatile donor $\hat{\text{A}}$ acceptor pair for probing generic changes of intraprotein distances. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3130-3140.	1.3	24
3582	Quantum-size effects in capped and uncapped carbon nanotubes. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2006, 102, 71.	4.4	16
3583	Ab initio and RRKM study of photodissociation of azulene cation. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1404.	1.3	44
3584	A computational study of oxidation of ruthenium porphyrins via ORu ^{IV} and ORu ^{VIO} species. <i>Dalton Transactions</i> , 2006, , 1867.	1.6	14
3585	On the role of alkylcobalamins in the vitamin B12-catalyzed reductive dehalogenation of perchloroethylene and trichloroethylene. <i>Chemical Communications</i> , 2006, , 558-560.	2.2	24
3586	Heteroleptic Iridium(III) Complexes with Phenylpyridine and Diphenylquinoline Derivative Ligands. <i>Molecular Crystals and Liquid Crystals</i> , 2006, 462, 197-207.	0.4	6
3587	Correlation between atomic rearrangement in defective fullerenes and migration behavior of encaged metal ions. <i>Physical Review B</i> , 2006, 73, .	1.1	14
3588	Canonical transformation theory for multireference problems. <i>Journal of Chemical Physics</i> , 2006, 124, 194106.	1.2	204

#	ARTICLE	IF	CITATIONS
3589	Experimental and Theoretical UV Characterizations of Acetylacetone and Its Isomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3920-3926.	1.1	51
3590	Relationship between NMR Shielding and Heme Binding Strength for a Series of 7-Substituted Quinolines. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7787-7792.	1.1	15
3591	Stability and Thermal Rearrangement of (E,E)-1,3-Cycloheptadiene and trans-Bicyclo[3.2.0]hept-6-ene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2034-2038.	1.1	5
3592	A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 14571-14578.	6.6	100
3593	Measurement of Long-Range ^1H - ^{19}F Scalar Coupling Constants and Their Glycosidic Torsion Dependence in 5-Fluoropyrimidine-Substituted RNA. <i>Journal of the American Chemical Society</i> , 2006, 128, 5851-5858.	6.6	64
3594	Gas and Liquid Phase Acidity of Natural Antioxidants. <i>Journal of Agricultural and Food Chemistry</i> , 2006, 54, 3078-3085.	2.4	108
3595	Reaction of N-Vinyl Phosphazenes with α,β -Unsaturated Aldehydes. Azatriene-Mediated Synthesis of Dihydropyridines and Pyridines Derived from β -Amino Acids. <i>Journal of Organic Chemistry</i> , 2006, 71, 6020-6030.	1.7	42
3596	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution: A Combined Monte Carlo and Quantum Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7253-7261.	1.1	42
3597	Molecular Structures of Tris(dipivaloylmethanato) Complexes of the Lanthanide Metals, $\text{Ln}(\text{dpm})_3$, Studied by Gas Electron Diffraction and Density Functional Theory Calculations: A Comparison of the $\text{Ln}-\text{O}$ Bond Distances and Enthalpies in $\text{Ln}(\text{dpm})_3$ Complexes and the Cubic Sesquioxides, Ln_2O_3 . <i>Inorganic Chemistry</i> , 2006, 45, 5179-5186.	1.9	25
3598	Organolanthanide-Catalyzed Hydroamination/Cyclization Reactions of Aminoalkynes. Computational Investigation of Mechanism, Lanthanide Identity, and Substituent Effects for a Very Exothermic $\text{C}-\text{N}$ Bond-Forming Process. <i>Organometallics</i> , 2006, 25, 5533-5539.	1.1	80
3599	Mechanism of Olefin Hydrosilylation Catalyzed by $\text{RuCl}_2(\text{CO})_2(\text{PPh}_3)_2$: A DFT Study. <i>Organometallics</i> , 2006, 25, 4504-4513.	1.1	49
3600	Theoretical models of directional proton molecular transport. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 3096.	1.5	15
3601	Photochemistry of 1,2,4-Oxadiazoles. A DFT Study on Photoinduced Competitive Rearrangements of 3-Amino- and 3-N-Methylamino-5-perfluoroalkyl-1,2,4-oxadiazoles. <i>Journal of Organic Chemistry</i> , 2006, 71, 2740-2749.	1.7	15
3602	DFT calculations of $\text{d}(\text{M}(\text{NR})(\text{CHtBu})(\text{X})(\text{Y}))$ ($\text{M} = \text{Mo}, \text{W}$; $\text{R} = \text{CPh}_3, 2,6\text{-iPr}_2\text{C}_6\text{H}_3$; X and $\text{Y} = \text{CH}_2\text{tBu}, \text{OtBu}$). <i>Journal of Organometallic Chemistry</i> , 2006, , 3077-3087.	1.6	58
3603	Theoretical Study of Reactant Activation in 1,3-Dipolar Cycloadditions of Cyclic Nitrones to Free and Pt-Bound Nitriles. <i>Journal of Organic Chemistry</i> , 2006, 71, 582-592.	1.7	52
3604	Olefin epoxidation with tert-butyl hydroperoxide catalyzed by $\text{MoO}_2\text{X}_2\text{L}$ complexes: a DFT mechanistic study. <i>Dalton Transactions</i> , 2006, , 1383.	1.6	88
3605	The oxidized soot surface: Theoretical study of desorption mechanisms involving oxygenated functionalities and comparison with temperature programmed desorption experiments. <i>Journal of Chemical Physics</i> , 2006, 125, 194706.	1.2	37
3606	MAGNETIC EXCHANGE IN POLYNUCLEAR TRANSITION METAL SYSTEM: AB INITIO CASPT2 AND DENSITY FUNCTIONAL THEORY STUDY ON TRIANGULAR COPPER(II) COMPLEXES. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 501-514.	1.8	3

#	ARTICLE	IF	CITATIONS
3607	Electronic Structure Studies of Tetrazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11110-11119.	1.2	63
3608	Ring Currents in Tangentially π -Bonded π -Aromatic Systems. <i>Journal of Organic Chemistry</i> , 2006, 71, 6459-6467.	1.7	13
3609	Adsorption of Methanol on Zeolites X and Y. An Atomistic and Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 6170-6178.	1.2	28
3610	Substituent Effect on a Family of Quinones in Aprotic Solvents: An Experimental and Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9411-9419.	1.1	69
3611	Interplay of Structure and Reactivity in a Most Unusual Furan Diels-Alder Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 13130-13141.	6.6	46
3612	Combined DFT and electrostatics study of the proton pumping mechanism in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2006, 1757, 1035-1046.	0.5	57
3613	Characterization of Weak $\text{NH} \cdots \text{N}$ Intermolecular Interactions of Ammonia with Various Substituted N -Systems. <i>Journal of the American Chemical Society</i> , 2006, 128, 5416-5426.	6.6	107
3614	Structure, Bonding, and Paramagnetism in the Manganese(II) Tris-Allyl Anions $[\text{Mn}(\text{C}_3\text{H}_3\text{R}_2)_3]^-$ (R = H, Me). <i>Journal of Physical Chemistry B</i> , 2006, 110, 7843-7851.	1.1	21
3615	How Does Ammonium Dynamically Interact with Benzene in Aqueous Media? A First Principle Study Using the Car Parrinello Molecular Dynamics Method. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5094-5098.	1.2	31
3616	First-Principle Computational Study on the Full Conformational Space of L-Threonine Diamide, the Energetic Stability of Cis and Trans Isomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11527-11536.	1.1	14
3617	The Chemistry of Dinuclear Analogues of the Anticancer Drug Cisplatin. A DFT/CDM Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 1654-1663.	6.6	62
3618	Remote Substituent Effects in Ruthenium-Catalyzed [2+2] Cycloadditions: An Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2006, 71, 3793-3803.	1.7	30
3619	Tunneling Splitting of Energy Levels and Rotational Constants in the Vinyl Radical C_2H_3 . <i>Journal of Physical Chemistry A</i> , 2006, 110, 5430-5435.	1.1	20
3620	Unprecedented C_{26} -Anion in $\text{Sc}_4\text{C}_2@C_{80}$. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11098-11102.	1.2	48
3621	Silyl, Hydrido Silylene or Alternative Bonding Modes: The Many Possible Structures of $[(\text{C}_5\text{H}_5)(\text{PH}_3)\text{IrX}]^+$ (X = SiHR ₂ and SiR ₃ ; R = H, CH ₃ , SiH ₃ , and Cl). <i>Organometallics</i> , 2006, 25, 4748-4755.	1.1	11
3622	Computational Insights into the Mechanism of Radical Generation in B12-Dependent Methylmalonyl-CoA Mutase. <i>Journal of the American Chemical Society</i> , 2006, 128, 1287-1292.	6.6	83
3623	Flexible 5-Guanidino-4-nitroimidazole DNA Lesions: Structures and Thermodynamics. <i>Biochemistry</i> , 2006, 45, 6644-6655.	1.2	13
3624	New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands: Consequences of Meridional vs Facial Geometry. <i>Inorganic Chemistry</i> , 2006, 45, 10520-10529.	1.9	41

#	ARTICLE	IF	CITATIONS
3625	Silapropargyl/Silaallenyl and Silylene Acetylide Complexes of [Cp(CO) ₂ W] ⁺ . Theoretical Study of Their Interesting Bonding Nature and Formation Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 11927-11939.	6.6	28
3626	Structure and Enhanced Reactivity Rates of the D _{5h} Sc ₃ N@C ₈₀ and Lu ₃ N@C ₈₀ Metallofullerene Isomers: The Importance of the Pyracylene Motif. <i>Journal of the American Chemical Society</i> , 2006, 128, 8581-8589.	6.6	172
3627	Intramolecular 1, <i>n</i> Palladium Migrations in Polycyclic Aromatic Hydrocarbons. Palladium(II) versus Palladium(IV) Mechanisms: A Theoretical Study. <i>Organometallics</i> , 2006, 25, 3130-3142.	1.1	48
3628	Amine-Catalyzed B ⁺ O ⁺ C Bond Formation: Mechanistic Insights from Density Functional Theory and Second-Order Møller-Plesset Perturbation Theory. <i>Organometallics</i> , 2006, 25, 2427-2436.	1.1	0
3629	Ring Slippage vs Charge Transfer in the Reductive Chemistry of [IndMo(CO) ₂ (\pm -diimine)] ⁺ Cations. <i>Organometallics</i> , 2006, 25, 5223-5234.	1.1	11
3630	Theoretical Investigation of Luminescence Behavior as a Function of Alkyl Chain Size in 4-Aminobenzonitrile Alicyclic Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11455-11461.	1.1	36
3631	Photochemical Reactivity of 2-Vinylbiphenyl and 2-Vinyl-1,3-terphenyl: The Balance between Nonadiabatic and Adiabatic Photocyclization. <i>Journal of the American Chemical Society</i> , 2006, 128, 10533-10540.	6.6	22
3632	Stable Gas-Phase Radical Cations of Dimeric Tryptophan and Tyrosine Derivatives. <i>Journal of Physical Chemistry B</i> , 2006, 110, 8517-8523.	1.2	14
3633	Modeling Styrene π -Styrene Interactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 519-525.	1.1	36
3634	N- and P-Channel Transport Behavior in Thin Film Transistors Based on Tricyanovinyl-Capped Oligothiophenes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14590-14597.	1.2	63
3635	Theoretical Study of Adsorption of Sarin and Soman on Tetrahedral Edge Clay Mineral Fragments. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21175-21183.	1.2	37
3636	Spin-Crossover in an Iron(III) π -Bispidine π -Alkylperoxide System. <i>Inorganic Chemistry</i> , 2006, 45, 7077-7082.	1.9	47
3637	Ligand Rearrangement Reactions of Cr(CO) ₆ in Alcohol Solutions: Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 996-1005.	1.2	22
3638	Monte Carlo Simulation of Cisplatin Molecule in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12047-12054.	1.2	55
3639	Soluble Molecular Compounds with the Mg π O π Al Structural Motif: A Model Approach for the Fixation of Organometallics on a MgO Surface. <i>Journal of the American Chemical Society</i> , 2006, 128, 13056-13057.	6.6	35
3640	Effects of Tris(pyrazolyl)borato Ligand Substituents on Dioxygen Activation and Stabilization by Copper Compounds. <i>Inorganic Chemistry</i> , 2006, 45, 3594-3601.	1.9	19
3641	Tuning Indenyl Hapticity in Zirconium Bis(indenyl) Complexes with the Nature of Complementary Ligands. <i>Organometallics</i> , 2006, 25, 4698-4701.	1.1	8
3642	Do B3LYP and CCSD(T) Predict Different Hydrosilylation Mechanisms? Influences of Theoretical Methods and Basis Sets on Relative Energies in Ruthenium π -Silylene-Catalyzed Ethylene Hydrosilylation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1416-1425.	1.1	24

#	ARTICLE	IF	CITATIONS
3643	On the Electronic Structure of Neutral and Ionic Azobenzenes and Their Possible Role as Surface Mounted Molecular Switches. <i>Journal of Physical Chemistry B</i> , 2006, 110, 16337-16345.	1.2	80
3644	Charge-Transfer $\pi\pi^*$ Excited State in the 7-Azaindole Dimer. A Hybrid Configuration Interactions Singles/Time-Dependent Density Functional Theory Description. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1145-1151.	1.1	30
3645	Hydrogen Bonding Pathways in Human Dihydroorotate Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19704-19710.	1.2	7
3646	On the Nature of Unrestricted Orbitals in Variational Active Space Wave Functions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9915-9920.	1.1	5
3647	Photostability Via Sloped Conical Intersections: A Computational Study of the Excited States of the Naphthalene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13591-13599.	1.1	40
3648	Density Functional Theory Study of ^{14}N Isotropic Hyperfine Coupling Constants of Organic Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13600-13608.	1.1	55
3649	Synthesis, Structure, and Solution Dynamics of Neutral Allylnickel Complexes of N-Heterocyclic Carbenes. <i>Organometallics</i> , 2006, 25, 4391-4403.	1.1	42
3650	Inelastic Neutron Scattering Spectrum of $\text{Cs}_2[\text{B}_{12}\text{H}_{12}]$: A Reproduction of Its Solid-State Vibrational Spectrum by Periodic DFT. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3744-3749.	1.1	19
3651	Mixed P^{N} and As^{N} Bis-Ylide Palladium Complexes: A Cooperative Intramolecular Interactions, Conformational Preferences, and C^{H} Bond Activations. <i>Organometallics</i> , 2006, 25, 4653-4664.	1.1	31
3652	Experimental and Theoretical Study of the Vibrational Spectra of 12-Crown-4 Alkali Metal Cation Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8676-8687.	1.1	29
3653	Adsorption Reactions of Dimethylaluminum Isopropoxide and Water on the $\text{H}/\text{Si}(100)-2 \times 1$ Surface: A Initial Reactions for Atomic Layer Deposition of Al_2O_3 . <i>Journal of Physical Chemistry B</i> , 2006, 110, 11277-11283.	1.2	18
3654	Modeling of Hydrogen Bonds in Monohydrated 2,4-Dithiothymine: An Ab Initio and AIM Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1416-1422.	1.2	3
3655	Theoretical Study of the Complexes of Horminone with Mg^{2+} and Ca^{2+} Ions and Their Relation with the Bacteriostatic Activity. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4564-4573.	1.1	13
3656	Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Significant Acceleration by Water Molecules. <i>Organometallics</i> , 2006, 25, 3352-3363.	1.1	96
3657	Supramolecular Structures from Three New Molecular Building Blocks Based on the Protonation/Deprotonation of 3,3-Bis(2-imidazolyl)propionic Acid (HBIP): $[\text{H}_3\text{BIP}](\text{C}_4\text{O}_4) \cdot \text{H}_2\text{O}$, $[\text{Cu}(\text{HBIP})_2](\text{HC}_4\text{O}_4)_2$, and $[\text{Cu}(\text{BIP})_2] \cdot 2\text{H}_2\text{O}$. <i>Crystal Growth and Design</i> , 2006, 6, 1124-1133.	1.4	31
3658	Gaseous Bradykinin and Its Singly, Doubly, and Triply Protonated Forms: A First-Principles Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 7528-7537.	1.2	41
3659	An Efficient Proton-Coupled Electron-Transfer Process during Oxidation of Ferulic Acid by Horseradish Peroxidase: A Coming Full Cycle. <i>Journal of the American Chemical Society</i> , 2006, 128, 13940-13949.	6.6	55
3660	Gate Effect of Vacancy-type Defect of Fullerene Cages on Metal-Atom Migrations in Metallofullerenes. <i>Nano Letters</i> , 2006, 6, 1389-1395.	4.5	16

#	ARTICLE	IF	CITATIONS
3661	Multireference Configuration Interaction Calculation of the σ - π^* Transition of Halogen- and Methyl-Substituted Vinyloxy Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12419-12426.	1.1	8
3662	Topology-Driven Physicochemical Properties of π -Electron Systems. 1. Does the Clar Rule Work in Cyclic π -Electron Systems with the Intramolecular Hydrogen or Lithium Bond? <i>Journal of Organic Chemistry</i> , 2006, 71, 7678-7682.	1.7	34
3663	Density Functional Theory (DFT) Calculations of the Infrared Absorption Spectra of Acetaminophen Complexes Formed with Ethanol and Acetone Species. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8986-9001.	1.1	17
3664	Theoretical UV Circular Dichroism of Cyclo(L-Proline-L-Proline). <i>Journal of Physical Chemistry A</i> , 2006, 110, 1925-1933.	1.1	12
3665	Diffusion and Overhauser NMR Studies on Dicationic Palladium Complexes of BINAP. <i>Organometallics</i> , 2006, 25, 4596-4604.	1.1	23
3666	EPR and ENDOR Study of Radiation-Induced Radical Formation in Purines: Sodium Inosine Crystals X-irradiated at 10 K. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6552-6562.	1.1	4
3667	Extension of the Single Amino Acid Chelate Concept (SAAC) to Bifunctional Biotin Analogues for Complexation of the $M(CO)_3+1$ Core ($M = Tc$ and Re): Syntheses, Characterization, Biotinidase Stability, and Avidin Binding. <i>Bioconjugate Chemistry</i> , 2006, 17, 579-589.	1.8	45
3668	Role of the Metal Ion in Formyl Peptide Bond Hydrolysis by a Peptide Deformylase Active Site Model. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1063-1072.	1.2	32
3669	Water-Catalyzed Hydrolysis of the Radical Cation of Ketene in the Gas Phase: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8266-8274.	1.1	12
3670	Theoretical Simulations of Clamping Levels in Optical Power Limiting. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20912-20916.	1.2	22
3671	Solid-State NMR and Computational Chemistry Study of Mononucleotides Adsorbed to Alumina. <i>Langmuir</i> , 2006, 22, 9281-9286.	1.6	46
3672	Karplus-Type Equations for $J(X^{\sim}Y)$ in Molecules $HmX^{\sim}YHn$: ($X, Y = N, O, P, S$). <i>Journal of Physical Chemistry A</i> , 2006, 110, 12543-12545.	1.1	12
3673	Is the Mechanism of the [2+2] Cycloaddition of Cyclopentyne to Ethylene Concerted or Biradical? A Completely Renormalized Coupled Cluster Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 367-378.	1.1	40
3674	Substituent Effects on Haptotropic Rearrangements of Bis(indenyl)zirconium Sandwich Complexes. <i>Organometallics</i> , 2006, 25, 2266-2273.	1.1	22
3675	Synthesis of Stannaindenyl Anions and a Dianion. <i>Organometallics</i> , 2006, 25, 2967-2971.	1.1	30
3676	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. <i>Journal of Organic Chemistry</i> , 2006, 71, 6388-6396.	1.7	39
3677	Structural and Electrochemical Investigations of the High Fluoride Affinity of Sterically Hindered 1,8-Bis(boryl)naphthalenes. <i>Inorganic Chemistry</i> , 2006, 45, 8136-8143.	1.9	110
3678	Kinetics and Mechanism of Ketone Enolization Mediated by Magnesium Bis(hexamethyldisilazide). <i>Journal of the American Chemical Society</i> , 2006, 128, 13599-13610.	6.6	35

#	ARTICLE	IF	CITATIONS
3679	Models for Solvation of Zirconocene Cations:Â Synthesis, Reactivity, and Computational Studies of Phenylsilyl-Substituted Cationic and Dicationic Zirconocene Compounds. <i>Organometallics</i> , 2006, 25, 2796-2805.	1.1	13
3680	Complexes of an Anionic Gallium(I) N-Heterocyclic Carbene Analogue with Group 14 Element(II) Fragments:â€ Synthetic, Structural and Theoretical Studies. <i>Inorganic Chemistry</i> , 2006, 45, 7242-7251.	1.9	80
3681	Computational Studies of Structures and Properties of Metallaboranes. 2. Transition-Metal Dicarbollide Complexes. <i>Organometallics</i> , 2006, 25, 2173-2181.	1.1	47
3682	Carbon Chemical Shift Tensor Components in Quinolines and Quinoline N-Oxides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 234-240.	1.1	8
3683	Heisenberg Exchange in Dinuclear Manganese Complexes:â€ A Density Functional Theory Study. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 981-989.	2.3	37
3684	Tunneling through Weak Interactions:Â Comparison of Through-Space-, H-Bond-, and Through-Bond-Mediated Tunneling. <i>Journal of Physical Chemistry A</i> , 2006, 110, 14018-14028.	1.1	24
3685	Structural and Spectroscopic Characterization of a Diruthenium-Dioxolene Complex Possessing a Singly Occupied Molecular Orbital Delocalized over the Entire Molecule, [Ru ₂ (3,6-DTBDiox) ₄]-. <i>Inorganic Chemistry</i> , 2006, 45, 3990-3997.	1.9	7
3686	Gas electron diffraction study of the vapour over dimethylamineâ€ gallane leading to an improved structure for dimeric dimethylamidogallane, [Me ₂ NGaH ₂] ₂ : a cautionary tale. <i>Dalton Transactions</i> , 2006, , 1204-1212.	1.6	5
3687	Torsional Anharmonicity in the Conformational Analysis of ¹² -d-Galactoseâ€. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3485-3492.	1.2	11
3688	Molecular Orbital Theory Study on Surface Complex Structures of Glyphosate on Goethite:â€ Calculation of Vibrational Frequencies. <i>Environmental Science & Technology</i> , 2006, 40, 3836-3841.	4.6	46
3689	Metal- and Ligation-Dependent Fragmentation of [M(1,10-Phenanthroline) _{1,2,3}] ₂ +Cations with M = Mn, Fe, Co, Ni, Cu, and Zn:Â Comparison between the Gas Phase and Solution. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10763-10769.	1.1	11
3690	Systematic ab Initio Study of ¹⁵ Nâ~ ¹⁵ N and ¹⁵ Nâ~ ¹ H Spinâ~Spin Coupling Constants Across Nâ~H+â~N Hydrogen Bonds:Â Predicting Nâ~N and Nâ~H Coupling Constants and Relating Them to Hydrogen Bond Type. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7496-7502.	1.1	38
3691	Charge Transfer Study through the Determination of the Ionization Energies of Tetrapeptides X ₃ -Tyr, X = Gly, Ala, or Leu. Influence of the Inclusion of One Glycine in Alanine and Leucine Containing Peptides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11975-11987.	1.1	1
3692	Computational Characterization of Low-Lying States and Intramolecular Charge Transfers in N-Phenylpyrrole and the Planar-Rigidized Fluorazene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1740-1748.	1.1	20
3693	Density Functional Theory Calculations of Tiâ~TEMPO Complexes:Â Influence of Ancillary Ligation on the Strength of the Tiâ~O Bond. <i>Organometallics</i> , 2006, 25, 3317-3323.	1.1	20
3694	Atomistic model of helium bubbles in gallium-stabilized plutonium alloys. <i>Physical Review B</i> , 2006, 73, .	1.1	69
3695	Methane Câ~H Bond Activation by Neutral Lanthanide and Thorium Atoms in the Gas Phase:Â A Theoretical Prediction. <i>Organometallics</i> , 2006, 25, 3407-3416.	1.1	39
3696	Calculation of Vibrational Spectra of Linear Tetrapyrroles. 4. Methine Bridge Câ~H Out-of-Plane Modes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10564-10574.	1.1	16

#	ARTICLE	IF	CITATIONS
3697	Photoelectron Spectroscopy of Free Multiply Charged Keggin Anions $\hat{\pm}$ -[PM12O40]3-(M = Mo, W) in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10737-10741.	1.1	28
3698	Correlated ab Initio Study of the Excited State of the Iron-Coordinated-Mode Noninnocent Glyoxalbis(mercaptoanil) Ligand. <i>Inorganic Chemistry</i> , 2006, 45, 3212-3216.	1.9	28
3699	Effect of Double Bonds on the Conducting Properties of Ciguatoxin 3C and Tetrahydropyrane-Based Polymers: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1172-1178.	1.2	3
3700	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Antimony Compounds in the Sb $\hat{\sim}$ H $\hat{\sim}$ C $\hat{\sim}$ O $\hat{\sim}$ Cl System. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5919-5928.	1.1	11
3701	Insights into the Chemomechanical Coupling of the Myosin Motor from Simulation of Its ATP Hydrolysis Mechanism. <i>Biochemistry</i> , 2006, 45, 5830-5847.	1.2	55
3702	BAC-MP4 Predictions of Thermochemistry for Gas-Phase Indium Compounds in the In $\hat{\sim}$ H $\hat{\sim}$ C $\hat{\sim}$ O $\hat{\sim}$ Cl System. <i>Journal of Physical Chemistry A</i> , 2006, 110, 281-290.	1.1	8
3703	Palladium Complexes of a Phosphorus Ylide with Two Stabilizing Groups: A Synthesis, Structure, and DFT Study of the Bonding Modes. <i>Inorganic Chemistry</i> , 2006, 45, 6803-6815.	1.9	49
3704	Directional Dependence of the Mean Excitation Energy and Spectral Moments of the Dipole Oscillator Strength Distribution of Glycine and Its Zwitterion. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8811-8817.	1.1	26
3705	An ab initio cluster-in-lattice model for the luminescence of K2NbOF5 crystal. <i>Computational Materials Science</i> , 2006, 38, 410-417.	1.4	2
3706	Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies. <i>Geochimica Et Cosmochimica Acta</i> , 2006, 70, 3803-3819.	1.6	35
3707	Calculation of Solvent Shifts on Electronic-Tensors with the Conductor-Like Screening Model (COSMO) and Its Self-Consistent Generalization to Real Solvents (Direct COSMO-RS). <i>Journal of Physical Chemistry A</i> , 2006, 110, 2235-2245.	1.1	573
3708	Structural Properties and Dynamics of Five-Coordinate Nickel(II) $\hat{\sim}$ -Allyl Complexes Containing Monodentate Phosphorus Ligands. <i>Organometallics</i> , 2006, 25, 2308-2330.	1.1	12
3709	Simulation of resonance Raman spectra of the solvated electron in water and methanol. , 2006, , 154-162.		1
3710	Synthesis and Characterization of Dimetallostannafluorenes. <i>Chemistry Letters</i> , 2006, 35, 940-941.	0.7	28
3711	Electron Transfer Reactions in Laser Desorption/Ionization and Matrix-Assisted Laser Desorption/Ionization: Factors Influencing Matrix and Analyte Ion Intensities. <i>European Journal of Mass Spectrometry</i> , 2006, 12, 345-358.	0.5	36
3712	DFT Calculations of Cubane-Type Mo2Ru2S4 Clusters. Stability of a Possible Dinitrogen Cluster and an Isolable Acetonitrile Cluster. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 53-58.	2.0	6
3713	Generalized Hybrid Orbitals in the FA-ADMA Method. <i>Zeitschrift Fur Physikalische Chemie</i> , 2006, 220, 927-944.	1.4	12
3714	Excitation Spectra of Dibenzoborole Containing $\hat{\sim}$ -Electron Systems: Controlling the Electronic Spectra by Changing the $\hat{\sim}$ Conjugation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2434-2439.	1.1	28

#	ARTICLE	IF	CITATIONS
3715	Ab Initio Study of Hydrogen Bonding and Proton Transfer in 3:1 FH:NH ₃ and FH:Collidine Complexes: Structures and One- and Two-Bond Coupling Constants across Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1128-1133.	1.1	15
3716	Many-body Brillouin-Wigner second-order perturbation theory using a multireference formulation: an application to bond breaking in the diatomic hydrides BH and FH. <i>Molecular Physics</i> , 2006, 104, 2367-2386.	0.8	14
3717	The localizability of valence space electron-electron correlations in pair-based coupled cluster models. <i>Molecular Physics</i> , 2006, 104, 1191-1206.	0.8	10
3718	Intermolecular interactions of sulfur trioxide and sulfuric acid dimers studied by the DFT method. <i>Journal of Chemical Research</i> , 2006, 2006, 790-793.	0.6	0
3719	Acetylene Elimination in Photodissociation of Neutral Azulene and Its Cation: An Ab Initio and RRKM Study. <i>Journal of the Chinese Chemical Society</i> , 2006, 53, 161-168.	0.8	10
3720	Characterizing High-Energy-Density Propellants for Space Propulsion Applications. , 2006, , .		4
3721	Theoretical Comparison of the Linear and Bent Structures for the Weakly Bound CO ₂ -HF Complex. <i>Journal of the Chinese Chemical Society</i> , 2006, 53, 519-530.	0.8	1
3722	Basis sets. , 0, , 178-216.		0
3723	anti-2-Hydroxy-2-methyl-1-tetralone oxime: X-ray and density functional theory study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o199-o202.	0.4	0
3724	Relationship between structure and photoinitiating abilities of selected bromide salts of 2-oxo-2,3-dihydro-1H-imidazo[1,2-a]pyridine (IMP): influence of the solvent and the substitution in benzaldehyde on the course of its reaction with IMP. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 135-142.	1.8	7
3725	Macrocyclic effect of auxiliary ligand on the gas-phase dissociation of ternary copper(II)-GGX complexes. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 790-796.	0.7	21
3726	Kernel energy method: Basis functions and quantum methods. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 447-457.	1.0	27
3727	Effects of H-bond type, backbone size, and halogen on structural and spectroscopic properties of hydrogen-bonded complexes of the X ₂ H ₂ type between alkenes or alkynes and haloacids (HF and HCl). <i>Journal of Physical Chemistry A</i> , 2006, 110, 1128-1133.	1.0	10
3728	Quantum chemical model study of the acyl migration in 2 ³ -formyl nucleosides. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1346-1356.	1.0	13
3729	Revealing the mechanism of Rh(I)-catalyzed hydroformylation of 4-pyridylethene derivatives: DFT study. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1844-1852.	1.0	12
3730	Analysis of exponent values in Gaussian-type functions for development of protonic and deuteronic basis functions. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1465-1476.	1.0	44
3731	Moletronics modeling toward molecular potentials. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1964-1969.	1.0	16
3732	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2129-2144.	1.0	35

#	ARTICLE	IF	CITATIONS
3733	Computational and spectroscopic studies concerning the solvatochromic behavior of 1,3-disubstituted azulenes. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2331-2338.	1.0	7
3734	Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3097-3107.	1.0	17
3735	Extension of the active-space equation-of-motion coupled-cluster methods to radical systems: The EA-EOMCCSDt and IP-EOMCCSDt approaches. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2854-2874.	1.0	28
3736	Application of electronic structure and transition state theory: Reaction of hydrogen with silicon radicals. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3149-3159.	1.0	3
3737	Detonation Velocities and Pressures, and their Relationships with Electric Spark Sensitivities for Nitramines. <i>Propellants, Explosives, Pyrotechnics</i> , 2006, 31, 102-109.	1.0	53
3738	Calculation of Detonation Velocity, Pressure, and Electric Sensitivity of Nitro Arenes Based on Quantum Chemistry. <i>Propellants, Explosives, Pyrotechnics</i> , 2006, 31, 361-368.	1.0	48
3739	Plain DFT and hybrid HF-DFT LCAO calculations of SnO ₂ (110) and (100) bare and hydroxylated surfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 1823-1834.	0.7	30
3740	Amino Acid Alanine Reactivity with the Fingerprint Reagent Ninhydrin. A Detailed Ab Initio Computational Study. <i>Journal of Forensic Sciences</i> , 2006, 51, 1267-1275.	0.9	21
3741	Structure-activity relationships in platelet-activating factor. Part 13: Synthesis and biological evaluation of piperazine derivatives with dual anti-PAF and anti-HIV-1 or pure antiretroviral activity. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 8109-8125.	1.4	14
3742	Structure-activity relationships in platelet-activating factor. Part 14: Synthesis and biological evaluation of piperazine derivatives with dual anti-PAF and anti-HIV-1 activity. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 7999-8013.	1.4	18
3743	Use of pyridine CH(D) vibrations for the study of Lewis acidity of metal oxides. <i>Applied Catalysis A: General</i> , 2006, 307, 98-107.	2.2	47
3744	Mechanism of methane oxidation by transition metal oxides: A cluster model study. <i>Catalysis Today</i> , 2006, 117, 133-137.	2.2	27
3745	Kinetic studies of the photoinduced formation of transition metal-dinitrogen complexes using time-resolved infrared and UV-vis spectroscopy. <i>Coordination Chemistry Reviews</i> , 2006, 250, 1681-1695.	9.5	15
3746	Mulliken-Hush elucidation of the encounter (precursor) complex in intermolecular electron transfer via self-exchange of tetracyanoethylene anion-radical. <i>Chemical Physics</i> , 2006, 324, 117-128.	0.9	28
3747	Initial driving force for proton transfer in Nafion. <i>Chemical Physics</i> , 2006, 324, 393-397.	0.9	16
3748	Effects of strong electron correlations in Ti ₈ C ₁₂ Met-Car. <i>Chemical Physics</i> , 2006, 326, 97-106.	0.9	8
3749	A quantum chemical ab initio study of the polymerization to polyhydridophosphazenes. <i>Chemical Physics</i> , 2006, 325, 291-298.	0.9	4
3750	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. <i>Chemical Physics</i> , 2006, 328, 307-317.	0.9	8

#	ARTICLE	IF	CITATIONS
3751	Ab initio MO and quasi-classical direct ab initio MD studies on the nitrogen inversion of trimethylamine. <i>Chemical Physics Letters</i> , 2006, 417, 316-319.	1.2	11
3752	Adaptive density partitioning technique in the auxiliary plane wave method. <i>Chemical Physics Letters</i> , 2006, 417, 241-245.	1.2	9
3753	A multi state-CASPT2 vs. TD-DFT study of the electronic excited states of RCo(CO) ₄ (R=H, CH ₃) organometallic complexes. <i>Chemical Physics Letters</i> , 2006, 417, 545-549.	1.2	10
3754	Single-reference, size-extensive, non-iterative coupled-cluster approaches to bond breaking and biradicals. <i>Chemical Physics Letters</i> , 2006, 418, 467-474.	1.2	180
3755	On the stability of dense versus cage-shaped water clusters: Quantum-chemical investigations of zero-point energies, free energies, basis-set effects and IR spectra of (H ₂ O) ₁₂ and (H ₂ O) ₂₀ . <i>Chemical Physics Letters</i> , 2006, 418, 361-367.	1.2	49
3756	Pople versus Dunning basis-sets for group IA metal hydrides and some other second row hydrides: The case against a De Facto standard. <i>Chemical Physics Letters</i> , 2006, 419, 254-258.	1.2	24
3757	Implementation of SurjÃ¡nâ€™s density matrix formulae for calculating second-order MÃ¶llerâ€™Plesset energy. <i>Chemical Physics Letters</i> , 2006, 420, 250-255.	1.2	37
3758	An efficient state-specific scheme of time-dependent density functional theory. <i>Chemical Physics Letters</i> , 2006, 420, 391-396.	1.2	20
3759	Determination of chromophore charge states in the low pH color transition of the fluorescent protein Rtm5H146S via time-dependent DFT. <i>Chemical Physics Letters</i> , 2006, 420, 507-511.	1.2	16
3760	Can superoxide species be formed at small Laâ€™O clusters in the presence of oxygen? A DFT study. <i>Chemical Physics Letters</i> , 2006, 423, 427-433.	1.2	4
3761	Natural atomic orbital based energy density analysis: Implementation and applications. <i>Chemical Physics Letters</i> , 2006, 424, 193-198.	1.2	23
3762	Triplet energies of Å–conjugated polymers. <i>Chemical Physics Letters</i> , 2006, 424, 23-27.	1.2	14
3763	Synthesis, X-ray, spectroelectrochemical, and theoretical studies of a tricyanovinyl-capped quaterthiophene: A correlation of semiconductor performance with physical properties. <i>Chemical Physics Letters</i> , 2006, 425, 251-256.	1.2	6
3764	transâ€™cis Isomerism and acylimine formation in DsRed chromophore models: Intrinsic rotation barriers. <i>Chemical Physics Letters</i> , 2006, 426, 159-162.	1.2	11
3765	CO ₂ adsorption in alkali cation exchanged Y faujasites: A quantum chemical study compared to experiments. <i>Chemical Physics Letters</i> , 2006, 426, 387-392.	1.2	62
3766	The initial mechanisms of Al ₂ O ₃ atomic layer deposition on OH/Si(100)-2Å–1 surface by tri-methylaluminum and water. <i>Chemical Physics Letters</i> , 2006, 426, 365-369.	1.2	31
3767	Ab initio study of the toluene dimer. <i>Chemical Physics Letters</i> , 2006, 427, 410-413.	1.2	25
3768	The structure of protonated HCP: A classical or non-classical ion?. <i>Chemical Physics Letters</i> , 2006, 429, 23-26.	1.2	7

#	ARTICLE	IF	CITATIONS
3769	Ultrafast photodissociation dynamics of HMX and RDX from their excited electronic states via femtosecond laser pump-probe techniques. <i>Chemical Physics Letters</i> , 2006, 430, 277-281.	1.2	55
3770	Do Eu@C82 and Gd@C82 have an anomalous endohedral structure?. <i>Chemical Physics Letters</i> , 2006, 431, 110-112.	1.2	35
3771	Parity violation energy of biomolecules III: RNA. <i>Chemical Physics Letters</i> , 2006, 432, 263-268.	1.2	10
3772	Enantiomers of cis-constrained and flexible 2-substituted GABA analogues exert opposite effects at recombinant GABAC receptors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 447-455.	1.4	23
3773	Molecular dynamics simulation of acetamide solvation using interaction energy components: Application to structural and energy properties. <i>Chemical Physics</i> , 2006, 327, 187-192.	0.9	13
3774	Electron momentum spectroscopy study of thiophene: Binding energy spectrum and valence orbital electron density distributions. <i>Chemical Physics</i> , 2006, 327, 269-277.	0.9	8
3775	Synthetic and theoretical study on proline-catalyzed Knoevenagel condensation in ionic liquid. <i>Journal of Molecular Catalysis A</i> , 2006, 253, 212-221.	4.8	68
3776	Conformational analysis of 8-oxabicyclo[3.2.1]oct-6-en-3-one derivatives by NMR and theoretical calculations. <i>Journal of Molecular Structure</i> , 2006, 791, 180-185.	1.8	14
3777	Synthesis and isomerisation of two metallated N,O-complexes of ruthenium: Models for the Murai reaction. <i>Inorganica Chimica Acta</i> , 2006, 359, 815-820.	1.2	17
3778	The synthesis and structural properties of [M(dippe)(η^2 -C ₄ H ₄ S)] complexes of Pd and Pt and comparison with their Ni analog. <i>Inorganica Chimica Acta</i> , 2006, 359, 2798-2805.	1.2	26
3779	Synthesis, characterization, structure and luminescence studies of dinuclear gold(I) alkynyls of bis(diphenylphosphino)alkyl- and aryl-amines. <i>Inorganica Chimica Acta</i> , 2006, 359, 3639-3648.	1.2	28
3780	Aliphatic C-X (X=halogen) bond activation by transition metal complexes containing the {Pt ₂ S ₂ } core: A theoretical study of the reaction mechanism. <i>Inorganica Chimica Acta</i> , 2006, 359, 3736-3744.	1.2	12
3781	Syntheses, crystal structures and properties of [K(2,2,2-crypt)] ₃ K(HP7)2 \cdot en, [K(18-crown-6)] ₂ HP7 and [K(db18-crown-6)] ₂ HP7 \cdot toluene. <i>Inorganica Chimica Acta</i> , 2006, 359, 4265-4273.	1.2	17
3782	Fragmentation of doubly charged metal-acetamide complexes: Second ionization energies and dissociation chemistries. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 251-264.	0.7	17
3783	Density functional study of hypophosphite adsorption on Ni (111) and Cu (111) surfaces. <i>Applied Surface Science</i> , 2006, 252, 2692-2701.	3.1	7
3784	DFT calculations of NMR J _C -H coupling constants: An additional tool to characterize the σ -agostic interaction in high oxidation state M-alkylidene complexes (M=Re, Mo and Ta). <i>Polyhedron</i> , 2006, 25, 339-348.	1.0	35
3785	Beryllium(II) complexes with (R ₂ N)P(O)F (R=Me or Et): Synthesis and characterisation by multinuclear (31P, 19F and 9Be) NMR in solution. <i>Polyhedron</i> , 2006, 25, 1373-1378.	1.0	5
3786	Phosphoramidic difluoride complexes of tin(IV) chloride: A multinuclear (119Sn, 31P, 19F and 1H) NMR characterisation in solution. <i>Polyhedron</i> , 2006, 25, 3299-3304.	1.0	18

#	ARTICLE	IF	CITATIONS
3787	Quantum-mechanical QSPR models for polymerization volume change of epoxides and methacrylates based on mercury dilatometry results. <i>Polymer</i> , 2006, 47, 8595-8603.	1.8	3
3788	Ge ₂ H ₂ a π -ligand in organometallic chemistry. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 2503-2511.	0.8	3
3789	Experimental and theoretical studies of a silver complex of O-functionalized N-heterocyclic carbene. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 3797-3805.	0.8	39
3790	Novel tetrahedral tetranickel cluster with alkylidyne ligand (NiCp) ₄ (η^3 -CR). <i>Journal of Organometallic Chemistry</i> , 2006, 691, 5825-5830.	0.8	3
3791	Solid-state structural properties of 2,4,6-trimethoxybenzene derivatives, determined directly from powder X-ray diffraction data in conjunction with other techniques. <i>Journal of Solid State Chemistry</i> , 2006, 179, 3214-3223.	1.4	7
3792	Investigation on the interactions between diperoxovanadate and substituted phenanthroline. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 64, 255-263.	2.0	5
3793	A theoretical study of hydrogen complexes of the XH- π type between propyne and HF, HCl or HCN. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 64, 412-417.	2.0	6
3794	Density functional theory study of vibronic structure of the first absorption Q _x band in free-base porphyrin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 308-323.	2.0	70
3795	Phase transition and intramolecular hydrogen bonding in nitro derivatives of ortho-hydroxy acetophenones. <i>Journal of Molecular Structure</i> , 2006, 785, 7-13.	1.8	11
3796	The intramolecular hydrogen bond in 2-hydroxy-benzamides. <i>Journal of Molecular Structure</i> , 2006, 790, 65-73.	1.8	17
3797	Synthesis, crystal structures and theoretical study of mixed ligand complexes of lanthanides acetylacetonates with o-phenanthroline and 2,2'-bipyridyl: The unexpected inverted electrostatic trend in stability. <i>Journal of Molecular Structure</i> , 2006, 789, 187-194.	1.8	12
3798	Band gap engineering at surfaces of insulating films by adsorption of organic molecules. <i>Surface Science</i> , 2006, 600, 1664-1669.	0.8	4
3799	Synthesis of arylboronates via Cp*RuCl-catalyzed cycloaddition of alkynylboronates. <i>Tetrahedron</i> , 2006, 62, 4294-4305.	1.0	58
3800	Analysis of the VROA signals of helical heptasilanes using an atomistic approach. <i>Vibrational Spectroscopy</i> , 2006, 42, 309-316.	1.2	12
3801	On the stability of the π -allyl intermediate in molybdenum-catalyzed asymmetric alkylations. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 716-724.	1.8	15
3802	Effect of phenyl substitution on the lifetime and product distribution of cyclobutylidene: preference change in the rearrangements via 1,2-carbon shift and 1,2-hydrogen shift. <i>Tetrahedron Letters</i> , 2006, 47, 3995-3999.	0.7	5
3803	Precision of total energy and orbital energies with the expansion method for the optimized effective Kohn-Sham potential. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 193-199.	1.5	22
3804	A simulation study of the interaction of sulfhydryl nucleophiles with several antifungal sesquiterpene lactones isolated from Greek <i>Centaurea</i> sp.. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 215-224.	1.5	5

#	ARTICLE	IF	CITATIONS
3805	Theoretical elucidation of the regioselectivity in a tandem 1,4-hydride addition/acylation of diethylphosphonocoumarin. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 177-187.	1.5	6
3806	The interaction between C28 (Td) and X (X=H and F). <i>Computational and Theoretical Chemistry</i> , 2006, 760, 53-57.	1.5	3
3807	A theoretical study on chemo- and regioselective Rh-catalyzed hydroformylation and hydrogenation of propyne. <i>Computational and Theoretical Chemistry</i> , 2006, 763, 75-81.	1.5	2
3808	Third-order generalized Van Vleck perturbation theory study of the ground and lowest excited states of C2. <i>Computational and Theoretical Chemistry</i> , 2006, 771, 73-78.	1.5	5
3809	Effect of the basis set selection on the electron momentum distribution in graphite. <i>Computational and Theoretical Chemistry</i> , 2006, 769, 53-59.	1.5	0
3810	Ab initio MO study on the S1 \rightarrow S0 origin transition energies of polychlorodibenzofurans (PCDFs). <i>Computational and Theoretical Chemistry</i> , 2006, 774, 7-12.	1.5	3
3811	Mg-H dissociation of magnesium hydride MgH ₂ catalyzed by 3d transition metals. <i>Thin Solid Films</i> , 2006, 509, 157-159.	0.8	36
3812	Dienamine Catalysis: Organocatalytic Asymmetric β^3 -Amination of β^2 -Unsaturated Aldehydes. <i>Journal of the American Chemical Society</i> , 2006, 128, 12973-12980.	6.6	380
3813	Interaction of a Transition Metal Atom with Intrinsic Defects in Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 13941-13946.	1.2	63
3814	Mechanism and Stereoselectivity of the Aza-Wittig Reaction between Phosphazenes and Aldehydes. <i>Journal of Organic Chemistry</i> , 2006, 71, 2839-2847.	1.7	63
3815	Photoelectron spectra of the nucleobases cytosine, thymine and adenine. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2006, 39, 305-329.	0.6	139
3816	Luminescent Molecular Copper(I) Alkynyl Open Cubes: Synthesis, Structural Characterization, Electronic Structure, Photophysics, and Photochemistry. <i>Chemistry - an Asian Journal</i> , 2006, 1, 273-286.	1.7	39
3817	Theoretical study of 1,3-dipolar cycloaddition of nitrones to doubly activated nitriles. <i>Russian Journal of Inorganic Chemistry</i> , 2006, 51, 1602-1612.	0.3	5
3818	Actinide Chemistry in Solution, Quantum Chemical Methods and Models. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 145-160.	0.5	114
3819	Iron Chelation by the Powerful Antioxidant Flavonoid Quercetin. <i>Journal of Agricultural and Food Chemistry</i> , 2006, 54, 6343-6351.	2.4	387
3820	Preparation, characterization, and the molecular structure of 2,4,6-trinitro-mesitylene. <i>Structural Chemistry</i> , 2006, 17, 351-357.	1.0	3
3821	The annular tautomerism of imidazoles and pyrazoles: The possible existence of nonaromatic forms. <i>Structural Chemistry</i> , 2006, 17, 439-444.	1.0	41
3822	Torsional barriers and nonlinear optical properties of 2-, 3-, 4-phenylpyridine molecules. <i>European Physical Journal D</i> , 2006, 56, 349-358.	0.4	11

#	ARTICLE	IF	CITATIONS
3823	Ab Initio Studies on the Molecular Conformation of Lignin Model Compounds I. Conformational Preferences of the Phenolic Hydroxyl and Methoxy Groups in Guaiacol. <i>Monatshefte für Chemie</i> , 2006, 137, 55-68.	0.9	28
3824	The axial ligand effect of oxo-iron porphyrin catalysts. How does chloride compare to thiolate?. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 168-178.	1.1	55
3825	Syn- and anti-conformations of 5'-deoxy- and 5'-O-methyl-uridine 2',3'-cyclic monophosphate. <i>Journal of Molecular Modeling</i> , 2006, 12, 205-212.	0.8	10
3826	Ab initio and DFT study on the electrophilic addition of bromine to endo-tricyclo[3.2.1.0 ^{2,4}]oct-6-ene. <i>Journal of Molecular Modeling</i> , 2006, 12, 290-296.	0.8	7
3827	Theoretical ⁴⁹ Ti NMR chemical shifts. <i>Journal of Molecular Modeling</i> , 2006, 12, 723-729.	0.8	8
3828	Ab initio and DFT study on the electrophilic addition reaction of bromine to tetracyclo[5.3.0.0 ^{2,6} .0 ^{3,10}]deca-4,8-diene. <i>Journal of Molecular Modeling</i> , 2006, 12, 991-995.	0.8	8
3829	Investigation of the structure of 6-amino-4-methylamino-5-nitrosopyrimidine by X-ray diffraction, NMR and molecular modeling. <i>Journal of Molecular Modeling</i> , 2006, 13, 219-224.	0.8	8
3830	Ab initio calculation of molecular chiroptical properties. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 227-245.	0.5	362
3831	Ab initio electronic structure theory as an aid to understanding excited state hydrogen transfer in moderate to large systems. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 355-372.	0.5	8
3832	Towards the Development and Applications of Manifestly Spin-free Multi-reference Coupled Electron-pair Approximation-like Methods: A State Specific Approach. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 621-636.	0.5	3
3833	Theoretical studies on the ground and excited states of blue phosphorescent cyclometalated Ir(III) complexes having ancillary ligand. <i>Current Applied Physics</i> , 2006, 6, 620-626.	1.1	61
3834	Physically based molecular device model in a transient circuit simulator. <i>Chemical Physics</i> , 2006, 326, 188-196.	0.9	5
3835	Geometries and stabilities of 3d-transition metal-cation benzene complexes, M+Bzn (M=Sc-Cu, n=1, 2). <i>Chemical Physics</i> , 2006, 326, 600-604.	0.9	30
3836	The dipole moment derivatives of gaseous benzene: A comparison of experimental and ab initio values. <i>Chemical Physics</i> , 2006, 327, 180-186.	0.9	3
3837	Steric and electronic effects in enantioselective hydrogenation of ketones on platinum modified by cinchonidine: Directing effect of the trifluoromethyl group. <i>Journal of Catalysis</i> , 2006, 240, 203-212.	3.1	23
3838	Simulation of ⁵⁹ Co NMR Chemical Shifts in Aqueous Solution. <i>Chemistry - A European Journal</i> , 2006, 12, 477-488.	1.7	63
3839	Mechanism of Nitrate Reduction by <i>Desulfovibrio desulfuricans</i> Nitrate Reductase—A Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2006, 12, 2532-2541.	1.7	70
3840	The Importance of Alkali Cations in the [RuCl ₂ (p-cymene)] ₂ —Pseudo-dipeptide-Catalyzed Enantioselective Transfer Hydrogenation of Ketones. <i>Chemistry - A European Journal</i> , 2006, 12, 3218-3225.	1.7	69

#	ARTICLE	IF	CITATIONS
3841	Calixarenes as Hosts for Ammonium Cations: A Quantum Chemical Study and Mass-Spectrometric Investigations. <i>Chemistry - A European Journal</i> , 2006, 12, 8995-9000.	1.7	19
3842	Ruthenium-Catalyzed Cycloaddition of 1,6-Diynes and Nitriles under Mild Conditions: Role of the Coordinating Group of Nitriles. <i>Chemistry - A European Journal</i> , 2006, 12, 5618-5631.	1.7	124
3843	Metal Nitrosyl Reactivity: Acetonitrile-Promoted Insertion of an Alkylidene into a Nitrosyl Ligand with Fission of the NO Bond. <i>Chemistry - A European Journal</i> , 2006, 12, 5199-5209.	1.7	8
3844	Ethylene Oligomerisation and Polymerisation with Nickel Phosphanolates Bearing Electron-Withdrawing Substituents: Structure–Reactivity Relationships. <i>Chemistry - A European Journal</i> , 2006, 12, 5210-5219.	1.7	62
3845	Deep Blue Mixed-Valent Pt(III)Pt(II) Complex [Pt ₃ Br ₂ ($\frac{1}{4}$ -pz) ₆] (pz=Pyrazolate) Showing Valence-Detrapping Behavior in Solution. <i>Chemistry - A European Journal</i> , 2006, 12, 6521-6527.	1.7	19
3846	Terminally Coordinated AsS and PS Ligands. <i>Chemistry - A European Journal</i> , 2006, 12, 8603-8608.	1.7	18
3847	Molecular dynamics simulation studies of a protein–RNA complex with a selectively modified binding interface. <i>Biopolymers</i> , 2006, 81, 256-269.	1.2	17
3848	Determination of the Relative Configuration of a Five-Membered Lactone from Residual Dipolar Couplings. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 4455-4460.	7.2	80
3849	C ₃₀ H ₁₂₆ ³⁺ : Self-Aggregation, High Charge Density, and Pyramidalization in a Supramolecular Structure of a Supercharged Hemifullerene. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3273-3277.	7.2	34
3850	A New Reaction Pathway in Organophosphorus Chemistry: Competing S _N 2 and A _E ² Pathways for Nucleophilic Attack at a Phosphorus–Carbon Cage Compound. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 3628-3631.	7.2	21
3851	Cyclic Carbodiphosphorane–Diphosphinocarbene Thermal Interconversion. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7447-7450.	7.2	30
3852	The Bromination of Bulky Trialkylphosphane Selenides R ₂ PSe (R, R' = iPr or tBu) Studied by Physical and Computational Methods. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 88-100.	1.0	35
3853	Self-Assembly and Characterization of Homo- and Heterodinuclear Complexes of Zinc(II) and Lanthanide(III) Ions with a Tridentate Schiff-Base Ligand. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 144-149.	1.0	35
3854	A Theoretical Study on Pd(II) Complexes Containing Hemilabile Pyrazole-Derived Ligands. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 447-454.	1.0	18
3855	Diamagnetic versus Paramagnetic Structure of SPS-Type Pincer-Based Co, Rh, and Ir Complexes. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2035-2039.	1.0	4
3856	Hydrogen Bonding and Proton Transfer to the Trihydride Complex [Cp*MoH ₃ (dppe)]: IR, NMR, and Theoretical Investigations. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2192-2209.	1.0	32
3857	A Cationic (N-Heterocyclic carbene)silver Complex as Catalyst for Bulk Ring-Opening Polymerization of L-Lactides. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2975-2984.	1.0	85
3858	DFT Investigation of the Potential of [H-M{(NHCH ₂ CH ₂) ₃ X}] Catalysts (M = Mo, Ru, Os; X = N, P) for the Reduction of N ₂ to NH ₃ by H ₂ . <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4407-4417.	1.0	35

#	ARTICLE	IF	CITATIONS
3859	â€œPincerâ€•N-Heterocyclic Carbene Complexes of Rhodium Functionalised with Pyridyl and Bipyridyl Donors. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 4857-4865.	1.0	40
3860	Radical Addition Reactions of Phosphorus Hydrides: Tuning the Reactivity of Phosphorus Hydrides, the Use of Microwaves and Hornerâ€•Wadsworthâ€•Emmons-Type Reactions. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 1547-1554.	1.2	63
3861	Nâ€²-(3-Amino-1H-isoindol-1-ylidene)-R-carbohydrazides and Their Amide-Type Isomerism. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 2833-2842.	1.2	11
3862	Systematic Studies on Photoluminescence of Oligo(arylene-ethynylene)s: Tunability of Excited States and Derivatization as Luminescent Labeling Probes for Proteins. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3125-3139.	1.2	17
3863	Simultaneous Regio- and Enantiodifferentiation in Carbohydrate Coupling. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3947-3959.	1.2	13
3864	4-Substituted-Phenyl(bisoxazoline)-Rhodium Complexes: Efficiency in the Catalytic Asymmetric Reductive Aldol Reaction. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 5594-5600.	1.2	46
3865	A theoretical study of thermal [1,3]-sigmatropic rearrangements of 3-trimethylsilyl-1-pyrazoline: Concerted vs. stepwise mechanisms. <i>Journal of Computational Chemistry</i> , 2006, 27, 228-237.	1.5	6
3866	A new method to determine electrostatic potential around a macromolecule in solution from molecular wave functions. <i>Journal of Computational Chemistry</i> , 2006, 27, 453-462.	1.5	72
3867	Hybrid density functional theory for π -stacking interactions: Application to benzenes, pyridines, and DNA bases. <i>Journal of Computational Chemistry</i> , 2006, 27, 491-504.	1.5	236
3868	Systematic QM/MM investigation of factors that affect the cytochrome P450-catalyzed hydrogen abstraction of camphor. <i>Journal of Computational Chemistry</i> , 2006, 27, 1324-1337.	1.5	84
3869	A DFT study on the relative affinity for oxygen of the α and β subunits of hemoglobin. <i>Journal of Computational Chemistry</i> , 2006, 27, 1446-1453.	1.5	10
3870	Correlation between computed gas-phase and experimentally determined solution-phase infrared spectra: Models of the ironâ€•iron hydrogenase enzyme active site. <i>Journal of Computational Chemistry</i> , 2006, 27, 1454-1462.	1.5	36
3871	Structure and Dynamics of Water Confined in Dimethyl Sulfoxide. <i>ChemPhysChem</i> , 2006, 7, 266-272.	1.0	46
3872	Adsorption of Functionalized Benzoic Acids on MgSO ₄ â€•xH ₂ O (100). <i>ChemPhysChem</i> , 2006, 7, 1055-1061.	1.0	6
3873	Electron Traps on Oxide Surfaces: (H ⁺)(e ⁻) Pairs Stabilized on the Surface of 17O Enriched CaO. <i>ChemPhysChem</i> , 2006, 7, 728-734.	1.0	24
3874	Ion-Pair Formation in the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(triflyl)imide as a Function of Temperature and Concentration. <i>ChemPhysChem</i> , 2006, 7, 1944-1949.	1.0	304
3875	Theoretical Determination of the Vibrational Raman Optical Activity Signatures of Helical Polypropylene Chains. <i>ChemPhysChem</i> , 2006, 7, 2366-2376.	1.0	37
3876	Theoretical Analysis of the Terahertz Spectrum of the High Explosive PETN. <i>ChemPhysChem</i> , 2006, 7, 2398-2408.	1.0	98

#	ARTICLE	IF	CITATIONS
3877	Interactions between pairs of antimalarial drugs studied by experimental and ab initio ^{13}C NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 276-282.	1.1	6
3878	Density-functional computation of ^{53}Cr NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 661-668.	1.1	22
3879	Computed coupling constants in $\text{X}(\text{CH}_3)_n\text{H}(4-n)$ moieties where $\text{X} = ^{13}\text{C}$ and ^{15}N , and $n = 0-4$: comparisons with experimental data. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 698-707.	1.1	14
3880	Substitution and protonation effects on spin-spin coupling constants in prototypical aromatic rings: C_6H_6 , $\text{C}_5\text{H}_5\text{N}$ and $\text{C}_5\text{H}_5\text{P}$. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 784-789.	1.1	15
3885	Solvent Effects on Anionic and Acid Forms of Nafion Side Chain. <i>Japanese Journal of Applied Physics</i> , 2006, 45, 5121-5125.	0.8	3
3886	Synthesis of an Aluminum Spirocyclic Hybrid with an Inorganic B_2O_3 and an Organic C_3N_2 Core. <i>Journal of the American Chemical Society</i> , 2006, 128, 12406-12407.	6.6	45
3887	Low-lying isomers and finite temperature behavior of $(\text{H}_2\text{O})_6^+$. <i>Journal of Chemical Physics</i> , 2006, 125, 174301.	1.2	43
3888	Sources of error in electronic structure calculations on small chemical systems. <i>Journal of Chemical Physics</i> , 2006, 124, 054107.	1.2	183
3889	A classical trajectory study of the photodissociation of T1 acetaldehyde: The transition from impulsive to statistical dynamics. <i>Journal of Chemical Physics</i> , 2006, 124, 044302.	1.2	34
3890	The water exchange process of tetraaquaplatinum(II): Density-functional theory and ab initio computational study. <i>Journal of Chemical Physics</i> , 2006, 124, 074511.	1.2	5
3891	The correlation-consistent composite approach: Application to the G3/99 test set. <i>Journal of Chemical Physics</i> , 2006, 125, 104111.	1.2	134
3892	Electron-electron and electron-nucleus correlation effects on exponent values of Gaussian-type functions for quantum protons and deuterons. <i>Journal of Chemical Physics</i> , 2006, 125, 144103.	1.2	39
3893	Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: Vibrational spectra and electronic structure of C_{28} , C_{60} , and C_{70} . <i>Journal of Chemical Physics</i> , 2006, 125, 214706.	1.2	40
3894	Arsacyclopentadienyl anions: Structure, properties and aromaticity. <i>Main Group Chemistry</i> , 2006, 5, 153-161.	0.4	3
3895	Ab Initio Study of the Vibrational Spectrum and Related Properties of Crystalline Compounds; the Case of CaCO_3 Calcite. <i>Zeitschrift Fur Physikalische Chemie</i> , 2006, 220, 893-912.	1.4	168
3896	Direct imaging of intracage structure in titanium-carbide endohedral metallofullerene. <i>Physical Review B</i> , 2006, 73, .	1.1	35
3897	Two-photon absorption cross sections: An investigation of the accuracy of calculated absolute and relative values. <i>Journal of Chemical Physics</i> , 2006, 124, 114108.	1.2	23
3898	Stretching of hydrogen-bonded OH in the lowest singlet excited electronic state of water dimer. <i>Journal of Chemical Physics</i> , 2006, 124, 044305.	1.2	47

#	ARTICLE	IF	CITATIONS
3899	Cation electric field is related to hydration energy. Journal of Chemical Physics, 2006, 124, 144507.	1.2	27
3900	The electronic structure of oxo-Mn(salen): Single-reference and multireference approaches. Journal of Chemical Physics, 2006, 124, 144314.	1.2	43
3901	Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. Journal of Chemical Physics, 2006, 124, 154306.	1.2	26
3902	An exploration of electronic structure and nuclear dynamics in tropolone. I. The X^1A_{11} ground state. Journal of Chemical Physics, 2006, 124, 204307.	1.2	21
3903	Electronic structure calculations of the phenalenyl-based neutral radical conductor bis(9-cyclohexylimino-1-phenalenyl) boron. Physical Review B, 2006, 74, .	1.1	16
3904	Polarization Propagator for X-Ray Spectra. Physical Review Letters, 2006, 97, 143001.	2.9	111
3905	Ab-initiomolecular orbital theory of hydrogenation of LiAl and Li ₂ Al ₂ : The magic clusters (LiAlH ₄) and (LiAlH ₄) ₂ . Physical Review B, 2006, 73, .	1.1	5
3906	Adiabatic approximations to internal rotation. Journal of Chemical Physics, 2006, 124, 224310.	1.2	26
3907	Ni adsorption on Stone-Wales defect sites in single-wall carbon nanotubes. Journal of Chemical Physics, 2006, 125, 084705.	1.2	24
3908	NONITERATIVE COUPLED-CLUSTER METHODS FOR EXCITED ELECTRONIC STATES. , 2006, , 45-106.		7
3909	A THEORETICAL INVESTIGATION OF STRUCTURAL, SPECTROSCOPIC AND THERMODYNAMIC PROPERTIES OF CYCLODECANE. Journal of Theoretical and Computational Chemistry, 2007, 06, 281-299.	1.8	4
3910	Synthesis and Optical Properties of SERS-active Nanocomposite Microspheres. Materials Research Society Symposia Proceedings, 2007, 1024, 1.	0.1	0
3911	A QUANTUM MECHANICAL "ELECTRODYNAMICAL APPROACH TO NONLINEAR PROPERTIES: APPLICATION TO OPTICAL POWER LIMITING WITH PLATINUM-ORGANIC COMPOUNDS. Journal of Nonlinear Optical Physics and Materials, 2007, 16, 157-169.	1.1	3
3912	Molecular Property Derivatives. Advances in Chemical Physics, 2007, , 99-153.	0.3	85
3913	Gaussian and finite-element Coulomb method for the fast evaluation of Coulomb integrals. Journal of Chemical Physics, 2007, 126, 144106.	1.2	20
3914	Fully automated implementation of the incremental scheme: Application to CCSD energies for hydrocarbons and transition metal compounds. Journal of Chemical Physics, 2007, 126, 154110.	1.2	154
3915	Molecular mechanics-valence bond method for planar conjugated hydrocarbon cations. Journal of Chemical Physics, 2007, 127, 134111.	1.2	17
3916	Biatomic substrates for bulk-molecule interfaces: The PtCo-oxygen interface. Journal of Chemical Physics, 2007, 127, 244706.	1.2	15

#	ARTICLE	IF	CITATIONS
3917	Evaluation of electronic correlation contributions for optical tensors of large systems using the incremental scheme. <i>Journal of Chemical Physics</i> , 2007, 127, 084108.	1.2	12
3918	Electronic circular dichroism spectra from the complex polarization propagator. <i>Journal of Chemical Physics</i> , 2007, 126, 134102.	1.2	61
3919	Photodissociation of S atom containing amino acid chromophores. <i>Journal of Chemical Physics</i> , 2007, 127, 064308.	1.2	7
3920	Dissociative electron attachment to the hydrogen-bound OH in water dimer through the lowest anionic Feshbach resonance. <i>Journal of Chemical Physics</i> , 2007, 127, 194309.	1.2	6
3921	UNDERSTANDING REACTIVE HAZARDS USING MOLECULAR SIMULATION: MECHANISMS OF HYDROXYLAMINE DECOMPOSITION. <i>Chemical Engineering Communications</i> , 2007, 194, 579-585.	1.5	3
3922	Adding electron-nuclear cusps to Gaussian basis functions for molecular quantum Monte Carlo calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	8
3923	Electronic states of the DNA polynucleotides poly(dG)-poly(dC) in the presence of iodine. <i>Physical Review B</i> , 2007, 75, .	1.1	16
3924	Factors affecting imine coordination in (iminoterpyridine)MX ₂ (M = Fe, Co, Ni, Zn): synthesis, structures, DFT calculations and ethylene oligomerisation studies. <i>New Journal of Chemistry</i> , 2007, 31, 75-85.	1.4	30
3925	Simulations on the effects of confinement and Ni-catalysis on the formation of tubular fullerene structures from peapod precursors. <i>Physical Review B</i> , 2007, 75, .	1.1	23
3926	Theoretical study of interaction of alkaline earth metal with and : structure, electronic properties and aromaticity. <i>Journal of Sulfur Chemistry</i> , 2007, 28, 537-546.	1.0	0
3927	Probing valence electronic wave-packet dynamics by all x-ray stimulated Raman spectroscopy: A simulation study. <i>Physical Review A</i> , 2007, 76, .	1.0	67
3928	Local electronic structure in MgB ₂ from B ₁ 2 ¹ -NMR. <i>Physical Review B</i> , 2007, 75, .	1.1	7
3929	Net Atomic Charge and Multipole Models for the ab Initio Molecular Electric Potential. <i>Reviews in Computational Chemistry</i> , 2007, , 219-271.	1.5	57
3930	Transfer of signatures from the vibrational spectrum of benzene to a silicon complex. <i>Physical Review A</i> , 2007, 75, .	1.0	1
3931	DFT Molecular Dynamics Study of Pyrene Biradical Species. <i>Petroleum Science and Technology</i> , 2007, 25, 67-80.	0.7	4
3932	Theoretical study of borathiin and its derivatives: structure and aromaticity. <i>Journal of Sulfur Chemistry</i> , 2007, 28, 505-511.	1.0	10
3933	Experimental and Theoretical Analysis of the Hydrogen-bonding Motifs Formed Between the Carboxyl and the Carboxylate Group: Towards a Systematic Classification of their Supramolecular Motifs. <i>Supramolecular Chemistry</i> , 2007, 19, 559-578.	1.5	22
3934	Electrochemical planarization of copper surfaces with submicron features. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2007, 25, 1019-1024.	0.9	0

#	ARTICLE	IF	CITATIONS
3935	Insights into Cu(I) Exchange in HAH1 Using Quantum Mechanical and Molecular Simulations. <i>Biochemistry</i> , 2007, 46, 8816-8826.	1.2	52
3936	Active-space symmetry-adapted-cluster configuration-interaction and equation-of-motion coupled-cluster methods for high accuracy calculations of potential energy surfaces of radicals. <i>Journal of Chemical Physics</i> , 2007, 126, 164111.	1.2	45
3937	Light-Matter Interaction of Strong Laser Pulses in the Micro-, Nano-, and Pico-second Regimes. <i>Materials Research Society Symposia Proceedings</i> , 2007, 1015, 1.	0.1	0
3938	Bound anionic states of adenine. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 4804-4807.	3.3	60
3939	Pressure-induced spectral changes for the special-pair radical cation of the bacterial photosynthetic reaction center. <i>Journal of Chemical Physics</i> , 2007, 126, 215102.	1.2	10
3940	An Overview of Computational Methods for Large Molecules. <i>Advances in Chemical Physics</i> , 2007, , 213-263.	0.3	12
3941	Electronic Excitations in a Ladder Type Fluoranthenopyracylene in its Neutral and Charged States: A Theoretical and Experimental Study. <i>Zeitschrift Fur Physikalische Chemie</i> , 2007, 221, 911-928.	1.4	0
3942	Theoretical Design of a Molecular Switch with Controlled Hydrogen Bonds: Electronic and Vibrational Spectra of [Co(2,2'-biimidazole)(C ₆ H ₄ O ₂)(NH ₃) ₂] ₂ . <i>Bulletin of the Chemical Society of Japan</i> , 2007, 80, 1335-1340.	2.0	7
3943	Theoretical Study of Geometries and Electronic Transition of Color-Switching Molecules: Tetra-Aza Macrocycle and Its Zinc Complexes. <i>Bulletin of the Chemical Society of Japan</i> , 2007, 80, 686-693.	2.0	4
3944	Quantum Mechanics for Organic Chemistry. , 0, , 1-41.		1
3945	Solid-Liquid Equilibrium in the System Propanoic Acid-Formamide. <i>Collection of Czechoslovak Chemical Communications</i> , 2007, 72, 899-907.	1.0	3
3946	Canonical Transformation Theory for Dynamic Correlations in Multireference Problems. <i>Advances in Chemical Physics</i> , 2007, , 343-384.	0.3	16
3947	Hole-vibronic coupling in oligothiophenes: impact of backbone torsional flexibility on relaxation energies. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2007, 365, 1435-1452.	1.6	59
3948	A parallel multi-configuration self-consistent field algorithm. <i>Molecular Physics</i> , 2007, 105, 2971-2976.	0.8	10
3949	Theoretical and Spectroscopic Study of 2-Substituted Indan-1,3-diones: A Coherent Picture of the Tautomeric Equilibrium. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9901-9913.	1.1	9
3950	A Structural Basis for the pH-dependent Increase in Fluorescence Efficiency of Chromoproteins. <i>Journal of Molecular Biology</i> , 2007, 368, 998-1010.	2.0	28
3951	A Comparison of Stigmatellin Conformations, Free and Bound to the Photosynthetic Reaction Center and the Cytochrome bc ₁ Complex. <i>Journal of Molecular Biology</i> , 2007, 368, 197-208.	2.0	47
3952	Study of michael-michael-retro michael addition catalyzed by 9-amino-9-deoxyepiquinine using ESI-MS. <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 2074-2080.	1.2	19

#	ARTICLE	IF	CITATIONS
3953	Direct location of the minimum point on intersection seams of potential energy surfaces with equation-of-motion coupled-cluster methods. <i>Molecular Physics</i> , 2007, 105, 2515-2525.	0.8	20
3954	On the Existence of Molecular Palladium(VI) Compounds: A Palladium Hexafluoride. <i>Inorganic Chemistry</i> , 2007, 46, 2700-2703.	1.9	17
3955	Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 407-433.	2.3	295
3956	Construction of Robust Open Metal-Organic Frameworks with Chiral Channels and Permanent Porosity. <i>Inorganic Chemistry</i> , 2007, 46, 2725-2734.	1.9	149
3957	Canonical transformation theory from extended normal ordering. <i>Journal of Chemical Physics</i> , 2007, 127, 104107.	1.2	122
3958	A Class of Luminescent Cyclometalated Alkynylgold(III) Complexes: A Synthesis, Characterization, and Electrochemical, Photophysical, and Computational Studies of $[Au(C^{\wedge}N^{\wedge}C)(C^{\wedge}CR)]$ ($C^{\wedge}N^{\wedge}C = \text{ip}^3C,N,C$) Tj 470q1 1 0894314	1.7	13
3959	Generation of $[La(\text{peptide})]_3^+$ Complexes in the Gas Phase: A Determination of the Number of Binding Sites Provided by Dipeptide, Tripeptide, and Tetrapeptide Ligands. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11562-11571.	1.1	22
3960	Synthesis and characterization of a new fluorescent probe for reactive oxygen species. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 1454.	1.5	25
3961	Diffusion of Methanol in Zeolite NaY: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2836-2844.	1.2	54
3962	Intramolecular General Acid Catalysis of the Hydrolysis of 2-(2-Imidazolium)phenyl Phosphate, and Bond Length-Reactivity Correlations for Reactions of Phosphate Monoester Monoanions. <i>Journal of Organic Chemistry</i> , 2007, 72, 3800-3807.	1.7	13
3963	Signature OH Absorption Spectrum from Cluster Models of Solvation: A Solvent-to-Solute Charge Transfer State. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10478-10482.	1.1	13
3964	Stereoselective Quaternization of \pm -Amino Phenylacetonitriles Mediated by a Remote Sulfinyl Group. <i>Journal of Organic Chemistry</i> , 2007, 72, 5994-6005.	1.7	16
3965	Alternative linear-scaling methodology for the second-order Møller-Plesset perturbation calculation based on the divide-and-conquer method. <i>Journal of Chemical Physics</i> , 2007, 127, 074103.	1.2	141
3966	Dual-basis self-consistent field methods: 6-31G* calculations with a minimal 6-4G primary basis. <i>Molecular Physics</i> , 2007, 105, 2455-2473.	0.8	25
3967	Anion-Selective Interaction and Colorimeter by an Optical Metalloreceptor Based on Ruthenium(II) 2,2'-Biimidazole: Hydrogen Bonding and Proton Transfer. <i>Inorganic Chemistry</i> , 2007, 46, 6427-6436.	1.9	146
3968	Mechanistic Insights into the Chemistry of Ru(II) Complexes Containing Cl and DMSO Ligands. <i>Inorganic Chemistry</i> , 2007, 46, 10707-10716.	1.9	53
3969	Ab Initio Study of the Two-Photon Circular Dichroism in Chiral Natural Amino Acids. <i>Journal of Physical Chemistry B</i> , 2007, 111, 446-460.	1.2	41
3970	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. <i>Annual Reports in Computational Chemistry</i> , 2007, 3, 177-193.	0.9	193

#	ARTICLE	IF	CITATIONS
3971	Anticancer and Antimicrobial Metallopharmaceutical Agents Based on Palladium, Gold, and Silver N-Heterocyclic Carbene Complexes. <i>Journal of the American Chemical Society</i> , 2007, 129, 15042-15053.	6.6	576
3972	Phosphine- and Pyridine-Functionalized N-Heterocyclic Carbene Methyl and Allyl Complexes of Palladium. Unexpected Regiospecificity of the Protonation Reaction of the Dimethyl Complexes. <i>Organometallics</i> , 2007, 26, 253-263.	1.1	118
3973	What is the Active Species of Cytochrome P450 during Camphor Hydroxylation? QM/MM Studies of Different Electronic States of Compound I and of Reduced and Oxidized Iron ^{IV} Oxo Intermediates. <i>Journal of the American Chemical Society</i> , 2007, 129, 8978-8987.	6.6	115
3974	Coordinatively Unsaturated Semisandwich Complexes of Ruthenium with Phosphinoamine Ligands and Related Species: A Complex Containing (R)-1,2-Bis((diisopropylphosphino)amino)cyclohexane in a New Coordination Form $P^3</math>-P</math>-N</math>-P</math>-N</math>. Inorganic Chemistry, 2007, 46, 6058-6067.$	1.9	34
3975	Master equation simulations of competing unimolecular and bimolecular reactions: application to OH production in the reaction of acetyl radical with O ₂ . <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4129.	1.3	62
3976	¹ H NMR Investigation of Paramagnetic Chromium(III) Olefin Polymerization Catalysts: Experimental Results, Shift Assignment and Prediction by Quantum Chemical Calculations. <i>Organometallics</i> , 2007, 26, 4402-4412.	1.1	80
3977	Understanding d ⁰ -Olefin Metathesis Catalysts: Which Metal, Which Ligands?. <i>Journal of the American Chemical Society</i> , 2007, 129, 8207-8216.	6.6	210
3978	Mechanism of Formation of Silver N-Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. <i>Organometallics</i> , 2007, 26, 6170-6183.	1.1	58
3979	Spectral Properties of Thioflavin T in Solvents with Different Dielectric Properties and in a Fibril-Incorporated Form. <i>Journal of Proteome Research</i> , 2007, 6, 1392-1401.	1.8	187
3980	Efficient Red Electrophosphorescent Devices Based on Iridium Complexes of Fluorinated 1-Phenylisoquinoline. <i>Japanese Journal of Applied Physics</i> , 2007, 46, 2735-2739.	0.8	6
3981	Ultrafast Deactivation Channel for Thymine Dimerization. <i>Journal of the American Chemical Society</i> , 2007, 129, 10996-10997.	6.6	125
3982	The Sila-Explosives Si(CH ₂ N ₃) ₄ and Si(CH ₂ ONO ₂) ₄ : Silicon Analogues of the Common Explosives Pentaerythryl Tetraazide, C(CH ₂ N ₃) ₄ , and Pentaerythritol Tetranitrate, C(CH ₂ ONO ₂) ₄ . <i>Journal of the American Chemical Society</i> , 2007, 129, 6908-6915.	6.6	65
3983	On the Keto [→] Enol Tautomerization of Malonaldehyde: An Effective Fragment Potential Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1659-1666.	1.1	17
3984	Gas Adsorption in Zeolites and Related Materials. <i>Studies in Surface Science and Catalysis</i> , 2007, 168, 555-XVI.	1.5	14
3985	Oxidation of Tertiary Silanes by Osmium Tetroxide. <i>Inorganic Chemistry</i> , 2007, 46, 5212-5219.	1.9	73
3986	Derivation of new interatomic potential for flexible metal-organic frameworks: a pre-requisite for understanding swelling under adsorption conditions.. <i>Studies in Surface Science and Catalysis</i> , 2007, , 918-925.	1.5	2
3987	Chapter 7 Using the reactivity-selectivity descriptor $f(r)$ in organic chemistry. <i>Theoretical and Computational Chemistry</i> , 2007, , 101-117.	0.2	8
3988	Water-Assisted H ⁺ H Bond Splitting Mediated by [CpRu(PTA)2Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. <i>Organometallics</i> , 2007, 26, 3289-3296.	1.1	57

#	ARTICLE	IF	CITATIONS
3989	Molecular Characterization of <i>p</i> -Alkyl Phenol- <i>n</i> -Heptane Interactions and Their Implication as Asphaltene Dispersants. <i>Energy & Fuels</i> , 2007, 21, 1127-1132.	2.5	14
3990	Vibronic Interaction in Metalloporphyrin π -Anion Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 852-857.	1.1	12
3991	Is the divide-and-conquer Hartree-Fock method valid for calculations of delocalized systems?. <i>Molecular Physics</i> , 2007, 105, 2799-2804.	0.8	42
3992	Synthesis and Photophysical Studies of Heteroleptic Tris-Cyclometalated Ir(III) Complex for Red OLED. <i>Molecular Crystals and Liquid Crystals</i> , 2007, 471, 235-244.	0.4	0
3993	State-specific multireference complete-active-space coupled-cluster approach versus other quantum chemical methods: dissociation of the N_2 molecule. <i>Molecular Physics</i> , 2007, 105, 1335-1357.	0.8	32
3994	Charge distribution in metal organic framework materials: transferability to a preliminary molecular simulation study of the CO ₂ adsorption in the MIL-53 (Al) system. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1059-1063.	1.3	112
3995	Chemoselectivity in σ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp ₂ LnR (R = CH ₃ , H, SiH ₃) with SiH ₄ and CH ₃ -SiH ₃ . <i>New Journal of Chemistry</i> , 2007, 31, 549-555.	1.4	37
3996	The [2,5,12-C ₃ B ₈ H ₁₅] ⁻ anion, the first representative of the eleven-vertex hypho family of tricarbaboranes. <i>Dalton Transactions</i> , 2007, , 1221-1228.	1.6	13
3997	Influence of the bridging ligand on the substitution behaviour of dinuclear Pt(II) complexes. An experimental and theoretical approach. <i>Dalton Transactions</i> , 2007, , 2295-2301.	1.6	58
3998	Organolanthanide mediated catalytic cycles: a computational perspective. <i>Dalton Transactions</i> , 2007, , 1743.	1.6	61
3999	Theoretical Studies on the Hydrolysis Mechanism of N-(2-oxo-1,2-dihydro-pyrimidinyl) Formamide. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2357-2364.	1.2	25
4000	Which One among Zn(II), Co(II), Mn(II), and Fe(II) is the Most Efficient Ion for the Methionine Aminopeptidase Catalyzed Reaction?. <i>Journal of the American Chemical Society</i> , 2007, 129, 7776-7784.	6.6	57
4001	Reaction and subsequent transformation of anionic acetylide-carbene complexes using the Ph ₃ PAu ⁺ fragment. <i>Dalton Transactions</i> , 2007, , 5684.	1.6	9
4002	Air-stable, convenient to handle Pd based PEPPSI (pyridine enhanced precatalyst preparation,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T utility in Suzuki-Miyaura cross-coupling reaction. <i>Dalton Transactions</i> , 2007, , 4546.	1.6	99
4003	Molecular recognition in molecular tweezers systems: quantum-chemical calculation of NMR chemical shifts. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4552.	1.3	21
4004	Inner-shell spectroscopy by the Gaussian and augmented plane wave method. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 1599.	1.3	82
4005	Torsional anharmonicity in the conformational analysis of tryptamine. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2065.	1.3	15
4006	Torsional anharmonicity in transition state theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2397.	1.3	19

#	ARTICLE	IF	CITATIONS
4007	The effects of alkyl sulfates on the analysis of phenolic compounds by microchip capillary electrophoresis with pulsed amperometric detection. <i>Analyst</i> , 2007, 132, 997.	1.7	26
4008	Vibrational overtone induced elimination reactions within hydrogen-bonded molecular clusters: the dynamics of water catalyzed reactions in CH ₂ FOH·(H ₂ O) _n . <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 3864-3871.	1.3	44
4009	Charge Model 4 and Intramolecular Charge Polarization. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2046-2054.	2.3	75
4010	Additivity of Ring Distortions in Halogen-Substituted Aromatics: a Gas-Phase Electron Diffraction and Computational Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7882-7887.	1.1	11
4011	Molecular Simulation of the Hydration of Ethene to Ethanol Using Ab Initio Potentials and Free Energy Curves. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13515-13520.	1.1	10
4012	Geometry Optimization of a Ru(IV) Allyl Dicationic Complex: A DFT Failure?. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 665-670.	2.3	17
4013	Extension of the Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian to Open-Shell Systems: A Benchmark Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11359-11382.	1.1	178
4014	Valence Anions in Complexes of Adenine and 9-Methyladenine with Formic Acid: Stabilization by Intermolecular Proton Transfer. <i>Journal of the American Chemical Society</i> , 2007, 129, 1216-1224.	6.6	37
4015	Structure Enhancement Methodology Using Theory and Experiment: Gas-Phase Molecular Structures Using a Dynamic Interaction between Electron Diffraction, Molecular Mechanics, and Ab Initio Data. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5913-5920.	1.1	5
4016	Spectroscopic Characterization and Langmuir-Blodgett Films of a Novel Azopolymer Material. <i>Langmuir</i> , 2007, 23, 1804-1809.	1.6	12
4017	DFT Study of Hydride Exchange in a Binuclear Ruthenium Complex. <i>Organometallics</i> , 2007, 26, 56-64.	1.1	11
4018	Models for the Structure and Electronic Transmission of Carbon Nanotubes Covalently Linked by a Molecular Bridge via Amide Couplings. <i>Journal of Physical Chemistry C</i> , 2007, 111, 3700-3704.	1.5	25
4019	Boron and Aluminum Complexes of Sterically Demanding Phosphinimines and Phosphinimides. <i>Inorganic Chemistry</i> , 2007, 46, 3623-3631.	1.9	41
4020	What Definitively Controls the Photochemical Activity of Methylbenzonnitriles and Methylanisoles? Insights from Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5775-5783.	1.1	3
4021	Effect of Hexafluorobenzene on the Photophysics of Pyrene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4884-4889.	1.1	22
4022	Theoretical Study of the Reaction Mechanisms Involved in the Thermal Intramolecular Reactions of 1,6-Fullerenynes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5253-5258.	1.1	12
4023	Gas-Phase Ionic Syntheses of Amino Acids: $\dot{\text{I}}^2$ versus $\dot{\text{I}}\pm$. <i>Journal of the American Chemical Society</i> , 2007, 129, 9910-9917.	6.6	39
4024	Computational Studies of Intramolecular Hydrogen Atom Transfers in the $\dot{\text{I}}^2$ -Hydroxyethylperoxy and $\dot{\text{I}}^2$ -Hydroxyethoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5032-5042.	1.1	37

#	ARTICLE	IF	CITATIONS
4025	Accurate Evaluation of Valence and Low-Lying Rydberg States with Standard Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5549-5556.	1.1	119
4026	CâˆO and CâˆS Bond Cleavage in Chelating Diethers and Thioethers Promoted by Î9,Î5-Bis(indenyl)zirconium Sandwich Complexes:Â A Combined Experimental and Computational Study. <i>Organometallics</i> , 2007, 26, 3191-3200.	1.1	45
4027	Scaled Density Functional Theory Correlation Functionalsâ€. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10390-10399.	1.1	0
4028	Photodissociation of 1,3,5-Triazine:â€% An Ab Initio and RRKM Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9591-9599.	1.1	22
4029	The Catalytic Effect of Dihydrofolate Reductase and Its Mutants Is Determined by Reorganization Energies. <i>Biochemistry</i> , 2007, 46, 6011-6025.	1.2	92
4030	Manganese(III)-Catalyzed Free Radical Reactions on Trimetallic Nitride Endohedral Metallofullerenes. <i>Journal of the American Chemical Society</i> , 2007, 129, 15710-15717.	6.6	70
4031	Electronic Structure of the PYP Chromophore in Its Native Protein Environment. <i>Journal of the American Chemical Society</i> , 2007, 129, 6798-6806.	6.6	72
4032	New generation of the reference interaction site model self-consistent field method: Introduction of spatial electron density distribution to the solvation theory. <i>Journal of Chemical Physics</i> , 2007, 126, 244504.	1.2	103
4033	A Dynamical Study of the Si+ + H2O Reaction. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10899-10906.	1.1	3
4034	Can Changes in One-bond Spinâˆspin Coupling Constants in Acids Be Related to Gas-Phase Proton Affinities of Bases?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6443-6448.	1.1	7
4035	Assessing the Efficacy of Nonsteroidal Anti-Inflammatory Drugs Through the Quantum Computation of Molecular Ionization Energies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7223-7226.	1.1	8
4036	Crucial Role of Anions on the Deprotonation of the Cationic Dihydrogen Complex trans-[FeH(Î2-H2)(dppe)2]+. <i>Journal of the American Chemical Society</i> , 2007, 129, 6608-6618.	6.6	51
4037	Hydrogen Bonding Mediated by Key Orbital Interactions Determines Hydration Enthalpy Differences of Phosphate Water Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10804-10814.	1.1	10
4038	Gas-Phase Structure, Rotational Barrier, and Vibrational Properties of Methyl Methanethiosulfonate, CH₃SO₂SCH₃:â€% An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9952-9960.	1.1	14
4039	Covalent and Ionic Nature of the Dative Bond and Account of Accurate Ammonia Borane Binding Enthalpies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13472-13483.	1.1	41
4040	Cerium(III) and Cerium(IV) Bis(Î8-pentalene) Sandwich Complexes:Â Synthetic, Structural, Spectroscopic, and Theoretical Studies. <i>Organometallics</i> , 2007, 26, 3111-3119.	1.1	57
4041	Can the Nonadiabatic Photodynamics of Aminopyrimidine Be a Model for the Ultrafast Deactivation of Adenine?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2852-2858.	1.1	67
4042	Conformational Preferences of <i>N</i>-Acetyl-<sc>l</sc>-leucine-<i>N</i>-methylamide. Gas-Phase and Solution Calculations on the Model Dipeptide. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10682-10691.	1.1	14

#	ARTICLE	IF	CITATIONS
4043	Energy Screening for the Incremental Scheme: Application to Intermolecular Interactions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9830-9837.	1.1	45
4044	Binding Energy of Transition-Metal Complexes with Large π -Conjugate Systems. Density Functional Theory vs Post-Hartree-Fock Methods. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7124-7132.	1.1	42
4045	Variation of One-bond $X\hat{\sim}Y$ Coupling Constants $1J(X\hat{\sim}Y)$ and the Components of $1J(X\hat{\sim}Y)$ with Rotation about the $X\hat{\sim}Y$ Bond for Molecules $H_mX\hat{\sim}YH_n$, with $X, Y = {}^{15}N, {}^{17}O, {}^{31}P, {}^{33}S$: The Importance of Nonbonding Pairs of Electrons. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2517-2526.	1.1	7
4046	Through-Space Intramolecular Palladium Rearrangement in Substituted Aryl Complexes: Theoretical Study of the Aryl to Alkylpalladium Migration Process. <i>Journal of Organic Chemistry</i> , 2007, 72, 9669-9678.	1.7	39
4047	Characterization of the Chemisorption of Methylsilane on a Au(1,1,1) Surface from the Silicon K- and L-Edge Spectra: A Theoretical Study Using the Four-Component Static Exchange Approximation. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13846-13850.	1.5	9
4048	Theoretical Study on the Motion of a La Atom Inside a C ₈₂ Cage. <i>Journal of Physical Chemistry A</i> , 2007, 111, 167-169.	1.1	38
4049	Direct-Dynamics VTST Study of the [1,7] Hydrogen Shift in 7-Methylocta-1,3(Z),5(Z)-triene. A Model System for the Hydrogen Transfer Reaction in Previtamin D ₃ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 719-725.	1.1	14
4050	New Complexes of Methyl-diphenylphosphonium Cyclopentadienylide, Representative of a Class of Ligands Heretofore Much Neglected. <i>Organometallics</i> , 2007, 26, 1433-1443.	1.1	31
4051	Transition State Infrared Spectra for the Trans \rightarrow Cis Isomerization of a Simple Peptide Model. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8384-8389.	1.1	6
4052	Haptotropic Shifts and Fluxionality of Cyclopentadienyl in Mixed-Hapticity Complexes: A DFT Mechanistic Study. <i>Organometallics</i> , 2007, 26, 1777-1781.	1.1	12
4053	An Ab Initio Study of the Excited States, Isomerization Energy Profiles and Conical Intersections of a Chiral Cyclohexylidene Derivative. <i>Journal of Physical Chemistry A</i> , 2007, 111, 238-243.	1.1	17
4054	Quantum Chemical Modeling of Ethene Epoxidation with Hydrogen Peroxide: The Effect of Microsolvation with Water. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9080-9086.	1.1	23
4055	Computational Studies on the Stabilities of trans-[Ir(OMe)(CO)(PPh ₃) ₂] and trans-[Ir(CH ₂ Me)(CO)(PPh ₃) ₂] toward β -H Elimination. <i>Organometallics</i> , 2007, 26, 3651-3659.	1.1	21
4056	Synthesis and Structure of Pentaorganostannate Having Five Carbon Substituents. <i>Journal of the American Chemical Society</i> , 2007, 129, 10974-10975.	6.6	30
4057	Selective Cyclopalladation of R ³ PNCH ₂ Aryl Iminophosphoranes. Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2007, 46, 10133-10142.	1.9	41
4058	Radiationless Decay of Red Fluorescent Protein Chromophore Models via Twisted Intramolecular Charge-Transfer States. <i>Journal of the American Chemical Society</i> , 2007, 129, 2054-2065.	6.6	80
4059	Quantifying the Intrinsic Effects of Two Point Mutation Models of Proline \rightarrow Proline Diamino Acid Diamide: A First-Principle Computational Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11592-11602.	1.2	15
4060	DFT Study of an Inner-Sphere Mechanism in the Hydrogen Transfer from a Hydroxycyclopentadienyl Ruthenium Hydride to Imines. <i>Organometallics</i> , 2007, 26, 2840-2848.	1.1	55

#	ARTICLE	IF	CITATIONS
4061	Carbon Dioxide Reduction by Pincer Rhodium η^2 -Dihydrogen Complexes: A Hydrogen-Binding Modes and Mechanistic Studies by Density Functional Theory Calculations. <i>Organometallics</i> , 2007, 26, 508-513.	1.1	62
4062	Theoretical Study of Tungsten η^3 -Silaallyl/ η^3 -Vinylsilyl and Vinyl Silylene Complexes: An Interesting Bonding Nature and Relative Stability. <i>Organometallics</i> , 2007, 26, 4413-4423.	1.1	23
4063	Production of Acrylic Acid through Nickel-Mediated Coupling of Ethylene and Carbon Dioxide: A DFT Study. <i>Organometallics</i> , 2007, 26, 6784-6792.	1.1	95
4064	Many-Photon Dynamics of Photobleaching. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11961-11975.	1.1	37
4065	Association Patterns in (HF) _m (H ₂ O) _n ($m > n$) Clusters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11976-11985.	1.1	26
4066	Chemisorbed and Physisorbed Structures for 1,10-Phenanthroline and Dipyrido[3,2- <i>a</i> :1',2'- <i>c</i>]phenazine on Au(111). <i>Journal of Physical Chemistry C</i> , 2007, 111, 17285-17296.	1.5	25
4067	Exploration of Mechanisms for the Transformation of 8-Hydroxy Guanine Radical to FAPyG by Density Functional Theory. <i>Chemical Research in Toxicology</i> , 2007, 20, 432-444.	1.7	46
4068	Oxidation Reaction by Xanthine Oxidase. Theoretical Study of Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2007, 129, 8131-8138.	6.6	39
4069	Nitrogen-Rich Oligoacenes: Candidates for <i>n</i> -Channel Organic Semiconductors. <i>Journal of the American Chemical Society</i> , 2007, 129, 1805-1815.	6.6	317
4070	Multidimensional Quantum Dynamical Study of η^2 -Hydrogen Transfer in a Cationic Rhodium Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2407-2419.	1.1	7
4071	Control of Electronic and Magnetic Coupling via Bridging Ligand Geometry in a Bimetallic Ytterbocene Complex. <i>Inorganic Chemistry</i> , 2007, 46, 5013-5022.	1.9	15
4072	Tunneling in the 1,5-Hydrogen Shift Reactions of 1,3-Cyclopentadiene and 5-Methyl-1,3-Cyclopentadiene. <i>Journal of the American Chemical Society</i> , 2007, 129, 164-168.	6.6	52
4073	Coordination and Rupture of Methyl C(sp ³)-H Bonds in Osmium Polyhydride Complexes with η^2 Agostic Interaction. <i>Organometallics</i> , 2007, 26, 5140-5152.	1.1	51
4074	Theoretical Investigation of the Binding of Small Molecules and the Intramolecular Agostic Interaction at Tungsten Centers with Carbonyl and Phosphine Ligands. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6815-6821.	1.2	11
4075	A Comparative Study of the Antioxidant Power of Flavonoid Catechin and Its Planar Analogue. <i>Journal of Agricultural and Food Chemistry</i> , 2007, 55, 7944-7949.	2.4	47
4076	Analysis of the Substituent Effect on the Reactivity Modulation during Self-Protonation Processes in 2-Nitrophenols. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8993-9002.	1.1	15
4077	Experimental and Theoretical Charge Density Distribution in Two Ternary Cobalt(III) Complexes of Aromatic Amino Acids. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10123-10133.	1.1	19
4078	Ab Initio Molecular Dynamics of Excited-State Intramolecular Proton Transfer Using Multireference Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11302-11310.	1.1	110

#	ARTICLE	IF	CITATIONS
4079	Enantioselective Synthesis of Chiral Sulfones by Rh-Catalyzed Asymmetric Addition of Boronic Acids to $\hat{I}\pm, \hat{I}^2$ -Unsaturated 2-Pyridyl Sulfones. <i>Journal of Organic Chemistry</i> , 2007, 72, 9924-9935.	1.7	94
4080	Calculations of the Effect of Tunneling on the Swain \hat{I} Schaad Exponents (SSEs) for the 1,5-Hydrogen Shift in 5-Methyl-1,3-cyclopentadiene. Can SSEs Be Used to Diagnose the Occurrence of Tunneling?. <i>Journal of the American Chemical Society</i> , 2007, 129, 16115-16118.	6.6	14
4081	Mechanism of the [RhF(PPh \hat{I}) \hat{I}] \hat{I} to cis-[RhPh(PPh \hat{I}) \hat{I} 2(PFPh \hat{I}) \hat{I}] Interconversion: \hat{I} P \hat{I} \hat{I} C Activation and F/Ph Exchange via a Metallophosphorane Pathway. <i>Organometallics</i> , 2007, 26, 1143-1149.	1.1	38
4082	Molecular Dynamics Simulation of the Reaction of Hydration of Formaldehyde Using a Potential Based on Solute \hat{I} Solvent Interaction Energy Components. <i>Journal of Physical Chemistry A</i> , 2007, 111, 339-344.	1.1	20
4083	Ab Initio Calculations on Low-Energy Conformers of $\hat{I}\pm$ -Cyclodextrin. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12127-12135.	1.1	34
4084	Ab Initio Computations of Polarizabilities and Hyperpolarizabilities of Atoms and Molecules. <i>Advances in Chemical Physics</i> , 2007, , 415-488.	0.3	21
4085	Calixarenes in a Membrane Environment: \hat{I} A Monolayer Study on the Miscibility of Three p-tert-Butylcalix[4]arene \hat{I}^2 -Lactam Derivatives with 1,2-Dimyristoyl-sn-glycero-3-phosphoethanolamine. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13231-13242.	1.2	37
4086	Polarization Consistent Basis Sets. 4: \hat{I} % The Elements He, Li, Be, B, Ne, Na, Mg, Al, and Ar. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11198-11204.	1.1	105
4087	Combined Theoretical and Experimental Analysis of the Bonding in the Heterobimetallic Cubane-Type Mo \hat{I} 3NiS \hat{I} 4 and Mo \hat{I} 3CuS \hat{I} 4 Core Clusters. <i>Inorganic Chemistry</i> , 2007, 46, 2159-2166.	1.9	22
4088	How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods. <i>Journal of Organic Chemistry</i> , 2007, 72, 2118-2126.	1.7	234
4089	Basis Sets for Ab Initio Molecular Orbital Calculations and Intermolecular Interactions. <i>Reviews in Computational Chemistry</i> , 2007, , 1-43.	1.5	36
4090	Mechanism of Activation of a Hafnium Pyridyl \hat{I} Amide Olefin Polymerization Catalyst: \hat{I} Ligand Modification by Monomer. <i>Journal of the American Chemical Society</i> , 2007, 129, 7831-7840.	6.6	128
4091	Synthesis and Properties of a Cationic Bidentate Lewis Acid. <i>Inorganic Chemistry</i> , 2007, 46, 8132-8138.	1.9	96
4092	Computational Study of Thioflavin T Torsional Relaxation in the Excited State. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4829-4835.	1.1	206
4093	Geometries of Second-Row Transition-Metal Complexes from Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2234-2242.	2.3	154
4094	Theoretical Study of Chemo-, Regio-, and Stereoselectivity in 1,3-Dipolar Cycloadditions of Nitrones and Nitrile Oxides to Free and Pt-Bound Bifunctional Dipolarophiles. <i>Journal of Organic Chemistry</i> , 2007, 72, 4475-4485.	1.7	47
4095	A Theoretical Study on the Hydrolysis Process of the Antimetastatic Ruthenium(III) Complex NAMI-A. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7862-7869.	1.2	54
4096	Ultralarge Hyperpolarizability Twisted \hat{I} -Electron System Electro-Optic Chromophores: \hat{I} Synthesis, Solid-State and Solution-Phase Structural Characteristics, Electronic Structures, Linear and Nonlinear Optical Properties, and Computational Studies. <i>Journal of the American Chemical Society</i> , 2007, 129, 3267-3286.	6.6	258

#	ARTICLE	IF	CITATIONS
4097	Assessment of Density Functional Theory Methods for the Computation of Heats of Formation and Ionization Potentials of Systems Containing Third Row Transition Metals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6044-6053.	1.1	94
4098	Principle and Mechanism of Direct Porphyrin Metalation: Joint Experimental and Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 2007, 129, 9476-9483.	6.6	167
4099	Stability of small Pd ⁿ (n=1-7) clusters on the basis of structural and electronic properties: A density functional approach. <i>Journal of Chemical Physics</i> , 2007, 127, 244306.	1.2	60
4100	Doorway mechanism for dissociative electron attachment to fructose. <i>Journal of Chemical Physics</i> , 2007, 126, 124301.	1.2	38
4101	The Structure, Stability, and Reactivity of Mo-oxo Species in H-ZSM5 Zeolites: Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 2081-2091.	1.5	20
4102	Experimental and Theoretical Examination of C≡N and C-H Bond Activations of Acetonitrile Using Zerovalent Nickel. <i>Journal of the American Chemical Society</i> , 2007, 129, 7562-7569.	6.6	139
4103	Computational Studies of Structures and Properties of Metallaboranes. Part 3: Protonated Iron Bis(dicarbollide), [3-Fe-(1,2-C ₂ B ₉ H ₁₁) ₂ H] ⁻ . <i>Inorganic Chemistry</i> , 2007, 46, 1771-1777.	1.9	16
4104	Ab Initio Molecular Dynamics and Time-Resolved Photoelectron Spectroscopy of Electronically Excited Uracil and Thymine. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8500-8508.	1.1	355
4105	Proton Hopping in Phosphoric Acid Solvated Nafion Membrane: A Molecular Simulation Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6357-6363.	1.2	43
4106	High resolution EPR spectroscopy of C ₆₀ F and C ₇₀ F in solid argon: Reassignment of C ₇₀ F regioisomers. <i>Journal of Chemical Physics</i> , 2007, 127, 084301.	1.2	51
4107	Theoretical Investigation of the Excited States of Coumarin Dyes for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5544-5548.	1.1	156
4109	Coupled-Cluster Approach in the Electronic-Structure Theory of Molecules. <i>Advances in Chemical Physics</i> , 2007, , 181-261.	0.3	26
4111	The Water-Exchange Mechanism of the [UO ₂ (OH) ₂] ₂ ⁺ Ion Revisited: The Importance of a Proper Treatment of Electron Correlation. <i>Chemistry - A European Journal</i> , 2007, 13, 800-811.	1.7	44
4112	Reaction Chemistry of Complexes Containing Pt ₂ H, Pt ₂ SH, or Pt ₂ S Fragments: From Their Apparent Simplicity to the Maze of Reactions Underlying Their Interconversion. <i>Chemistry - A European Journal</i> , 2007, 13, 1047-1063.	1.7	17
4113	The Preferred Reaction Path for the Oxidation of Methanol by PQQ-Containing Methanol Dehydrogenase: Addition vs Elimination versus Hydride-Transfer Mechanism. <i>Chemistry - A European Journal</i> , 2007, 13, 2109-2117.	1.7	48
4114	2,2-Biphosphinines and 2,2-Bipyridines in Homoleptic Dianionic Group ₄ Complexes and Neutral 2,2-Biphosphine Group ₆ d ₆ Metal Complexes: Octahedral versus Trigonal-Prismatic Geometries. <i>Chemistry - A European Journal</i> , 2007, 13, 2953-2965.	1.7	13
4115	Computational Mutation Analysis of Hydrogen Abstraction and Radical Rearrangement Steps in the Catalysis of Coenzyme B ₁₂ -Dependent Diol Dehydratase. <i>Chemistry - A European Journal</i> , 2007, 13, 7864-7873.	1.7	39
4116	Catalyzing Aldehyde Hydrosilylation with a Molybdenum(VI) Complex: A Density Functional Theory Study. <i>Chemistry - A European Journal</i> , 2007, 13, 3934-3941.	1.7	72

#	ARTICLE	IF	CITATIONS
4117	Cobalt-Mediated [2+2+2] Cycloaddition versus C ₁ H and Ni ₁ H Activation of 2-Pyridones and Pyrazinones with Alkynes: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2007, 13, 7466-7478.	1.7	36
4118	π-π Stacking versus Steric Effects in Stereoselectivity Control: Highly Diastereoselective Synthesis of syn-1,2-Diarylpropylamines. <i>Chemistry - A European Journal</i> , 2007, 13, 6179-6195.	1.7	57
4119	Intramolecular Spin Alignment in Photomagnetic Molecular Devices: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2007, 13, 5360-5377.	1.7	44
4120	Application of AIM Parameters at Ring Critical Points for Estimation of π-Electron Delocalization in Six-Membered Aromatic and Quasi-Aromatic Rings. <i>Chemistry - A European Journal</i> , 2007, 13, 7996-8006.	1.7	159
4121	⁵¹ V...NMR Chemical Shifts Calculated from QM/MM Models of Vanadium Chloroperoxidase. <i>Chemistry - A European Journal</i> , 2007, 13, 4723-4732.	1.7	95
4122	Cobalt(I)-Mediated Preparation of Polyborylated Cyclohexadienes: Scope, Limitations, and Mechanistic Insight. <i>Chemistry - A European Journal</i> , 2007, 13, 5408-5425.	1.7	61
4123	Alkali Metal Diphenylmethanides: Synthetic, Computational and Structural Studies. <i>Chemistry - A European Journal</i> , 2007, 13, 9899-9911.	1.7	14
4124	An Explanation for the Very Large Breathing Effect of a Metal-Organic Framework during CO ₂ Adsorption. <i>Advanced Materials</i> , 2007, 19, 2246-2251.	11.1	501
4125	Ligand Influence on Metathesis Activity of Ruthenium Carbene Catalysts: A DFT Study. <i>Advanced Synthesis and Catalysis</i> , 2007, 349, 204-214.	2.1	93
4126	How does the Achiral Base Decide the Stereochemical Outcome in the Dynamic Kinetic Resolution of Sulfinyl Chlorides? A Computational Study. <i>Advanced Synthesis and Catalysis</i> , 2007, 349, 2103-2110.	2.1	18
4127	Electrostatic energy in the effective fragment potential method: Theory and application to benzene dimer. <i>Journal of Computational Chemistry</i> , 2007, 28, 276-291.	1.5	108
4128	Theoretical study of the electronic spectra of oxidized and reduced states of lumiflavin and its derivative. <i>Journal of Computational Chemistry</i> , 2007, 28, 727-739.	1.5	36
4129	On the quality of the hardness kernel and the Fukui function to evaluate the global hardness. <i>Journal of Computational Chemistry</i> , 2007, 28, 574-583.	1.5	48
4130	Electronic reorganization: Origin of sigma trans promotion effect. <i>Journal of Computational Chemistry</i> , 2007, 28, 423-441.	1.5	10
4131	Origin of intrinsic 310-helix versus strand stability in homopolypeptides and its implications for the accuracy of the Amber force field. <i>Journal of Computational Chemistry</i> , 2007, 28, 1648-1657.	1.5	11
4132	Can an OH radical form a strong hydrogen bond? A theoretical comparison with H ₂ O. <i>Journal of Computational Chemistry</i> , 2007, 28, 1357-1363.	1.5	21
4133	Excited states of GFP chromophore and active site studied by the SAC-Cl method: Effect of protein environment and mutations. <i>Journal of Computational Chemistry</i> , 2007, 28, 2443-2452.	1.5	78
4134	Vibrational corrections to geometries of transition metal complexes from density functional theory. <i>Journal of Computational Chemistry</i> , 2007, 28, 1531-1537.	1.5	27

#	ARTICLE	IF	CITATIONS
4135	Common system setup for the entire catalytic cycle of cytochrome P450cam in quantum mechanical/molecular mechanical studies. <i>Journal of Computational Chemistry</i> , 2007, 28, 2147-2158.	1.5	46
4136	Implementation of divide-and-conquer method including Hartree-Fock exchange interaction. <i>Journal of Computational Chemistry</i> , 2007, 28, 2003-2012.	1.5	130
4137	Orthogonal natural atomic orbitals form an appropriate one-electron basis for expanding CASSCF wave functions into localized bonding schemes and their weights. <i>Journal of Computational Chemistry</i> , 2007, 28, 2013-2019.	1.5	6
4138	Efficient algorithm for "on-the-fly" error analysis of local or distributed serially correlated data. <i>Journal of Computational Chemistry</i> , 2007, 28, 2309-2316.	1.5	16
4139	Model transition states for methane diazonium ion methylation of guanine runs in oligomeric DNA. <i>Journal of Computational Chemistry</i> , 2007, 28, 2352-2365.	1.5	11
4140	Gas-Phase Structure and Vibrational Properties of Trifluoromethyl Trifluoromethanesulfonate, CF ₃ SO ₂ OCF ₃ . <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 1381-1389.	1.0	22
4141	Synthesis, Reactivity and DFT Investigation of a Cationic Zirconocene Benzyl Compound with an Appended Phenyl Group. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2327-2333.	1.0	13
4142	Electronic Structure of Linearly Coordinated EQ Complexes of the Type [(N ₃ N)W(EQ)] [N ₃ N = N(CH ₂ CH ₂ NSiMe ₃) ₃ ; E = P, As, Sb, Bi; Q = O, S, Se, Te]: A DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2443-2453.	1.0	3
4143	C-S Bond Activation and Partial Hydrogenation of Thiophene by a Dinuclear Trihydride Platinum Complex. <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 5707-5719.	1.0	17
4144	[2.2.2]Propellane Isomerization by Grob Rearrangement: An Ab Initio MR-AQCC Study. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3173-3178.	1.2	11
4145	Base-Catalyzed Anti-Markovnikov Hydroamination of Vinylarenes " Scope, Limitations and Computational Studies. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 3311-3325.	1.2	84
4146	A Density Functional Study on the Hydrolysis Process of Non-classical Transplatin(II) with Two Same Planar Heterocycle Amines. <i>Chinese Journal of Chemistry</i> , 2007, 25, 1604-1611.	2.6	2
4147	On the Origin of Red and Blue Shifts of X-H and C-H Stretching Vibrations in Formic Acid (Formate) Tj ETQq0 0.0 rgBT /Overlock 10	1.0	28
4148	Conformational and tautomeric eccentricities of 2-acetyl-1,8-dihydroxynaphthalenes. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 106-117.	1.1	17
4149	Intramolecular hydrogen bonding of novelo-hydroxythioacetophenones and related compounds evaluated by deuterium isotope effects on ¹³ C chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 245-252.	1.1	19
4150	Probing the proton-transfer coordinate of complexes with F-H...P hydrogen bonds using one- and two-bond spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2007, 45, 714-719.	1.1	20
4151	Vibrational spectroscopic study of budesonide. <i>Journal of Raman Spectroscopy</i> , 2007, 38, 903-908.	1.2	14
4152	Observation of an unusually facile fragmentation pathway of gas-phase peptide ions: a study on the gas-phase fragmentation mechanism and energetics of tryptic peptides modified with 4-sulfophenyl isothiocyanate (SPITC) and 4-chlorosulfophenyl isocyanate (SPC) and their 18-crown-6 complexes. <i>Journal of Mass Spectrometry</i> , 2007, 42, 380-388.	0.7	4

#	ARTICLE	IF	CITATIONS
4153	Ruthenium-catalyzed [2+2] cycloadditions between substituted alkynes and norbornadiene: a theoretical study. <i>Tetrahedron</i> , 2007, 63, 7659-7666.	1.0	16
4154	Theoretical studies on the role of bridging group of Cp ligands for the Ziegler-Natta catalysis. <i>Computational and Theoretical Chemistry</i> , 2007, 804, 35-39.	1.5	1
4155	Photo-rearrangement of N-substituted pyridinium and meta-alkoxy pyridinium ions. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 25-32.	1.5	3
4156	How the topological analysis of the electron localization function accounts for the inductive effect. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 69-76.	1.5	13
4157	Theoretical study of structure and properties of a molecular reactor based on the urea-linked β -cyclodextrin dimer. <i>Computational and Theoretical Chemistry</i> , 2007, 809, 95-102.	1.5	13
4158	Methanol dehydrogenation promoted by a heterobimetallic Ru(II)-Sn(II) complex as catalyst: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 77-84.	1.5	7
4159	On the origin of diastereofacial selectivity in the interaction of β -pinene with rhodium carbonyl: A density functional study. <i>Computational and Theoretical Chemistry</i> , 2007, 816, 109-117.	1.5	15
4160	On the formation of Al ₄ N ₁₂ H ₂₄ from triethylaluminum and ammonia: A pathway to crystalline AlN with the Wurtzite structure. <i>Computational and Theoretical Chemistry</i> , 2007, 817, 61-76.	1.5	1
4161	Reactions of NO ₂ with CH ₃ NHNH and CH ₃ NNH ₂ : A direct molecular dynamics study. <i>Computational and Theoretical Chemistry</i> , 2007, 818, 119-124.	1.5	21
4162	Performance of Time Dependent Density Functional Theory on excitations of medium sized molecules – Test on ionic forms of anthraquinone dihydroxy derivatives. <i>Computational and Theoretical Chemistry</i> , 2007, 823, 78-86.	1.5	28
4163	Study of charge transfer transition in benzene-ICl complex in gas phase and in CCl ₄ medium by ab initio and TDDFT methods. <i>Chemical Physics Letters</i> , 2007, 433, 427-431.	1.2	16
4164	The triplet state decay kinetics and deactivation funnel geometry of a series of nonplanar saddle-shaped porphyrins. <i>Chemical Physics Letters</i> , 2007, 434, 116-120.	1.2	8
4165	Parity violation energy of 5-pyrimidyl alkanol, a chiral autocatalytic molecule. <i>Chemical Physics Letters</i> , 2007, 435, 346-349.	1.2	11
4166	Extension of energy density analysis to periodic boundary condition calculation: Evaluation of locality in extended systems. <i>Chemical Physics Letters</i> , 2007, 438, 132-138.	1.2	31
4167	Insertion reaction of ethylene into the Rh-H bond: A comparative theoretical study. <i>Chemical Physics Letters</i> , 2007, 439, 69-75.	1.2	13
4168	Assignment of the lowest-lying THz absorption signatures in biotin and lactose monohydrate by solid-state density functional theory. <i>Chemical Physics Letters</i> , 2007, 440, 203-209.	1.2	101
4169	Adsorption structures of thiophene on Si(100)-(2 \times 1) studied by scanning tunneling microscopy and density functional theory. <i>Chemical Physics Letters</i> , 2007, 443, 347-351.	1.2	15
4170	Electrostatic interaction energies with overlap effects from a localized approach. <i>Chemical Physics Letters</i> , 2007, 445, 315-320.	1.2	11

#	ARTICLE	IF	CITATIONS
4171	Phosphorescent iridium(III) complexes with hetero (CĒ†N) ligands. <i>Current Applied Physics</i> , 2007, 7, 390-395.	1.1	8
4172	A critical analysis of the performance of conventional ab initio and DFT methods in the computation of Si6 ground state. <i>Chemical Physics</i> , 2007, 331, 417-426.	0.9	20
4173	Chain length dependence of singlet and triplet excited states of oligofluorenes: A density functional study. <i>Chemical Physics</i> , 2007, 336, 91-98.	0.9	26
4174	Error analysis of incremental electron correlation calculations and applications to clusters and potential energy surfaces. <i>Chemical Physics</i> , 2007, 338, 33-43.	0.9	34
4175	A unified approach to the analysis of the chemical bond in hydrides and hydrocarbons. <i>Acta Materialia</i> , 2007, 55, 6673-6680.	3.8	14
4176	Steric and electronic effects on Siâ€“Ge bond lengths: An experimental and theoretical structural study of Me2Ge(SiCl3)2 and Me3GeSiCl3. <i>Inorganica Chimica Acta</i> , 2007, 360, 1323-1331.	1.2	7
4177	Hydrogen atom abstraction from HOOCl by chlorine atom and OH radical. <i>Inorganica Chimica Acta</i> , 2007, 360, 837-841.	1.2	3
4178	Kinetics and thermodynamics of proton transfer to Cpâˆ—Ru(dppe)H: Via dihydrogen bonding and (Î2-H2)-complex to the dihydride. <i>Inorganica Chimica Acta</i> , 2007, 360, 149-162.	1.2	38
4179	Intermolecular proton transfer induced by excess electron attachment to adenine(formic acid)n (n=2), Tj ETQq0 0 0 rgBT /Overlock 10 T	0.9	20
4180	C 1s near edge X-ray absorption fine structure (NEXAFS) of substituted benzoic acidsâ€”A theoretical and experimental study. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2007, 154, 109-118.	0.8	26
4181	Dehydrogenation of hydroxymatairesinol to oxomatairesinol over carbon nanofibre-supported palladium catalysts. <i>Journal of Molecular Catalysis A</i> , 2007, 274, 42-49.	4.8	31
4182	Furfuraldenevalinate system: Solution chemistry of denticity reduction, gas and solid phase complexing behavior. <i>Journal of Molecular Liquids</i> , 2007, 131-132, 196-199.	2.3	3
4183	Density functional and X-ray diffraction studies of bis(isocinchomeric acid) trihydrated. <i>Journal of Molecular Structure</i> , 2007, 837, 58-62.	1.8	11
4184	The vibrational spectra of the boron halides and their molecular complexes. Part 9. Ab initio studies of the complexes of boron trifluoride with methanol, methanethiol and some related bases. <i>Journal of Molecular Structure</i> , 2007, 834-836, 30-41.	1.8	14
4185	Investigation of torsional barriers and nonlinear optical (NLO) properties of phenyltriazines. <i>Journal of Molecular Structure</i> , 2007, 834-836, 516-520.	1.8	59
4186	Experimental and theoretical study of the compound [Pd(dmba)(NCO)(imz)]. <i>Journal of Molecular Structure</i> , 2007, 829, 195-201.	1.8	20
4187	Crystal structure of olanzapine and its solvates. Part 3. Two and three-component solvates with water, ethanol, butan-2-ol and dichloromethane. <i>Journal of Molecular Structure</i> , 2007, 830, 188-197.	1.8	38
4188	N(4)-Methyl-4-nitroacetophenone thiosemicarbazone and its nickel(II) complex: Experimental and theoretical structural studies. <i>Polyhedron</i> , 2007, 26, 1449-1458.	1.0	17

#	ARTICLE	IF	CITATIONS
4189	A computational study on mixed-ligand N2P3 donor-set iron(II) and ruthenium(II) classical and non-classical hydrides. <i>Polyhedron</i> , 2007, 26, 4936-4940.	1.0	4
4190	Electronic structure and conformations of ortho-, meta-, and para-aminobenzenesulfonic acid and its dimers. <i>Polymer</i> , 2007, 48, 5431-5439.	1.8	0
4191	Internal carbon monoxide exchange and CO dissociation in cobalt carbonyl carbene complexes. A density functional study. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 1825-1833.	0.8	14
4192	The molecular structure of using gas-phase electron diffraction and ab initio and DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 1161-1167.	0.8	12
4193	New Pd ^{II} -NHC-complexes for the Mizoroki-Heck reaction. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 1519-1529.	0.8	68
4194	1-D Polymeric divalent metal m-ferrocenylbenzoates: Structures, NLO and electrochemical properties. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 1584-1592.	0.8	21
4195	Mechanism of olefin hydrosilylation catalyzed by [RuCl(NCCH3)5] ⁺ : A DFT study. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 2282-2290.	0.8	30
4196	Substituent effect in para substituted Cr(CO)5-pyridine complexes. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 3866-3873.	0.8	53
4197	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 228-240.	2.0	422
4198	SAC-CI theoretical study on the excited states of lumiflavin: Structure, excitation spectrum, and solvation effect. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 189, 205-210.	2.0	58
4199	Electronic states and phosphorescence of dendron functionalized platinum(II) acetylides. <i>Journal of Luminescence</i> , 2007, 124, 302-310.	1.5	45
4200	Adsorption of organic probes on silica through Lewis interactions: A comparison of experimental results and quantum chemical calculations. <i>Journal of Colloid and Interface Science</i> , 2007, 310, 369-376.	5.0	17
4201	Theory of chemical bonds in metalloenzymes III: Full geometry optimization and vibration analysis of ferredoxin-type [2Fe-2S] cluster. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 116-133.	1.0	33
4202	Theory of chemical bonds in metalloenzymes IV: Hybrid-DFT study of Rieske-type [2Fe-2S] clusters. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 609-627.	1.0	32
4203	Cascade configuration of logical gates processing information encoded in molecular potentials. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 754-761.	1.0	14
4204	Influence of BH3 and alkaline cation released from the reduction agent on a tandem reduction/acylation reaction-A computational study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1814-1825.	1.0	1
4205	Can an excess electron localize on a purine moiety in the adenine-thymine Watson-Crick base pair? A computational study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2224-2232.	1.0	8
4206	A force field for simulating ethanol adsorption on Au(111) surfaces. A DFT study. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2169-2177.	1.0	20

#	ARTICLE	IF	CITATIONS
4207	Investigation of the nanoscale self-assembly of donor- π -acceptor molecules. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2233-2242.	1.0	7
4208	An improved 6-31G basis set for atoms Ga through Kr. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3028-3038.	1.0	4
4209	Theory of chemical bonds in metalloenzymes. IX. Theoretical study on the active site of the ribonucleotide reductase and the related species. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3250-3265.	1.0	13
4210	Hybrid density functional study of ligand coordination effects on the magnetic couplings and the dioxygen binding of the models of hemocyanin. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 3103-3119.	1.0	16
4211	Theory of chemical bonds in metalloenzymes. VII. Hybrid density functional theory studies on the electronic structures of P450. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 631-650.	1.0	20
4212	The effects of pyridine derivative additives on interface processes at nanocrystalline TiO ₂ thin film in dye-sensitized solar cells. <i>Surface and Interface Analysis</i> , 2007, 39, 809-816.	0.8	45
4213	Are aromatic carbon donor hydrogen bonds linear in proteins?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 489-497.	1.5	28
4214	A computational study into the reactivity of epichlorohydrin and epibromohydrin under basic conditions in the gas phase and solution. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 19-29.	0.9	7
4215	A computational study into the reactivity of epichlorohydrin and epibromohydrin under acidic conditions in the gas phase and aqueous solution. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1058-1071.	0.9	5
4216	Carbon and secondary deuterium kinetic isotope effects on S _N 2 methyl transfer reactions. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 1114-1120.	0.9	2
4217	Electronic and spatial structure of dimethyl orthophosphate and orthophosphate. <i>Biophysics (Russian Federation)</i> , 2007, 52, 355-364.	0.2	3
4218	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity. <i>Photochemistry and Photobiology</i> , 2005, 81, 924-933.	1.3	1
4219	Ab Initio Study of Non-Peptidic Antihypertensives. <i>Chemical Biology and Drug Design</i> , 2007, 69, 251-257.	1.5	3
4220	Gem-diamines as highly active organocatalysts for carbon-carbon bond formation. <i>Journal of Catalysis</i> , 2007, 246, 136-146.	3.1	59
4221	Bicyclic proline analogues as organocatalysts for stereoselective aldol reactions: an in silico DFT study. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 1287.	1.5	65
4222	A New Class of Supramolecular Wires. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18912-18916.	1.5	12
4223	A mathematical and computational review of Hartree-Fock SCF methods in quantum chemistry. <i>Molecular Physics</i> , 2007, 105, 3057-3098.	0.8	82
4224	An ab initio investigation of bismuth hydration. <i>Canadian Journal of Chemistry</i> , 2007, 85, 945-950.	0.6	19

#	ARTICLE	IF	CITATIONS
4225	Crystal and Molecular Structure of 4,6-Bis(nitroimino)-1,3,5-triazinan-2-one: A Theoretical and X-ray Studies. <i>Journal of Physical Chemistry A</i> , 2007, 111, 150-158.	1.1	15
4226	Local Modifications of Single-Wall Carbon Nanotubes Induced by Bond Formation with Encapsulated Fullerenes. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1099-1109.	1.2	32
4227	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in Hypericin. <i>Photochemistry and Photobiology</i> , 2007, 74, 157-163.	1.3	1
4228	Direct and Remarkably Efficient Conversion of Methane into Acetic Acid Catalyzed by Amavadin and Related Vanadium Complexes. A Synthetic and a Theoretical DFT Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 10531-10545.	6.6	151
4229	A Computational Study of O ⁺ -O Bond Formation Catalyzed by Mono- and Bis-MnIV ⁺ Corrole Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 7075-7086.	1.9	56
4231	New perspectives in multireference perturbation theory: the n-electron valence state approach. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 743-754.	0.5	238
4232	Germyl mesolytic dissociations in the allylgermane and penta-2,4-dienylgermane radical anions. A theoretical study. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 253-264.	0.5	0
4233	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 589-595.	0.5	9
4234	Cavity cooling of translational and ro-vibrational motion of molecules: ab initio-based simulations for OH and NO. <i>Applied Physics B: Lasers and Optics</i> , 2007, 89, 459-467.	1.1	10
4235	Preparation, crystal structure and characterization of 2,4,6-trinitro-3,5-dimethylbenzoic acid monohydrate. <i>Structural Chemistry</i> , 2007, 18, 75-80.	1.0	1
4236	Ab initio studies of push-pull systems. <i>Structural Chemistry</i> , 2007, 18, 399-407.	1.0	26
4237	Structure, bioactivity and theoretical study of 1-cyano-N-p-tolylcyclo-propanecarboxamide. <i>Structural Chemistry</i> , 2007, 18, 563-568.	1.0	9
4238	Local dipole interactions induce helicity of (S)-2-butyl-N-(1,8-naphthaloyl)-2-aminobenzoate molecules containing 1,8-naphthalimide rings utilized as a column building blocks: X-ray and quantum mechanical studies. <i>Structural Chemistry</i> , 2007, 18, 379-386.	1.0	6
4239	Aromaticity changes along the reaction coordinate connecting the cyclobutadiene dimer to cubane and the benzene dimer to hexaprismane. <i>Structural Chemistry</i> , 2007, 18, 773-783.	1.0	18
4240	An efficient methodology to study cyclodextrin clusters: application to Î±-CD hydrated monomer, dimer, trimer and tetramer. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2007, 59, 265-277.	1.6	16
4241	Relaxation of STO-3G and 6-31G* basis set functions in the series of LiF isoelectronic molecules of second row elements. <i>Journal of Structural Chemistry</i> , 2007, 48, 6-15.	0.3	3
4242	Adsorption of CO ₂ in metal organic frameworks of different metal centres: Grand Canonical Monte Carlo simulations compared to experiments. <i>Adsorption</i> , 2007, 13, 461-467.	1.4	123
4243	Halogen bonding: the f-hole. <i>Journal of Molecular Modeling</i> , 2007, 13, 291-296.	0.8	2,004

#	ARTICLE	IF	CITATIONS
4244	Ab initio and DFT investigation of electrophilic addition reaction of bromine to endo,endo-tetracyclo[4.2.1.13.6.02,7]dodeca-4,9-diene. <i>Journal of Molecular Modeling</i> , 2007, 13, 425-430.	0.8	6
4245	Quantum chemical study of the mechanism of ethylene elimination in silylative coupling of olefins. <i>Journal of Molecular Modeling</i> , 2007, 13, 477-483.	0.8	7
4246	A step on the path in the discovery of new latent fingerprint development reagents: substituted Ruhemann's purples and implications for the law. <i>Journal of Molecular Modeling</i> , 2007, 13, 943-948.	0.8	6
4247	Ab initio and DFT study of the inner mechanism and dynamic stereochemistry of electrophilic addition reaction of bromine to bisbenzotetracyclo[6.2.2.23,6.02,7]tetradeca-4,9,11,13-tetraene. <i>Journal of Molecular Modeling</i> , 2007, 13, 1215-1220.	0.8	6
4248	Phenylalkylamines as calcium channel blockers. <i>Journal of Chemical Sciences</i> , 2007, 119, 565-570.	0.7	3
4249	Thermochemistry of 2- and 4-biphenylmethanol. <i>Journal of Chemical Thermodynamics</i> , 2007, 39, 1384-1391.	1.0	6
4250	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. <i>Chemical Physics</i> , 2007, 333, 157-167.	0.9	154
4251	Vibrational dynamics and molecular structure of 1H- and 3H-1,2,3-triazolo[4,5-b]pyridine and its methyl-derivatives based on DFT chemical quantum calculations. <i>Chemical Physics</i> , 2007, 334, 90-108.	0.9	4
4252	Heteroleptic tris-cyclometalated iridium(III) complexes with phenylpyridine and diphenylquinoline derivative ligands. <i>Thin Solid Films</i> , 2007, 515, 5084-5089.	0.8	22
4253	Modelling water adsorption on Au(210) surfaces. I. A force field for water-Au interactions by DFT. <i>Journal of Electroanalytical Chemistry</i> , 2007, 609, 140-146.	1.9	20
4254	Synthesis, electrochemistry, geometric and electronic structure of oxo-molybdenum compounds involved in an oxygen atom transferring system. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 748-756.	1.5	24
4255	Cytotoxic studies of substituted titanocene and ansa-titanocene anticancer drugs. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 1558-1570.	1.5	59
4256	A study of the valence shell electronic structure of the 5-halouracils. <i>Chemical Physics</i> , 2008, 352, 205-216.	0.9	18
4257	Calculation of free-energy curves for the study of hydrolysis reactions in aqueous solution from ab initio potentials and molecular dynamics simulation. <i>Chemical Physics</i> , 2008, 353, 73-78.	0.9	14
4258	Structure of the doubly charged $\langle \text{mml:math altimg="si1.gif" overflow="scroll" \rangle$ xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/	0.7	3
4259	Experimental and theoretical studies on the asymmetric cyanosilylation of C2-symmetric hydrazones. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 998-1004.	1.8	11
4260	Synthesis and rhodium complexation of enantiomerically enriched bicyclo[3.3.1]nona-2,6-diene. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 1328-1332.	1.8	16
4261	An efficient one-pot synthesis of 3-glyoxylic acids of electron-deficient substituted azaindoles by ionic liquid imidazolium chloroaluminate-promoted Friedel-Crafts acylation. <i>Tetrahedron Letters</i> , 2008, 49, 6250-6253.	0.7	27

#	ARTICLE	IF	CITATIONS
4262	A computational study of the conformations of the boric acid (B(OH) ₃), its conjugate base ((HO) ₂ BO ⁻) and borate anion. Computational and Theoretical Chemistry, 2008, 853, 33-38.	1.5	13
4263	The molecular structure of disulfiram and its complexation with silica. A quantum chemical study. Computational and Theoretical Chemistry, 2008, 861, 57-61.	1.5	11
4264	The isomers of phenalene and their singlet and triplet states: A Hartree-Fock and density functional computational investigation. Computational and Theoretical Chemistry, 2008, 863, 50-54.	1.5	10
4265	Theoretical investigation of photoelectron spectra of furan, pyrrole, thiophene, and selenole. Chemistry of Heterocyclic Compounds, 2008, 44, 1101-1112.	0.6	20
4266	Proton transfer in C-halogen pyrazole cyclamers. A theoretical study. Structural Chemistry, 2008, 19, 191-198.	1.0	15
4267	Adsorption of dimethyl methylphosphonate and trimethyl phosphate on calcium oxide: an ab initio study. Structural Chemistry, 2008, 19, 307-320.	1.0	33
4268	Theoretical and experimental NMR studies of the Swern oxidation of methyl 6,7-dihydroxyvouacapan-17-oate. Structural Chemistry, 2008, 19, 625-631.	1.0	11
4269	X-ray Diffraction and DFT Studies of 2-Methoxy-5-phenylaniline. Journal of Chemical Crystallography, 2008, 38, 295-299.	0.5	4
4270	Propeller-like Conformation of Diphenylacetic Acid. Journal of Chemical Crystallography, 2008, 38, 403-406.	0.5	7
4271	Pyrene-1-Carboxylate in Water and Glycerol Solutions: Origin of the Change of pK Upon Excitation. Journal of Fluorescence, 2008, 18, 41-49.	1.3	15
4272	X-ray emission and absorption spectra of Cr(CO) ₆ : A comparison of quantum-chemical and full multiple scattering calculations with experiment. Journal of Structural Chemistry, 2008, 49, 1-18.	0.3	3
4273	Direct determination of absolute configuration: a vibrational circular dichroism study on dimethyl-substituted phenyloxiranes synthesized by Shi epoxidation. Theoretical Chemistry Accounts, 2008, 119, 133-142.	0.5	8
4274	Cluster study of surface radicals of Si(111)-7 × 7 reconstructed surface. Theoretical Chemistry Accounts, 2008, 120, 79-83.	0.5	8
4275	A microsolvation approach to the prediction of the relative enthalpies and free energies of hydration for ammonium ions. Theoretical Chemistry Accounts, 2008, 120, 5-22.	0.5	6
4276	trans-1,2-Dicyano-cyclopropane and other cyano-cyclopropane derivatives. Theoretical Chemistry Accounts, 2008, 119, 211-229.	0.5	8
4277	Regioselectivity preference of testosterone hydroxylation by cytochrome P450 3A4. Theoretical Chemistry Accounts, 2008, 121, 313-319.	0.5	12
4278	Investigation into mercury bound to biothiols: structural identification using ESI-ion-trap MS and introduction of a method for their HPLC separation with simultaneous detection by ICP-MS and ESI-MS. Analytical and Bioanalytical Chemistry, 2008, 390, 1753-1764.	1.9	99
4279	A computational approach to the synthesis of 1,3,5-thiadiazinane-2-thiones in aqueous medium: theoretical evidence for water-promoted heterocyclization. Journal of Molecular Modeling, 2008, 14, 641-647.	0.8	9

#	ARTICLE	IF	CITATIONS
4280	A density functional theory study of phenyl formation initiated by ethynyl radical (C ₂ H ₃) and ethyne (C ₂ H ₂). <i>Journal of Molecular Modeling</i> , 2008, 14, 1203-1208.	0.8	10
4281	New Insight into Carbon-Nanotube Electronic Structure Selectivity. <i>Small</i> , 2008, 4, 2035-2042.	5.2	21
4282	Estimation of Water Solubility of Polycyclic Aromatic Hydrocarbons Using Quantum Chemical Descriptors and Partial Least Squares. <i>QSAR and Combinatorial Science</i> , 2008, 27, 618-626.	1.5	32
4283	Computational study of the fluorination effect on nitrogen-boron bond. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 84-89.	1.0	3
4284	Modeling intercalation through the sandwich-type interactions between benzene and 14 polyaromatic molecules: DFT and <i>ab initio</i> results. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 112-118.	1.0	5
4285	Improving the TDDFT calculation of low-lying excited states for polycyclic aromatic hydrocarbons using the Tamm-Dancoff approximation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 430-439.	1.0	62
4286	Theoretical electronic structure of the molecule ScBr. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 456-461.	1.0	11
4287	Analytical optimization of exponent values in protonic and deuteronic Gaussian-type functions by elimination of translational and rotational motions from multi-component molecular orbital scheme. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 472-481.	1.0	5
4288	<i>Ab initio</i> study of the photochemistry of aminopyrimidine. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1266-1276.	1.0	12
4289	Solvent effect on the reactivity of <i>cis</i> -platinum (II) complexes: A density functional approach. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1400-1409.	1.0	36
4290	Insertion and carbonylation reactions of styrene promoted by [HRh(CO) _x](PMe ₃) _{3-x} (<i>x</i> = 1, 2) compounds: A theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2358-2373.	1.0	4
4291	Structure and properties of disiloxane: An <i>ab initio</i> and post-Hartree-Fock study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2088-2096.	1.0	13
4292	Biorthogonal method of moments of coupled-cluster equations: Alternative derivation, further considerations, and application to a model magnetic system. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2128-2149.	1.0	14
4293	Spin-spin coupling across intramolecular N-H...N hydrogen bonds in models for proton sponges: an <i>ab initio</i> investigation. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 457-463.	1.1	18
4294	<i>Z</i> , <i>E</i> isomerization mechanism for <i>N</i> -arythio-1,4-benzoquinonimines: DNMR and DFT investigations. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 811-817.	1.1	9
4295	Density-functional computation of ⁹⁹ Tc NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, S36-S44.	1.1	22
4296	NMR spectroscopic investigation of <i>o</i> -nitrosobenzoic acid. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 1163-1167.	1.1	4
4297	Resolving an apparent discrepancy between theory and experiment: spin-spin coupling constants for FCCF. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 1003-1006.	1.1	27

#	ARTICLE	IF	CITATIONS
4298	Detection of platinum dihydride bisphosphine complexes and studies of their reactivity through para-hydrogen-enhanced NMR methods. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, S107-S114.	1.1	8
4299	Vibrational spectra, X-ray and molecular structure of 1H- and 3H-imidazo[4,5-b]pyridine and their methyl derivatives: DFT quantum chemical calculations. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 1-15.	1.2	14
4300	Crystal and molecular structure of 2-aminopyridinium-4-hydroxybenzenesulfonate"IR and Raman spectra, DFT calculations and physicochemical properties. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 569-581.	1.2	14
4301	Molecular structure and vibrational spectra of 3 (or 4 or 6)-methyl-5-nitro-2-pyridinethiones: FT-IR, FT-Raman and DFT quantum chemical calculations. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 832-841.	1.2	10
4302	Crystal and molecular structure of 2-amino-5-chloropyridinium hydrogen selenate"its IR and Raman spectra, DFT calculations and physicochemical properties. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 863-872.	1.2	22
4303	The Rate-Determining Step in the Rhodium-Xantphos-Catalysed Hydroformylation of 1-Octene. <i>Chemistry - A European Journal</i> , 2008, 14, 1843-1853.	1.7	75
4304	Intramolecular Alkyl Phosphine Dehydrogenation in Cationic Rhodium Complexes of Tris(cyclopentylphosphine). <i>Chemistry - A European Journal</i> , 2008, 14, 1004-1022.	1.7	42
4305	Amavadin and Other Vanadium Complexes as Remarkably Efficient Catalysts for One-Pot Conversion of Ethane to Propionic and Acetic Acids. <i>Chemistry - A European Journal</i> , 2008, 14, 1828-1842.	1.7	67
4306	New Insights into the Polymerization of Methyl Methacrylate Initiated by Rare-Earth Borohydride Complexes: A Combined Experimental and Computational Approach. <i>Chemistry - A European Journal</i> , 2008, 14, 1881-1890.	1.7	31
4307	Luminescent Alkynylplatinum(II) Complexes of 2,6-Bis(alkylbenzimidazol-2-yl)pyridine-Type Ligands with Ready Tunability of the Nature of the Emissive States by Solvent and Electronic Property Modulation. <i>Chemistry - A European Journal</i> , 2008, 14, 4562-4576.	1.7	119
4308	On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retro-Prato) Tj ETQqO 0 0 rgBT /Overlock 10 Tf 50 342	1.7	56
4309	A Structural and Computational Study of Synthetically Important Alkali-Metal/Tetramethylpiperidide (TMP) Amine Solvates. <i>Chemistry - A European Journal</i> , 2008, 14, 8025-8034.	1.7	47
4310	PGSE NMR Diffusion Overhauser Studies on [Ru(Cp*)(η^6 -arene)][PF ₆] ₂ , Plus a Variety of Transition-Metal, Inorganic, and Organic Salts: An Overview of Ion Pairing in Dichloromethane. <i>Chemistry - A European Journal</i> , 2008, 14, 5617-5629.	1.7	25
4311	Reductive Degradation of nido-1-CB8H ₁₂ into Smaller-Cage Carborane Systems via New Monocarbaboranes [arachno-5-CB8H ₁₃] and closo-2-CB6H8. <i>Chemistry - A European Journal</i> , 2008, 14, 6529-6533.	1.7	12
4312	Highly Convenient Amine-Free Sonogashira Coupling in Air in a Polar Mixed Aqueous Medium by trans- and cis-(NHC) ₂ PdX ₂ (X=Cl, Br) Complexes of N/O-Functionalized N-Heterocyclic Carbenes. <i>Chemistry - A European Journal</i> , 2008, 14, 6646-6655.	1.7	122
4313	A DFT Study of the Mechanism of Polymerization of ϵ -Caprolactone Initiated by Organolanthanide Borohydride Complexes. <i>Chemistry - A European Journal</i> , 2008, 14, 5507-5518.	1.7	70
4314	Do the Local Softness and Hardness Indicate the Softest and Hardest Regions of a Molecule?. <i>Chemistry - A European Journal</i> , 2008, 14, 8652-8660.	1.7	85
4315	Construction of Titanasiloxanes by Incorporation of Silanols to the Metal Oxide Model [Ti(η^5 -C ₅ Me ₅)(η^4 -O) ₃ CR]: DFT Elucidation of the Reaction Mechanism. <i>Chemistry - A European Journal</i> , 2008, 14, 7930-7938.	1.7	20

#	ARTICLE	IF	CITATIONS
4316	Bonding and Bending in Zirconium(IV) and Hafnium(IV) Hydrazides. <i>Chemistry - A European Journal</i> , 2008, 14, 8131-8146.	1.7	38
4317	Reaction Mechanism of Molybdoenzyme Formate Dehydrogenase. <i>Chemistry - A European Journal</i> , 2008, 14, 8674-8681.	1.7	47
4318	Effect of the Nature of the Metal Atom on Hydrogen Bonding and Proton Transfer to [Cp* <i>M</i> H ₃ (dppe)]: Tungsten versus Molybdenum. <i>Chemistry - A European Journal</i> , 2008, 14, 9921-9934.	1.7	28
4319	Comparative Study on the Structural, Optical, and Electrochemical Properties of Bithiophene-Fused Benzo[<i>c</i>]phospholes. <i>Chemistry - A European Journal</i> , 2008, 14, 8102-8115.	1.7	75
4320	Mechanism of the Palladium-Catalyzed Carbohydroxylation of Allene-Substituted Conjugated Dienes: Rationalization of the Recently Observed Nucleophilic Attack by Water on a (i-allyl)palladium Intermediate. <i>Chemistry - A European Journal</i> , 2008, 14, 9175-9180.	1.7	31
4321	Living Radical Polymerization of Acrylates Mediated by 1,3-Bis(2-pyridylimino)isoindolatocobalt(II) Complexes: Monitoring the Chain Growth at the Metal. <i>Chemistry - A European Journal</i> , 2008, 14, 10267-10279.	1.7	70
4322	Reaching Optimal Light-Induced Intramolecular Spin Alignment within Photomagnetic Molecular Device Prototypes. <i>Chemistry - A European Journal</i> , 2008, 14, 11385-11405.	1.7	28
4323	Ab Initio Study of the Magneto-Optical Rotation of Diastereoisomers. <i>ChemPhysChem</i> , 2008, 9, 462-469.	1.0	1
4324	Exploring the Optical Activity Tensor by Anisotropic Rayleigh Optical Activity Scattering. <i>ChemPhysChem</i> , 2008, 9, 265-271.	1.0	13
4325	Thin-Film Properties of DNA and RNA Bases: A Combined Experimental and Theoretical Study. <i>ChemPhysChem</i> , 2008, 9, 740-747.	1.0	27
4326	Electronic and Vibrational Spectroscopy of 1-Methylthymine and its Water Clusters: The Dark State Survives Hydration. <i>ChemPhysChem</i> , 2008, 9, 1570-1577.	1.0	35
4327	Two-electron integral evaluation on the graphics processor unit. <i>Journal of Computational Chemistry</i> , 2008, 29, 334-342.	1.5	144
4328	A DFT study of solvation effects on the tautomeric equilibrium and catalytic ylide generation of thiamin models. <i>Journal of Computational Chemistry</i> , 2008, 29, 1037-1047.	1.5	14
4329	Linear-scaling Cholesky decomposition. <i>Journal of Computational Chemistry</i> , 2008, 29, 1004-1010.	1.5	34
4330	The hardness kernel as the basis for global and local reactivity indices. <i>Journal of Computational Chemistry</i> , 2008, 29, 1064-1072.	1.5	34
4331	A dual-level state-specific time-dependent density-functional theory. <i>Journal of Computational Chemistry</i> , 2008, 29, 1187-1197.	1.5	12
4332	Efficient model chemistries for peptides. I. General framework and a study of the heterolevel approximation in RHF and MP2 with Pople split-valence basis sets. <i>Journal of Computational Chemistry</i> , 2008, 29, 1408-1422.	1.5	16
4333	Gaussian basis set of double zeta quality for atoms K through Kr: Application in DFT calculations of molecular properties. <i>Journal of Computational Chemistry</i> , 2008, 29, 2434-2444.	1.5	80

#	ARTICLE	IF	CITATIONS
4334	The Cyclooligomerisation of Acetylene at Metal Centres. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 2874-2883.	1.0	19
4335	Ruthenium Dihydrogen Complex for C-H Activation: Catalytic H/D Exchange under Mild Conditions. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 3493-3500.	1.0	39
4336	Synthesis, X-ray Crystallography, Spectroelectrochemistry and Computational Studies on Potential Copper-Based Radiopharmaceuticals. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 3549-3560.	1.0	18
4337	Inter- and Intramolecular C-H...O Bonding in the Anions of 1,3-Indandione Derivatives. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 673-683.	1.2	11
4338	DFT/MM Study on Copper-Catalyzed Cyclopropanation - Enantioselectivity with No Enthalpy Barrier. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 5614-5621.	1.2	18
4339	[2+1]-Cycloaddition of Nitrene onto C ₆₀ Revisited: Interconversion between an Aziridinofullerene and an Azafulleroid. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 1298-1300.	7.2	54
4340	Dipositively Charged Protonated a ₃ and a ₂ Ions: Generation by Fragmentation of [La(GGG)(CH ₃ CN) ₂] ³⁺ . <i>Angewandte Chemie - International Edition</i> , 2008, 47, 8288-8291.	7.2	12
4341	Observation of ¹³ C-NMR Chemical Shifts of Metal Carbides Encapsulated in Fullerenes: Sc ₂ C ₂ @C ₈₂ , Sc ₂ C ₂ @C ₈₄ , and Sc ₃ C ₂ @C ₈₀ . <i>Angewandte Chemie - International Edition</i> , 2008, 47, 7905-7908.	7.2	71
4345	Chemically stable silver nanoparticle-crosslinked polymer microspheres. <i>Journal of Colloid and Interface Science</i> , 2008, 319, 572-576.	5.0	44
4346	Synthesis, spectroscopic and structural studies of 2,2,2-trifluoroethyl phosphorodiamidate complexes with tin(IV) chloride. <i>Polyhedron</i> , 2008, 27, 1754-1760.	1.0	11
4347	Studies of degradation enhancement of polystyrene by flame retardant additives. <i>Polymer Degradation and Stability</i> , 2008, 93, 1664-1673.	2.7	70
4348	Quantum chemical study of the intermediate complex required for iron-mediated reactivity and antimalarial activity of dispiro-1,2,4-trioxolanes. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 27, 394-400.	1.3	11
4349	Regioselective control of the nickel-mediated coupling of acetylene and carbon dioxide - A DFT study. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 2703-2710.	0.8	43
4350	Mapping Potential Energy Surfaces by Neural Networks: The ethanol/Au(111) interface. <i>Journal of Electroanalytical Chemistry</i> , 2008, 624, 109-120.	1.9	20
4351	Spectroelectrochemical study of the adsorption of acetate anions at gold single crystal and thin-film electrodes. <i>Electrochimica Acta</i> , 2008, 53, 2309-2321.	2.6	53
4352	How the site of ionisation influences side-chain fragmentation in histidine radical cation. <i>Chemical Physics Letters</i> , 2008, 451, 276-281.	1.2	14
4353	Coupled cluster study of the phenyl-acetylide anion. <i>Chemical Physics Letters</i> , 2008, 454, 404-408.	1.2	4
4354	Adsorption states of dinitrogen on small tungsten nanoclusters. <i>Chemical Physics Letters</i> , 2008, 455, 261-264.	1.2	3

#	ARTICLE	IF	CITATIONS
4355	Initial adsorption mechanisms of TiCl ₄ on OH/Si(100)-2 \bar{A} -1. <i>Chemical Physics Letters</i> , 2008, 457, 69-73.	1.2	16
4356	Large-scale parallel calculations with combined coupled cluster and molecular mechanics formalism: Excitation energies of zinc \bar{A} porphyrin in aqueous solution. <i>Chemical Physics Letters</i> , 2008, 458, 205-209.	1.2	46
4357	Mechanistic theoretical insight of Ru(II) catalysts with a meridional \bar{A} facial bpea fashion competition. <i>Chemical Physics Letters</i> , 2008, 458, 200-204.	1.2	10
4358	Reactivity of nitrobenzofurazan towards nucleophiles: Insights from DFT. <i>Chemical Physics Letters</i> , 2008, 461, 16-20.	1.2	15
4359	Adsorption of TiCl ₄ on H/Si(1 0 0)-2 \bar{A} - 1 Surface. <i>Chemical Physics Letters</i> , 2008, 461, 249-253.	1.2	14
4360	Theoretical analysis of the solid-state terahertz spectrum of the high explosive RDX. <i>Chemical Physics Letters</i> , 2008, 463, 84-89.	1.2	60
4361	The solid-state terahertz spectrum of MDMA (Ecstasy) \bar{A} A unique test for molecular modeling assignments. <i>Chemical Physics Letters</i> , 2008, 463, 353-356.	1.2	30
4362	Projector Monte Carlo method based on configuration state functions. Test applications to the H ₄ system and dissociation of LiH. <i>Chemical Physics Letters</i> , 2008, 463, 431-434.	1.2	44
4363	The electronic structure of N,N \bar{A} 2-bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexane-diamino cobalt(II). <i>Chemical Physics Letters</i> , 2008, 464, 31-37.	1.2	13
4364	Synthesis, dopaminergic profile, and molecular dynamics calculations of N-aralkyl substituted 2-aminoindans. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3233-3244.	1.4	10
4365	A theoretical and experimental study of the near edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectra (XPS) of nucleobases: Thymine and adenine. <i>Chemical Physics</i> , 2008, 347, 360-375.	0.9	142
4366	Towards the elaboration of a QM method to describe molecular solutes under the effect of a very high pressure. <i>Chemical Physics</i> , 2008, 344, 135-141.	0.9	59
4367	The effect of protonation on the photodissociation processes in formamide \bar{A} An ab initio surface hopping dynamics study. <i>Chemical Physics</i> , 2008, 349, 308-318.	0.9	20
4368	A study of the valence shell electronic structure of uracil and the methyluracils. <i>Chemical Physics</i> , 2008, 353, 47-58.	0.9	16
4369	¹⁹ F \bar{A} ¹⁹ F and ¹⁹ F \bar{A} ¹ H spin \bar{A} spin coupling constants in cyclic FH polymers (FH) _n , n=2 \bar{A} 6. <i>Solid State Nuclear Magnetic Resonance</i> , 2008, 34, 86-92.	1.5	14
4370	⁵¹ V solid-state NMR investigations and DFT studies of model compounds for vanadium haloperoxidases. <i>Solid State Nuclear Magnetic Resonance</i> , 2008, 34, 52-67.	1.5	29
4371	Synthesis and structure of a heterocyclic ansa pyrrole amino acid. <i>Tetrahedron</i> , 2008, 64, 3005-3016.	1.0	13
4372	Theory-guided design of Br \bar{A} nsted acid-assisted phosphine catalysis: synthesis of dihydropyrones from aldehydes and allenates. <i>Tetrahedron</i> , 2008, 64, 6935-6942.	1.0	50

#	ARTICLE	IF	CITATIONS
4373	Theoretical studies of stereoselectivities in the direct syn- and anti-Mannich reactions catalyzed by different amino acids. <i>Tetrahedron: Asymmetry</i> , 2008, 19, 2285-2292.	1.8	15
4374	Some physical organic aspects of salicylaldehydes oximes, a theoretical study. <i>Tetrahedron Letters</i> , 2008, 49, 631-635.	0.7	16
4375	A unique and novel cyclopropylmethyl cation intermediate: a DFT study. <i>Tetrahedron Letters</i> , 2008, 49, 5894-5898.	0.7	9
4376	The prediction of gas-phase and aqueous basicities for alkyl amines. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 84-97.	1.5	9
4377	A conceptual DFT study of hydrazino peptides: Assessment of the nucleophilicity of the nitrogen atoms by means of the dual descriptor $\rho^{\text{eff}}(r)$. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 46-51.	1.5	54
4378	Ab initio study of luminescent substituted 8-hydroxyquinoline metal complexes with application in organic light emitting diodes. <i>Computational and Theoretical Chemistry</i> , 2008, 850, 127-134.	1.5	24
4379	Theoretical study of the properties of fluoroborathiin and fluoroboroxine. <i>Computational and Theoretical Chemistry</i> , 2008, 853, 77-81.	1.5	17
4380	Hydrogen atom transfer in the reaction of hydroxycinnamic acids with OH and HO ₂ radicals: DFT study. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 53-59.	1.5	19
4381	Assessment of density functionals for the investigation of iridium(III) complexes. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 97-102.	1.5	19
4382	Computational study on optical and electronic properties of the α -CH ₂ N substituted emitting materials based on spiroilabifluorene derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 85-91.	1.5	25
4383	The α -hydrazinoturn α -hydrogen bonding network in hydrazinopeptides and aza- β 3-peptides as probed by an AIM topological analysis of the electronic density. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 41-46.	1.5	8
4384	Using symmetry in the framework of the incremental scheme: Molecular applications. <i>Chemical Physics</i> , 2008, 346, 266-274.	0.9	28
4385	Ground and excited state intramolecular proton transfer controlled intramolecular charge separation and recombination: A new type of charge and proton transfer reaction. <i>Chemical Physics</i> , 2008, 348, 181-186.	0.9	21
4386	Synthesis and photophysical study of iridium(III) complex with 6-pentafluorophenyl-2,4-diphenylquinolines. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008, 313-314, 435-438.	2.3	2
4387	New heteroleptic Tris-cyclometalated iridium complex for red electrophosphorescent light-emitting diodes. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008, 313-314, 426-430.	2.3	1
4388	Electronic structure and reactivity analysis for a set of Zn-chelates with substituted 8-hydroxyquinoline ligands and their application in OLED. <i>Organic Electronics</i> , 2008, 9, 625-634.	1.4	24
4389	Solution structure of molybdic acid from Raman spectroscopy and DFT analysis. <i>Inorganica Chimica Acta</i> , 2008, 361, 1000-1007.	1.2	75
4390	On the oxidation of alkyl and aryl sulfides by [(Me ₃ TACN)MnVO(OH) ₂] ⁺ : A density functional study. <i>Inorganica Chimica Acta</i> , 2008, 361, 1079-1086.	1.2	11

#	ARTICLE	IF	CITATIONS
4391	Structure of Co ₂ (CO) ₆ (dppm) and Co ₂ (CO) ₅ (CHCO ₂ Et)(dppm) (dppm=Ph ₂ PCH ₂ PPh ₂) and exchange reaction with ¹³ CO: An experimental and computational study. <i>Inorganica Chimica Acta</i> , 2008, 361, 1832-1842.	1.2	6
4392	Experimental and computational studies of two new mono- and dinuclear iridium complexes containing a Buchwald biphenyl phosphine ligand. <i>Inorganica Chimica Acta</i> , 2008, 361, 2623-2630.	1.2	5
4393	Selective decarbonylation by a pincer PCP-rhodium(I) complex. <i>Inorganica Chimica Acta</i> , 2008, 361, 3327-3331.	1.2	23
4394	Proton affinity of S-containing aromatic compounds: Implications for crude oil hydrodesulfurization. <i>Journal of Molecular Catalysis A</i> , 2008, 281, 79-84.	4.8	32
4395	An intermediate structure trapped in solid-state tautomerization process of (E)-4-[(4-chlorophenylimino)methyl]benzene-1,2,3-triol. <i>Journal of Molecular Structure</i> , 2008, 873, 130-136.	1.8	44
4396	Molecular geometry of antimalarial amodiaquine in different crystalline environments. <i>Journal of Molecular Structure</i> , 2008, 875, 32-41.	1.8	12
4397	Phosphine oxide adducts of tin(IV) chloride: Experimental NMR and DFT computational study. <i>Journal of Molecular Structure</i> , 2008, 892, 103-109.	1.8	13
4398	Quantum mechanical ab initio simulation of the electron screening effect in metal deuteride crystals. <i>European Physical Journal A</i> , 2008, 35, 243-252.	1.0	5
4399	Access to Enantioenriched $\hat{1}\pm$ -Amino Esters via Rhodium-Catalyzed 1,4-Addition/Enantioselective Protonation. <i>Journal of the American Chemical Society</i> , 2008, 130, 6159-6169.	6.6	124
4400	Hydrogen activation by high-valent oxo-molybdenum(vi) and -rhenium(vii) and -(v) compounds. <i>Dalton Transactions</i> , 2008, , 1727.	1.6	80
4401	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1449-1459.	2.3	421
4402	Ionic Hydrogenation of Ketones with Molybdenum Pentabenzylcyclopentadienyl Hydride Catalysts. <i>Organometallics</i> , 2008, 27, 4589-4599.	1.1	33
4403	The Reaction Mechanism for the Organocatalytic Ring-Opening Polymerization of $\langle \text{sc} \rangle \langle \text{sc} \rangle$ -Lactide Using a Guanidine-Based Catalyst: Hydrogen-Bonded or Covalently Bound?. <i>Journal of the American Chemical Society</i> , 2008, 130, 6749-6754.	6.6	230
4404	Low-Temperature FTIR Spectroscopic and Theoretical Study on an Energetic Nitroimine: $\hat{a}\epsilon\%$ Dinitroammeline (DNAM). <i>Journal of Physical Chemistry A</i> , 2008, 112, 3432-3443.	1.1	9
4405	Estimation of n-octanol/water partition coefficients of polycyclic aromatic hydrocarbons by quantum chemical descriptors. <i>Open Chemistry</i> , 2008, 6, 310-318.	1.0	9
4406	Study of the electronic structure of M(CO) ₅ Cl complexes (M = Mn, Re) using X-ray spectroscopy and density-functional theory. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2008, 72, 476-482.	0.1	1
4407	An <i>Ab Initio</i> Study of At ₂ Antagonists. <i>Chemical Biology and Drug Design</i> , 2008, 71, 271-277.	1.5	1
4408	Effect of Dimerization on Vibrational Spectra of Eumelanin Precursors ^{$\hat{a}\epsilon\%$} . <i>Photochemistry and Photobiology</i> , 2008, 84, 613-619.	1.3	15

#	ARTICLE	IF	CITATIONS
4409	Absorption Spectrum of OH Radical in Water. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13372-13381.	1.1	38
4410	Synthesis and Characterization of a Non-IPR Fullerene Derivative: Sc ₃ N@C ₆₈ [C(COOC ₂ H ₅) ₂]. <i>Journal of Physical Chemistry C</i> , 2008, 112, 19203-19208.	1.5	41
4411	Comparison of Nitroaldol Reaction Mechanisms Using Accurate Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10635-10649.	1.1	9
4412	Computational Analysis of Amine-Borane Adducts as Potential Hydrogen Storage Materials with Reversible Hydrogen Uptake. <i>Inorganic Chemistry</i> , 2008, 47, 5910-5918.	1.9	91
4413	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6794-6810.	1.5	55
4414	A generalization of the state-specific complete-active-space coupled-cluster method for calculating electronic excited states. <i>Journal of Chemical Physics</i> , 2008, 128, 074101.	1.2	46
4415	Rearrangement of a Cyclohexyl Radical to a Cyclopentylmethyl Radical on the Avermectin Skeleton. <i>Organic Letters</i> , 2008, 10, 2255-2258.	2.4	16
4416	Dinitrogen and Acetylide Complexes of Low-Valent Chromium. <i>Inorganic Chemistry</i> , 2008, 47, 4639-4647.	1.9	36
4417	Density Functional Study of Protonated Formylmetallocenes. <i>Organometallics</i> , 2008, 27, 394-401.	1.1	6
4418	Highly Regioselective Derivatization of Trimetallic Nitride Templated Endohedral Metallofullerenes via a Facile Photochemical Reaction. <i>Journal of the American Chemical Society</i> , 2008, 130, 17755-17760.	6.6	72
4419	Ab Initio EOM-CCSD Spin-Spin Coupling Constants for Hydrogen-Bonded Formamide Complexes: Bridging Complexes with NH ₃ , (NH ₃) ₂ , H ₂ O, (H ₂ O) ₂ , FH, and (FH) ₂ . <i>Journal of Physical Chemistry A</i> , 2008, 112, 6338-6343.	1.1	18
4420	Experimental and Theoretical Examination of C≡CN Bond Activation of Benzonitrile Using Zerovalent Nickel. <i>Organometallics</i> , 2008, 27, 3811-3817.	1.1	97
4421	Three-Dimensional Through-Space/Through-Bond Delocalization in Cyclophane Systems: A Molecule-in-Molecule Approach. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2948-2954.	1.1	10
4422	A New Cyclization to Fused Pyrazoles Tunable for Pericyclic or Pseudopericyclic Route: An Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 3900-3906.	1.7	13
4423	Theoretical Investigations on the Stereoselectivity of the Proline Catalyzed Mannich Reaction in DMSO. <i>Journal of Organic Chemistry</i> , 2008, 73, 9388-9392.	1.7	38
4424	Ultrafast transformation of graphite to diamond: An <i>ab initio</i> study of graphite under shock compression. <i>Journal of Chemical Physics</i> , 2008, 128, 184701.	1.2	84
4425	Extrapolation to the complete-basis-set limit and the implications of avoided crossings: The X ¹ Σ ⁺ g ⁺ , B ¹ Σ ⁺ g ⁺ , and B ² Σ ⁺ g ⁺ states of C ₂ . <i>Journal of Chemical Physics</i> , 2008, 129, 234103.	1.2	60
4426	DFT Calculations of ⁵¹ V Solid-State NMR Parameters of Vanadium(V) Model Complexes. <i>Zeitschrift Fur Physikalische Chemie</i> , 2008, 222, 1389-1406.	1.4	18

#	ARTICLE	IF	CITATIONS
4427	Assessment of Density Functionals for Intramolecular Dispersion-Rich Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1610-1619.	2.3	65
4428	Theoretical study on the mechanism of a ring-opening reaction of oxirane by the active-site aspartic dyad of HIV-1 protease. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 359-365.	1.5	9
4429	Accelerating Density Functional Calculations with Graphics Processing Unit. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1230-1236.	2.3	136
4430	Quantum Chemical Approach to the Mechanism for the Biological Conversion of Tyrosine to Dopamine. <i>Journal of the American Chemical Society</i> , 2008, 130, 16890-16897.	6.6	70
4431	Reaction mechanism of the direct gas phase synthesis of H ₂ O ₂ catalyzed by Au ₃ . <i>Journal of Chemical Physics</i> , 2008, 129, 124705.	1.2	9
4432	A Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin-Spin Coupling Constants for Selected Singly Bonded Molecules, and the Hydrides NH ₃ , H ₂ O, and HF and Their Protonated and Deprotonated Ions and Hydrogen-Bonded Complexes. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 967-973.	2.3	48
4433	From Large 12-Membered Macrometallacycles to Ionic (NHC) ₂ M+Cl ⁻ Type Complexes of Gold and Silver by Modulation of the N-Substituent of Amido-Functionalized N-Heterocyclic Carbene (NHC) Ligands. <i>Inorganic Chemistry</i> , 2008, 47, 4153-4165.	1.9	71
4434	Supramolecular Self-Assembly of Cyclodextrin and Higher Water Soluble Guest: Thermodynamics and Topological Studies. <i>Journal of the American Chemical Society</i> , 2008, 130, 8426-8436.	6.6	79
4435	Reactivity of (TiO ₂) _n Clusters (n = 1-10): Probing Gas-Phase Acidity and Basicity Properties. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16087-16095.	1.5	66
4436	Investigations of Coupling Characters in Ionic Liquids Formed between the 1-Ethyl-3-methylimidazolium Cation and the Glycine Anion. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5088-5097.	1.2	37
4437	Addition of POSS-T ₈ to the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 754-761.	1.5	6
4438	Mechanism for the Substitution of an Aqua Ligand of UO ₂ (OH) ₂ ·5H ₂ O by Chloride. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1654-1658.	2.3	8
4439	Correlation of Hydrogen-Atom Abstraction Reaction Efficiencies for Aryl Radicals with their Vertical Electron Affinities and the Vertical Ionization Energies of the Hydrogen-Atom Donors. <i>Journal of the American Chemical Society</i> , 2008, 130, 17697-17709.	6.6	46
4440	Electronic flexoelectricity in low-dimensional systems. <i>Physical Review B</i> , 2008, 77, .	1.1	157
4441	On the Electronically Excited States of Uracil. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9983-9992.	1.1	115
4442	Accurate Gas-Phase Experimental Structures of Octasilsesquioxanes (Si ₈ O ₁₂ X ₈ ; X = H, Me). <i>Organometallics</i> , 2008, 27, 4183-4187.	1.1	56
4443	A DFT Study on the Mechanism of Palladium-Catalyzed Alkyne Hydrogenation: Neutral versus Cationic Pathways. <i>Organometallics</i> , 2008, 27, 43-52.	1.1	23
4444	Theoretical Study of Ni Adsorption on Single-Walled Boron Nitride Nanotubes with Intrinsic Defects. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5778-5783.	1.5	44

#	ARTICLE	IF	CITATIONS
4445	Quadratic response functions in the relativistic four-component Kohn-Sham approximation. <i>Journal of Chemical Physics</i> , 2008, 128, 024105.	1.2	71
4446	Low-Energy Structures of Ligand Passivated Si Nanoclusters: Theoretical Investigation of Si_{2L4} and Si_{10L16} ($L = \text{H}, \text{CH}_3, \text{OH}, \text{and F}$). <i>Journal of Physical Chemistry C</i> , 2008, 112, 1819-1824.	1.5	2
4447	Substitution behaviour of amine-bridged dinuclear Pt(II) complexes with bio-relevant nucleophiles. <i>Dalton Transactions</i> , 2008, , 2759.	1.6	34
4448	Computational Electrochemistry of Ruthenium Anticancer Agents. Unprecedented Benchmarking of Implicit Solvation Methods. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 499-506.	2.3	31
4449	Mechanism of Spectral Tuning Going from Retinal in Vacuo to Bovine Rhodopsin and its Mutants: Multireference ab Initio Quantum Mechanics/Molecular Mechanics Studies. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16883-16890.	1.2	85
4450	Extremely narrow SiON angles in siloxy-substituted nitrogen-containing rings: a computational investigation. <i>Dalton Transactions</i> , 2008, , 5999.	1.6	3
4451	Competing $\text{C}=\text{F}$ Activation Pathways in the Reaction of Pt(0) with Fluoropyridines: Phosphine-Assistance versus Oxidative Addition. <i>Journal of the American Chemical Society</i> , 2008, 130, 15499-15511.	6.6	101
4452	Calculation of pK_a Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16860-16873.	1.2	179
4453	Origin of Enantioselection in Hetero-Diels-Alder Reactions Catalyzed by Naphthyl-TADDOL. <i>Organic Letters</i> , 2008, 10, 2749-2752.	2.4	78
4454	Ruthenium Carbene and Allenylidene Complexes Supported by the Tertiary Amine-Aromatic Diimine Ligand Set: Structural, Spectroscopic, and Theoretical Studies. <i>Organometallics</i> , 2008, 27, 5806-5814.	1.1	29
4455	Electron scattering from gas-phase glycine molecules. <i>Journal of Chemical Physics</i> , 2008, 129, 164308.	1.2	16
4456	Preparation of tris(azolyl)phosphine gold complexes: digold coordination and variation in solid state intermolecular interactions. <i>New Journal of Chemistry</i> , 2008, 32, 138-150.	1.4	13
4457	A Valence Bond Modeling of Trends in Hydrogen Abstraction Barriers and Transition States of Hydroxylation Reactions Catalyzed by Cytochrome P450 Enzymes. <i>Journal of the American Chemical Society</i> , 2008, 130, 10128-10140.	6.6	232
4458	Tropospheric Oxidation of Ethyne and But-2-yne. 1. Theoretical Mechanistic Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3656-3665.	1.1	22
4459	Mechanism of Ultrafast Photodecay in Restricted Motions in Protonated Schiff Bases: The Pentadieniminium Cation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1189-1199.	2.3	32
4460	Barrier-free proton transfer in the valence anion of 2'-deoxyadenosine-5'-monophosphate. II. A computational study. <i>Journal of Chemical Physics</i> , 2008, 128, 044315.	1.2	21
4461	Structure, stability, and infrared spectroscopy of $(\text{H}_2\text{O})_n\text{NH}_4^+$ clusters: A theoretical study at zero and finite temperature. <i>Journal of Chemical Physics</i> , 2008, 129, 154305.	1.2	34
4462	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1369-1377.	2.3	83

#	ARTICLE	IF	CITATIONS
4463	Prediction of Activation Energies for Aromatic Oxidation by Cytochrome P450. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13058-13065.	1.1	55
4464	Molybdophosphonate Clusters as Building Blocks in the Oxomolybdate-Organodiphosphonate/Cobalt(II)-Organoinimine System: Structural Influences of Secondary Metal Coordination Preferences and Diphosphonate Tether Lengths. <i>Inorganic Chemistry</i> , 2008, 47, 832-854.	1.9	96
4465	Complete Mechanism of O_2 Intramolecular Aromatic Hydroxylation through O_2 Activation by a Macrocyclic Dicopper(I) Complex. <i>Journal of the American Chemical Society</i> , 2008, 130, 17710-17717.	6.6	62
4466	Probing the Adsorption Sites for CO_2 in Metal Organic Frameworks Materials MIL-53 (Al). <i>TJ ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5</i>	1.5	137
4467	Shorter Argentophilic Interaction than Auophilic Interaction in a Pair of Dimeric $\{(\text{NHC})\text{MCl}\}_2$ (M = Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.9	137
4468	Nature of the Fe^{O_2} Bonding in Oxy-Myoglobin: Effect of the Protein. <i>Journal of the American Chemical Society</i> , 2008, 130, 14778-14790.	6.6	234
4469	Quantum Mechanical/Molecular Mechanical Study of Mechanisms of Heme Degradation by the Enzyme Heme Oxygenase: The Strategic Function of the Water Cluster. <i>Journal of the American Chemical Society</i> , 2008, 130, 1953-1965.	6.6	71
4470	Quantum and Molecular Mechanical Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450cam and Its Mutant D251N. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5126-5138.	1.2	35
4471	Mechanisms of Catalyst Poisoning in Palladium-Catalyzed Cyanation of Haloarenes. Remarkably Facile C-N Bond Activation in the $[(\text{Ph})_3\text{P}]_4\text{Pd}[\text{Bu}_4\text{N}]^+\text{CN}^-$ System. <i>Journal of the American Chemical Society</i> , 2008, 130, 4828-4845.	6.6	122
4472	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1849-1868.	2.3	956
4473	Substituent Effects on the Vibronic Coupling for the Phenoxyl/Phenol Self-Exchange Reaction. <i>Journal of Physical Chemistry B</i> , 2008, 112, 336-343.	1.2	12
4474	Density Functional Theory Study of the Adsorption of Formaldehyde on Pd_4 and on $\text{Pd}_4/\text{Al}_2\text{O}_3$ Clusters. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8929-8937.	1.1	29
4475	One- and two-photon Absorptions in asymmetrically substituted free-base porphyrins: A density functional theory study. <i>Journal of Chemical Physics</i> , 2008, 128, 074302.	1.2	11
4476	Binding of CO, NO, and O_2 to Heme by Density Functional and Multireference ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11824-11832.	1.1	218
4477	Construction of Aryliridium-Salen Complexes: Enantio- and <i>Cis</i> -Selective Cyclopropanation of Conjugated and Nonconjugated Olefins. <i>Journal of the American Chemical Society</i> , 2008, 130, 10327-10337.	6.6	110
4478	Probing Silver Nanoparticles During Catalytic H_2 Evolution. <i>Journal of the American Chemical Society</i> , 2008, 130, 7067-7076.	6.6	49
4479	Photophysics and Deactivation Pathways of Thymine. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8273-8279.	1.1	66
4480	Chapter 17 The Supporting Role of Molecular Modelling and Computational Chemistry in Polymer Analysis. <i>Comprehensive Analytical Chemistry</i> , 2008, 53, 685-734.	0.7	0

#	ARTICLE	IF	CITATIONS
4481	Triplet Pathways in Diarylethene Photochromism: Photophysical and Computational Study of Dyads Containing Ruthenium(II) Polypyridine and 1,2-Bis(2-methylbenzothiophene-3-yl)maleimide Units. <i>Journal of the American Chemical Society</i> , 2008, 130, 7286-7299.	6.6	163
4482	Synthesis, Reactivity, and Electronic Structure of [<i>n</i>]Vanadoarenophanes: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 11376-11393.	6.6	52
4483	Thermochemical properties and relative stability of polychlorinated biphenyls. <i>Environmental Toxicology and Pharmacology</i> , 2008, 25, 148-155.	2.0	11
4484	Unraveling high precision stereocontrol in a triple cascade organocatalytic reaction. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3921.	1.5	43
4485	Experimental and Theoretical Study of the Reactions between Small Neutral Iron Oxide Clusters and Carbon Monoxide. <i>Journal of the American Chemical Society</i> , 2008, 130, 15879-15888.	6.6	156
4486	Nonadiabatic excited-state dynamics of polar π -systems and related model compounds of biological relevance. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 482-494.	1.3	80
4487	Spectral Tuning in Visual Pigments: An ONIOM(QM:MM) Study on Bovine Rhodopsin and its Mutants. <i>Journal of Physical Chemistry B</i> , 2008, 112, 6814-6827.	1.2	110
4488	Inclusion of explicit electron-proton correlation in the nuclear-electronic orbital approach using Gaussian-type geminal functions. <i>Journal of Chemical Physics</i> , 2008, 129, 014101.	1.2	69
4489	Redefining the atom: atomic charge densities produced by an iterative stockholder approach. <i>Chemical Communications</i> , 2008, , 5909.	2.2	111
4490	Pristine Multiwalled Carbon Nanotube/Polyethylene Nanocomposites by Immobilized Catalysts. <i>Chemistry of Materials</i> , 2008, 20, 4588-4594.	3.2	44
4491	New Ruthenium(II) Complexes with Enantiomerically Pure Bis- and Tris(pinene)-Fused Tridentate Ligands. Synthesis, Characterization and Stereoisomeric Analysis. <i>Inorganic Chemistry</i> , 2008, 47, 8016-8024.	1.9	16
4492	Influence of Sequential Guanidinium Methylation on the Energetics of the Guanidinium-Guanine Dimer and Guanidinium-Guanine-Cytosine Trimer: Implications for the Control of Protein-DNA Interactions by Arginine Methyltransferases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16995-17002.	1.2	3
4493	Complexation of Metal Ions in Langmuir Films Formed with Two Amphiphilic Dioxadithia Crown Ethers. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10953-10963.	1.2	8
4494	³¹ P Chemical Shift of Adsorbed Trialkylphosphine Oxides for Acidity Characterization of Solid Acids Catalysts. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7349-7356.	1.1	92
4495	Rational Enhancement of Second-Order Nonlinearity: Bis-(4-methoxyphenyl)hetero-aryl-amino Donor-Based Chromophores: Design, Synthesis, and Electrooptic Activity. <i>Journal of the American Chemical Society</i> , 2008, 130, 10565-10575.	6.6	186
4496	Synthesis and Characterization of a Thiol-Tethered Tripyridyl Porphyrin on Au(111). <i>Journal of Physical Chemistry C</i> , 2008, 112, 6110-6118.	1.5	37
4497	Synthesis, structure and reactions of a trianion equivalent, trilitiostannane. <i>Chemical Communications</i> , 2008, , 6495.	2.2	6
4498	Pre-catalyst resting states: a kinetic, thermodynamic and quantum mechanical analyses of [PdCl ₂ (2-oxazoline) ₂] complexes. <i>Dalton Transactions</i> , 2008, , 3115.	1.6	19

#	ARTICLE	IF	CITATIONS
4499	Materials for hydrogen storage: structure and dynamics of borane ammonia complex. Dalton Transactions, 2008, , 4514.	1.6	43
4500	The role of substrate in unmasking oxyl character in oxomanganese complexes: the key to selectivity?. Dalton Transactions, 2008, , 6141.	1.6	22
4501	Links between through-bond interactions and assembly structure in simple piperidones. New Journal of Chemistry, 2008, 32, 1924.	1.4	10
4502	A ground-state-directed optimization scheme for the Kohn-Sham energy. Physical Chemistry Chemical Physics, 2008, 10, 5344.	1.3	16
4503	Tighter multipole-based integral estimates and parallel implementation of linear-scaling AO-MP2 theory. Physical Chemistry Chemical Physics, 2008, 10, 3335.	1.3	74
4504	Molecular structures of M(Bu ^t) ₃ (M = Al, Ga, In) using gas-phase electron diffraction and ab initio calculations: experimental and computational evidence for charge-transfer processes leading to photodissociation. Dalton Transactions, 2008, , 404-410.	1.6	9
4505	Implementation of an iterative algorithm for optimal control of molecular dynamics into MCTDH. Physical Chemistry Chemical Physics, 2008, 10, 850-856.	1.3	25
4506	Spin-rotation and nuclear shielding constants of sulfur hexafluoride. Molecular Physics, 2008, 106, 1241-1247.	0.8	3
4507	Design of Energetic Ionic Liquids. , 2008, , .		6
4508	CCSD calculations on C14, C18, and C22 carbon clusters. Journal of Chemical Physics, 2008, 128, 114301.	1.2	82
4509	Theoretical investigation of the reaction mechanism for the phosphate diester hydrolysis using an asymmetric dinuclear metal complex as a biomimetic model of the purple acid phosphatase enzyme. Physical Chemistry Chemical Physics, 2008, 10, 7039.	1.3	30
4510	Reactivity of Pt- and Pd-bound nitriles towards nitrile oxides and nitrones: substitution vs. cycloaddition. Dalton Transactions, 2008, , 1312.	1.6	25
4511	Prototropic rearrangements in cycloheptatrienyl PCP pincer iridium complexes. Dalton Transactions, 2008, , 527-532.	1.6	21
4512	Fluoride ion complexation by a B2/Hg heteronuclear tridentate lewis acid. Dalton Transactions, 2008, , 4442.	1.6	55
4513	TLC Separation of Isomeric Diazinodithiins and Diazinyl Sulfides as the Smiles Rearrangement Products. Journal of Liquid Chromatography and Related Technologies, 2008, 31, 3020-3031.	0.5	1
4514	The gas-phase structure of 1-selena-closo-dodecaborane(11), 1-SeB ₁₁ H ₁₁ , determined by the concerted use of electron diffraction and computational methods. Dalton Transactions, 2008, , 96-100.	1.6	15
4515	Construction of building blocks for extended porphyrin arrays by nitration of porphyrin-2,3-diones and quinoxalino[2,3-b]porphyrins. New Journal of Chemistry, 2008, 32, 340-352.	1.4	25
4516	More user-friendly phosphines? Molecular structure of methylphosphine and its adduct with borane, studied by gas-phase electron diffraction and quantum chemical calculations. Dalton Transactions, 2008, , 5041.	1.6	11

#	ARTICLE	IF	CITATIONS
4517	An efficient synthesis of chiral phosphinyl oxide pyrrolidines and their application to asymmetric direct aldol reactions. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3997.	1.5	49
4518	Metathesis of Nitrogen Atoms within Triple Bonds Involving Carbon, Tungsten, and Molybdenum. <i>Inorganic Chemistry</i> , 2008, 47, 5377-5385.	1.9	25
4519	Theoretical and Experimental Vibrational Characterizations of Amine-Coated Silver Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2008, 112, 13851-13855.	1.5	7
4520	Gold Micrometer Crystals Modified with Carboranethiol Derivatives. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14446-14455.	1.5	48
4521	Catalytic Oxidation of H ₂ by N ₂ O in the Gas Phase: O-Atom Transport with Atomic Metal Cations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10141-10146.	1.1	21
4522	Optimizing Conical Intersections without Derivative Coupling Vectors: Application to Multistate Multireference Second-Order Perturbation Theory (MS-CASPT2). <i>Journal of Physical Chemistry B</i> , 2008, 112, 405-413.	1.2	340
4523	Multireference Ab Initio Quantum Mechanics/Molecular Mechanics Study on Intermediates in the Catalytic Cycle of Cytochrome P450 _{cam} . <i>Journal of Physical Chemistry A</i> , 2008, 112, 12904-12910.	1.1	45
4524	Nonlinear Response Properties of Ultralarge Hyperpolarizability Twisted π -System Donor-Acceptor Chromophores. Dramatic Environmental Effects on Response. <i>Journal of Physical Chemistry B</i> , 2008, 112, 44-50.	1.2	58
4525	Interactions of the Hormone Oxytocin with Divalent Metal Ions. <i>Journal of the American Chemical Society</i> , 2008, 130, 5993-6000.	6.6	76
4526	Peptide Hydrolysis Catalyzed by Matrix Metalloproteinase 2: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8412-8424.	1.2	32
4527	Excess Electrons Bound to Small Ammonia Clusters. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11817-11823.	1.1	21
4528	Oligosaccharide Trans-Glycoside ³ J _{COCC} Karplus Curves Are Not Equivalent: Effect of Internal Electronegative Substituents. <i>Journal of Organic Chemistry</i> , 2008, 73, 3255-3257.	1.7	23
4529	Understanding the Reactivity of the Tetrahedrally Coordinated High-Valence d ⁰ Transition Metal Oxides toward the C-H Bond Activation of Alkanes: A Cluster Model Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 717-721.	1.1	28
4530	Formal and Standard Ruthenium-Catalyzed [2 + 2 + 2] Cycloaddition Reaction of 1,6-Diynes to Alkenes: A Mechanistic Density Functional Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 1320-1332.	1.7	42
4531	Ion-Pairing of Octyl Viologen Diiodide in Low-Polar Solvents: An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7987-7995.	1.1	26
4532	Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10226-10235.	1.1	24
4533	Multinuclear NMR, X-ray, and DFT Studies on RhCl(diene)(phosphoramidite) Complexes. <i>Organometallics</i> , 2008, 27, 4580-4588.	1.1	9
4534	Synthesis, Structure and Magnetic Behavior of Five-Coordinate Bis(iminopyrrolyl) Complexes of Cobalt(II) containing PMe ₃ and THF Ligands. <i>Inorganic Chemistry</i> , 2008, 47, 8896-8911.	1.9	48

#	ARTICLE	IF	CITATIONS
4535	Experimental Observation of Supramolecular Carbonyl- π -Carbonyl and Carbonyl- π -anion Assemblies Supported by Theoretical Studies. <i>Crystal Growth and Design</i> , 2008, 8, 3773-3784.	1.4	64
4536	Quantum Mechanical/Molecular Mechanical Study on the Mechanisms of Compound I Formation in the Catalytic Cycle of Chloroperoxidase: An Overview on Heme Enzymes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9490-9500.	1.2	60
4537	RGe(I)Ge(I)R Compound (R = PhC(N \rightarrow Bu) ₂) with a Ge \rightarrow Ge Single Bond and a Comparison with the Gauche Conformation of Hydrazine. <i>Organometallics</i> , 2008, 27, 5459-5463.	1.1	175
4538	Regioselectivity in the Ligand-Assisted Addition of Vinylmagnesium Bromide: An Experimental and Theoretical Study on the 1 ³ -Alkoxy-cyclobutenone Model. <i>Journal of Organic Chemistry</i> , 2008, 73, 6521-6533.	1.7	7
4539	Photochromism of an Organorhodium Dithionite Complex in the Crystalline-State: Molecular Motion of Pentamethylcyclopentadienyl Ligands Coupled to Atom Rearrangement in a Dithionite Ligand. <i>Journal of the American Chemical Society</i> , 2008, 130, 17836-17845.	6.6	42
4540	An Interface between the Universal Force Field and the Effective Fragment Potential Method. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12753-12760.	1.2	6
4541	Probing the Electronic Communication of the Isocyanide Bridge Through the Luminescence Properties of the d ⁹ -d ⁹ [ClPt($\frac{1}{4}$ -dppm)Pt(Ci \rightarrow Ni-PCP)] ⁺ and A-Frame [ClPd($\frac{1}{4}$ -dppm) ₂ ($\frac{1}{4}$ -Ci \rightarrow Ni-PCP)PdCl] Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 10816-10824.	1.0	10
4542	Assessing the Role of Polarization in Docking. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12157-12163.	1.1	42
4543	1,2-Addition versus π -Bond Metathesis Reactions in Transient Bis(cyclopentadienyl)zirconium Imides: Evidence for a d ⁰ Dihydrogen Complex. <i>Organometallics</i> , 2008, 27, 872-879.	1.1	22
4544	Computational Study of the C \rightarrow H Bond Activation in Ethylene on a Binuclear Ruthenium Complex. <i>Organometallics</i> , 2008, 27, 3681-3692.	1.1	8
4545	Photostability via Sloped Conical Intersections: A Computational Study of the Pyrene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10881-10886.	1.1	28
4546	Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Druglike Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1718-1732.	2.3	13
4547	Toward a Consistent Treatment of Polarization in Model QM/MM Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12151-12156.	1.1	13
4548	Selectivity in the Oxidative Addition of C \rightarrow S Bonds of Substituted Thiophenes to the (C ₅ Me ₅)Rh(PMe ₃) Fragment: A Comparison of Theory with Experiment. <i>Inorganic Chemistry</i> , 2008, 47, 10889-10894.	1.9	26
4549	2D NMR Study of the DNA Duplex d(CTCTC [*] A [*] ACTTCC) \rightarrow d(GGAAGTTGAGAG) Cross-Linked by the Antitumor-Active Dirhodium(II,II) Unit at the Cytosine \rightarrow Adenine Step. <i>Biochemistry</i> , 2008, 47, 2265-2276.	1.2	33
4550	Proton Affinity of Methyl Peroxynitrate. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1981-1985.	1.1	4
4551	Spin Coupling and Resonance. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13197-13202.	1.1	7
4552	Origin of Stereoselectivity in the Reduction of a Planar Oxacarbenium. <i>Organic Letters</i> , 2008, 10, 3769-3772.	2.4	23

#	ARTICLE	IF	CITATIONS
4553	A Valence Bond Study of Three-Center Four-Electron π Bonding: Electronegativity vs Electroneutrality. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12806-12811.	1.1	18
4554	¹³ C-Labeled <i>N</i> -Acetyl-neuraminic Acid in Aqueous Solution: Detection and Quantification of Acyclic Keto, Keto Hydrate, and Enol Forms by ¹³ C NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 11892-11900.	6.6	41
4555	Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11873-11884.	1.1	28
4556	Theoretical Modeling of the Doping Process in Polypyrrole by Calculating UV/Vis Absorption Spectra of Neutral and Charged Oligomers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11842-11853.	1.1	33
4557	Ab Initio Molecular Dynamics Simulation of a Medium-Sized Water Cluster Anion: From an Interior to a Surface-Located Excess Electron via a Delocalized State. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6125-6133.	1.1	79
4558	Oxidative Addition of the C $\hat{=}$ S Bond of Thiophene to the (C ₅ Me ₅)Rh(PMe ₃) ₃ Fragment: A Theoretical Study Revisited. <i>Organometallics</i> , 2008, 27, 3666-3670.	1.1	22
4559	A Deeper Look into Thiophene Coordination Prior to Oxidative Addition of the C $\hat{=}$ S Bond to Platinum(0): A Computational Study Using DFT and MO Methods. <i>Organometallics</i> , 2008, 27, 53-60.	1.1	26
4560	Regioselective Ortho Palladation of Stabilized Iminophosphanes in Exo Positions: Scope, Limitations, and Mechanistic Insights. <i>Organometallics</i> , 2008, 27, 2929-2936.	1.1	41
4561	Bond Selection in the Photoisomerization Reaction of Anionic Green Fluorescent Protein and Kindling Fluorescent Protein Chromophore Models. <i>Journal of the American Chemical Society</i> , 2008, 130, 8677-8689.	6.6	149
4562	A Model for Proton Transfer to Metal Electrodes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10814-10826.	1.5	42
4563	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6860-6868.	1.5	157
4564	Structural Investigation of Encapsulated Fluoride in Polyhedral Oligomeric Silsesquioxane Cages Using Ion Mobility Mass Spectrometry and Molecular Mechanics. <i>Chemistry of Materials</i> , 2008, 20, 4299-4309.	3.2	82
4565	Understanding Selectivity in the Oxidative Addition of the Carbon $\hat{=}$ Sulfur Bonds of 2-Cyanothiophene to Pt(0). <i>Inorganic Chemistry</i> , 2008, 47, 4596-4604.	1.9	20
4566	Cationic Methyl Complexes of the Rare-Earth Metals: An Experimental and Computational Study on Synthesis, Structure, and Reactivity. <i>Inorganic Chemistry</i> , 2008, 47, 9265-9278.	1.9	49
4567	Helical Supramolecular Assemblies of {2,4,6-[Cp $\hat{=}$ -Rh(E2-1,2-C2B10H10)(NC5H4CH2S)] ₃ (triazine)} (E = S, Se) Shaped by Cp $\hat{=}$ - $\hat{=}$ Toluene $\hat{=}$ Cp $\hat{=}$ $\hat{=}$ -Stacking Forces and BH $\hat{=}$ Pyridine Hydrogen Bonding. <i>Inorganic Chemistry</i> , 2008, 47, 2940-2942.	1.9	28
4568	DFT Study on Chemical N ₂ Fixation by Using a Cubane-Type Ru ₃ S ₄ Cluster: Energy Profile for Binding and Reduction of N ₂ to Ammonia via Ru $\hat{=}$ N $\hat{=}$ NH ₂ ($\hat{=}$ = 1 $\hat{=}$) Intermediates with Unique Structures. <i>Journal of the American Chemical Society</i> , 2008, 130, 9037-9047.	6.6	49
4569	Why Does Fluoride Anion Accelerate Transmetalation between Vinylsilane and Palladium(II) $\hat{=}$ Vinyl Complex? Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 12975-12985.	6.6	88
4570	Molecular Structure of the Octatetrayl Anion, C ₈ H $\hat{=}$: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7717-7722.	1.1	7

#	ARTICLE	IF	CITATIONS
4571	Density Functional Theory Calculations of the Lowest Energy Quintet and Triplet States of Model Hemes: Role of Functional, Basis Set, and Zero-Point Energy Corrections. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3700-3711.	1.1	25
4572	Proton Affinity of Methyl Nitrite and Methyl Peroxynitrite: Implications for Measuring Branching Ratios of Alkyl Nitrates and Nitrites. <i>Journal of the American Chemical Society</i> , 2008, 130, 11234-11239.	6.6	5
4573	Theoretical Study of Pyrazolate-Bridged Dinuclear Platinum(II) Complexes: Interesting Potential Energy Curve of the Lowest Energy Triplet Excited State and Phosphorescence Spectra. <i>Inorganic Chemistry</i> , 2008, 47, 4329-4337.	1.9	51
4574	Catalytic Asymmetric Alkylations of Ketoimines. Enantioselective Synthesis of <i>i</i> -N-Substituted Quaternary Carbon Stereogenic Centers by Zr-Catalyzed Additions of Dialkylzinc Reagents to Aryl-, Alkyl-, and Trifluoroalkyl-Substituted Ketoimines. <i>Journal of the American Chemical Society</i> , 2008, 130, 5530-5541.	6.6	180
4575	Facile Ruthenium(IV)-Catalyzed Single and Double Allylation of Indole Compounds using Alcohols as Substrates: Aspects of Ruthenium(IV) Allyl Chemistry. <i>Organometallics</i> , 2008, 27, 3796-3805.	1.1	48
4576	Computational Studies of Intramolecular Carbon-Heteroatom Bond Activation of N-Aryl Heterocyclic Carbene Ligands. <i>Organometallics</i> , 2008, 27, 938-944.	1.1	28
4577	Origins of Stereoselectivity in the Oxido-Alkylidenation of Alkynes. <i>Organic Letters</i> , 2008, 10, 4597-4600.	2.4	22
4578	Synthesis, Reactivity, and Computational Studies of $[\text{Ir}^{\text{III}}\text{-C}^{\text{sp}5}\text{-H}^{\text{sp}5}\text{-C}^{\text{sp}5}\text{-H}^{\text{sp}4}\text{-CMe}_2\text{-C}^{\text{sp}6}\text{-H}^{\text{sp}6}]^+$ Aromatic C-H Bond Activation at ~ 50 Å°C. <i>Organometallics</i> , 2008, 27, 1996-2003.		
4579	^{31}P Chemical Shift Tensors for Canonical and Non-canonical Conformations of Nucleic Acids: A DFT Study and NMR Implications. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3470-3478.	1.2	25
4580	Cubic Nonlinear Optical Properties of Platinum-Terminated Polyynediyl Chains. <i>Inorganic Chemistry</i> , 2008, 47, 9946-9957.	1.9	66
4581	Computational Study of C-H Activation of 1,3-Dimesitylimidazol-2-ylidene (IMes) at Ruthenium: The Role of Ligand Bulk in Accessing Reactive Intermediates. <i>Organometallics</i> , 2008, 27, 617-625.	1.1	36
4582	Room-Temperature First-Order Phase Transition in a Charge-Disproportionated Molecular Conductor (MeEDO-TTF) $_2$ PF $_6$. <i>Chemistry of Materials</i> , 2008, 20, 7551-7562.	3.2	25
4583	Origins of Opposite Syn-Anti Diastereoselectivities in Primary and Secondary Amino Acid-Catalyzed Intermolecular Aldol Reactions Involving Unmodified β -Hydroxyketones. <i>Journal of Organic Chemistry</i> , 2008, 73, 5264-5271.	1.7	15
4584	Mechanism and Control of Rare Tautomer Trapping at a Metal-Metal Bond: Adenine Binding to Dirhodium Antitumor Agents $[\text{Rh}^{\text{II}}]_2$. <i>Journal of the American Chemical Society</i> , 2008, 130, 665-675.	6.6	31
4585	Refining the Active Site Structure of Iron-Iron Hydrogenase Using Computational Infrared Spectroscopy. <i>Inorganic Chemistry</i> , 2008, 47, 2380-2388.	1.9	40
4586	A Rational Basis for the Axial Ligand Effect in C-H Oxidation by $[\text{MnO}(\text{porphyrin})(\text{X})]^+$ (X = H $_2$ O, OH $^-$). <i>J. Phys. Chem. B</i> , 2008, 112, 7843-7847.	1.9	87
4587	Contributions of the 8-Methyl Group to the Vibrational Normal Modes of Flavin Mononucleotide and Its 5-Methyl Semiquinone Radical. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6179-6189.	1.1	20
4588	H $_2$ O-Involved Hydrogen Bonds in Pseudo-Double-Decker Supramolecular Structure of 1,8,15,22-Tetrasubstituted Phthalocyaninato Zinc Complex. <i>Crystal Growth and Design</i> , 2008, 8, 4454-4459.	1.4	15

#	ARTICLE	IF	CITATIONS
4589	Binding to DNA Purine Base and Structure-Activity Relationship of a Series of Structurally Related Ru(II) Antitumor Complexes: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 9966-9974.	1.2	20
4590	Quantitative Three Dimensional Structure Linear Interaction Energy Model of 5-(Salicyl)sulfamoyl]adenosine and the Aryl Acid Adenylating Enzyme MbtA. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7154-7160.	2.9	21
4591	Mechanism for Iron-Catalyzed Alkene Isomerization in Solution. <i>Organometallics</i> , 2008, 27, 4370-4379.	1.1	44
4592	Theoretical Study of the Acid-Promoted Hydrolysis of Oxazolin-5-one: A Microhydration Model. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10659-10667.	1.2	16
4593	Theoretical Study of the Mechanism and Rate Constant of the B + CO ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8148-8153.	1.1	3
4594	Theoretical Predictions of ³¹ P NMR Chemical Shift Threshold of Trimethylphosphine Oxide Adsorbed on Solid Acid Catalysts. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4496-4505.	1.2	143
4595	Theoretical Investigation of the Magnetic Interactions of Ni ⁹ Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4020-4028.	1.1	7
4596	Low-energy electron scattering from methanol and ethanol. <i>Physical Review A</i> , 2008, 77, .	1.0	69
4597	Single Crystal Structure of Zeolite A (LTA) Containing Ag ₄ Cl ₄ Nanoclusters and Reduced 1,3,5-Tripyrylium Dimers with Remarkably Short 2.43 Å... Interplanar Spacings. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11181-11193.	1.5	6
4598	Mixed Valence Creutz-Taube Ion Analogues Incorporating Thiocrowns: Synthesis, Structure, Physical Properties, and Computational Studies. <i>Inorganic Chemistry</i> , 2008, 47, 11633-11643.	1.9	17
4599	Matrix Isolation FTIR Spectroscopic and Theoretical Study of 3,3-Dichloro-1,1,1-Trifluoropropane (HCFC-243). <i>Journal of Physical Chemistry A</i> , 2008, 112, 11641-11648.	1.1	5
4600	Mechanism of Hydride Donor Generation Using a Ru(II) Complex Containing an NAD ⁺ Model Ligand: Pulse and Steady-State Radiolysis Studies. <i>Inorganic Chemistry</i> , 2008, 47, 3958-3968.	1.9	78
4601	Carbene Proton Attachment Energies: Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5269-5277.	1.1	7
4602	Understanding the Behavior of N-Tosyl and N-2-Pyridylsulfonyl Imines in Cu ^{II} -Catalyzed Aza-Friedel-Crafts Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 6401-6404.	1.7	59
4603	Substituent Effects on the Rearrangements of Cyclohexyl to Cyclopentyl Radicals Involving Avermectin-Related Radicals. <i>Journal of Organic Chemistry</i> , 2008, 73, 8175-8181.	1.7	20
4604	Indirect Photolysis of Organic Compounds: Prediction of OH Reaction Rate Constants through Molecular Orbital Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11391-11399.	1.1	15
4605	Synthesis and Molecular and Electronic Structure of an Unusual Paramagnetic Borohydride Complex Mo(NAr) ₂ (PMe ₃) ₂ (i ⁻ BH ₄). <i>Inorganic Chemistry</i> , 2008, 47, 999-1006.	1.9	13
4606	Flexible-Boundary Quantum-Mechanical/Molecular-Mechanical Calculations: Partial Charge Transfer between the Quantum-Mechanical and Molecular-Mechanical Subsystems. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 414-425.	2.3	45

#	ARTICLE	IF	CITATIONS
4607	Computational Study of the Reaction of C ₆ F ₆ with [IrMe(PEt ₃) ₃] ₃ : Identification of a Phosphine-Assisted C ⁺ F Activation Pathway via a Metallophosphorane Intermediate. <i>Journal of the American Chemical Society</i> , 2008, 130, 15490-15498.	6.6	81
4608	Chemisorption-induced Structural Changes and Transition from Chemisorption to Physisorption in Au ₆ (CO) _n (n = 4 ⁹). <i>Journal of Physical Chemistry C</i> , 2008, 112, 11920-11928.	1.5	51
4609	¹³ C ⁺ H and ¹³ C ⁺ C NMR J-Couplings in ¹³ C-Labeled N-Acetyl-neuraminic Acid: Correlations with Molecular Structure. <i>Journal of Organic Chemistry</i> , 2008, 73, 4376-4387.	1.7	26
4610	Surface Reaction of 1,2-Dichloroethylene on Si(100)-2 Å ¹ : Importance of Surface Isomerization Channel. <i>Journal of Physical Chemistry C</i> , 2008, 112, 9327-9335.	1.5	7
4611	Computational Investigation on Stereochemistry in Titanium ⁺ Salicylaldehydes-Catalyzed Cyanation of Benzaldehyde. <i>Journal of Organic Chemistry</i> , 2008, 73, 4840-4847.	1.7	10
4612	Combined Experimental and Theoretical Approach To Understand the Reactivity of a Mononuclear Cu(II) ⁺ Hydroperoxo Complex in Oxygenation Reactions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13102-13108.	1.1	25
4613	Influence of the Solvent Description on the Predicted Mechanism of SN2 Reactions. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12414-12419.	1.2	7
4614	Simultaneous analytical optimization of variational parameters in Gaussian-type functions with full configuration interaction of multicomponent molecular orbital method by elimination of translational and rotational motions: Application to isotopomers of the hydrogen molecule. <i>Journal of Chemical Physics</i> , 2008, 128, 164118.	1.2	22
4615	Ligand-Derived Oxidase Activity. Catalytic Aerial Oxidation of Alcohols (Including Methanol) by Cu(II)-Diradical Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 8943-8956.	1.9	62
4616	Thermochemical Properties of Polychlorinated Biphenylenes. <i>Journal of Chemical & Engineering Data</i> , 2008, 53, 48-52.	1.0	1
4617	M ₂ @C ₇₉ N (M = Y, Tb): Isolation and Characterization of Stable Endohedral Metallofullerenes Exhibiting M ⁺ M Bonding Interactions inside Aza[80]fullerene Cages. <i>Journal of the American Chemical Society</i> , 2008, 130, 12992-12997.	6.6	155
4618	Thermal Decomposition Mechanisms of Methanol, Ethanol, and 1-Propanol on the Si(100)-2 Å ¹ Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6907-6913.	1.5	11
4619	Chiral Modification of Rh and Pt Surfaces: Effect of Rotational Flexibility of Cinchona-Type Modifiers on Their Adsorption Behavior. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3866-3874.	1.5	20
4620	Water Cluster Anions Studied by the Long-Range Corrected Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9845-9853.	1.1	36
4621	Growth pattern and electronic properties of acetonitrile clusters: A density functional study. <i>Journal of Chemical Physics</i> , 2008, 128, 214307.	1.2	17
4622	Exploring Photobiology and Biospectroscopy with the Sac-Ci (Symmetry-Adapted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 147 Tid and Physics, 2008, , 93-124.	0.6	9
4623	Nonadiabatic Excited-State Dynamics of Aromatic Heterocycles: Toward the Time-Resolved Simulation of Nucleobases. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 209-235.	0.6	4
4624	Stable Valence Anions of Nucleic Acid Bases and DNA Strand Breaks Induced by Low Energy Electrons. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 619-667.	0.6	15

#	ARTICLE	IF	CITATIONS
4625	Highly asymmetric coordination of trimethylsilyl groups to tetrazole and triazole rings: an experimental and computational study in gaseous and crystalline phases. Dalton Transactions, 2008, , 3817.	1.6	3
4626	Theoretical study of the potential energy surface for the interaction of cisplatin and their aquated species with water. Journal of Chemical Physics, 2008, 128, 165103.	1.2	30
4627	Extension of linear-scaling divide-and-conquer-based correlation method to coupled cluster theory with singles and doubles excitations. Journal of Chemical Physics, 2008, 129, 044103.	1.2	135
4628	High-efficiency, low-voltage phosphorescent organic light-emitting diode devices with mixed host. Journal of Applied Physics, 2008, 104, .	1.1	143
4629	Electronic structure of the organic semiconductor copper phthalocyanine: Experiment and theory. Journal of Chemical Physics, 2008, 128, 034703.	1.2	32
4630	Calculated interactions of a nitro group with aromatic rings of crystalline picryl bromide. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13720-13723.	3.3	35
4631	Density functional studies on Lewis acidity of alkaline earth metal exchanged faujasite zeolite. Molecular Simulation, 2008, 34, 1121-1128.	0.9	3
4632	ESTIMATION OF DISSOLVABILITY OF CHLORIC AND ALKYL BENZENE DERIVATIVES USING QUANTUM CHEMICAL DESCRIPTORS AND PARTIAL LEAST SQUARES. Journal of Theoretical and Computational Chemistry, 2008, 07, 989-999.	1.8	2
4633	Probing interactions between core-electron transitions by ultrafast two-dimensional x-ray coherent correlation spectroscopy. Journal of Chemical Physics, 2008, 128, 184307.	1.2	15
4634	H $\hat{\alpha}$ • D isotope effect of methyl internal rotation for acetaldehyde in ground state as calculated from a multicomponent molecular orbital method. Journal of Chemical Physics, 2008, 128, 184309.	1.2	14
4635	Dipole switching in large molecules described by explicitly time-dependent configuration interaction. Journal of Chemical Physics, 2008, 128, 234307.	1.2	22
4636	Rototranslational sum rules for electromagnetic hypershielding at the nuclei and related atomic Cartesian derivatives of the optical rotatory power. Journal of Chemical Physics, 2008, 128, 244107.	1.2	2
4637	<i>Ab initio</i> multiple spawning dynamics of excited state intramolecular proton transfer: the role of spectroscopically dark states. Molecular Physics, 2008, 106, 537-545.	0.8	31
4638	<i>Ab initio</i> spectroscopy and photoinduced cooling of the trans-stilbene molecule. Journal of Chemical Physics, 2008, 128, 164303.	1.2	75
4639	An atomic orbital-based reformulation of energy gradients in second-order Møller-Plesset perturbation theory. Journal of Chemical Physics, 2008, 128, 154101.	1.2	62
4640	<i>Ab initio</i> study of the one- and two-photon circular dichroism of R-(+)-3-methyl-cyclopentanone. Journal of Chemical Physics, 2008, 128, 164312.	1.2	50
4641	X-ray absorption and natural circular dichroism spectra of C84: A theoretical study using the complex polarization propagator approach. Journal of Chemical Physics, 2008, 128, 234304.	1.2	16
4642	Negative ions of nitroethane and its clusters. Journal of Chemical Physics, 2008, 129, 064308.	1.2	15

#	ARTICLE	IF	CITATIONS
4643	Oligo(vinylidene fluoride) Langmuir-Blodgett films studied by spectroscopic ellipsometry and the density functional theory. <i>Journal of Chemical Physics</i> , 2008, 129, 064704.	1.2	7
4644	Energetics and molecular dynamics of the reaction of HOCO with HO ₂ radicals. <i>Journal of Chemical Physics</i> , 2008, 129, 214307.	1.2	20
4645	Plasma Chemistry of Octafluorocyclopentene/Argon/Oxygen Mixtures. <i>Japanese Journal of Applied Physics</i> , 2008, 47, 6843-6848.	0.8	8
4646	Synthesis and structural characterization of a new self-assembled disulfide linked meso-tetrakis-porphyrin macromolecular array. <i>Journal of Porphyrins and Phthalocyanines</i> , 2008, 12, 845-848.	0.4	4
4647	X-ray Crystallographic Investigations of an Azacryptand and its Bis-Protonated Salt: Interactions of Acyclic Water Trimer and C-H...N Interactions in T-shaped Benzene Dimer. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , 2008, 38, 2-11.	0.6	3
4648	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The formula for general active spaces and its applications for multibond breaking systems. <i>Journal of Chemical Physics</i> , 2008, 128, 224107.	1.2	41
4649	Synthesis and Photophysical Studies of New Blue Phosphorescent Iridium Complexes of Fluorinated 2-phenyl-4-methoxypyridine. <i>Molecular Crystals and Liquid Crystals</i> , 2008, 491, 209-216.	0.4	5
4650	Double-quantum-coherence attosecond x-ray spectroscopy of spatially separated, spectrally overlapping core-electron transitions. <i>Physical Review A</i> , 2008, 78, .	1.0	26
4651	Geometrical and Kinetic Isotope Effects on R-H(D)-A...R Type Intramolecular Hydrogen Bonds (R = CH ₂), <i>Tj ETQq0 0 0 rgBT /Overloc</i> <i>Japan</i> , 2008, 81, 820-825.	2.0	15
4652	Theoretical Studies on Electronic Structures and Chemical Indices of the Active Site of Oxygenated and Deoxygenated Hemerythrin. <i>Bulletin of the Chemical Society of Japan</i> , 2008, 81, 91-102.	2.0	14
4653	Photo-Induced State Conversion Mechanism of an Optically Durable Molecular Memory with Controlled Hydrogen Bonding: A Spin-Orbit CI Study of [{Co(2,2'-biimidazole)(C ₆ H ₄ O ₂)(NH ₃) ₂ } ₂]. <i>Bulletin of the Chemical Society of Japan</i> , 2008, 81, 235-240.	2.0	0
4654	Analysis on Excitation of Molecules with <i>h_v</i> Symmetry: Frozen Orbital Analysis and General Rules. <i>Chemistry Letters</i> , 2008, 37, 322-323.	0.7	7
4655	Cis-trans, trans-cis isomerizations and N=O bond dissociation of nitrous acid (HONO) on an ab initio potential surface obtained by novelty sampling and feed-forward neural network fitting. <i>Journal of Chemical Physics</i> , 2008, 128, 194310.	1.2	45
4656	New Expression of the Chemical Bond in Hydrides Using Atomization Energies. <i>Advances in Quantum Chemistry</i> , 2008, , 145-160.	0.4	7
4657	An Exploration of Mechanisms for the Transformation of 8-Oxoguanine to Guanidinohydantoin and Spiroiminodihydantoin by Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2008, 130, 5245-5256.	6.6	85
4659	Local reactivity of O ₂ with Pt ₃ on Co ₃ Pt and related backgrounds. <i>Journal of Chemical Physics</i> , 2008, 128, 204701.	1.2	7
4660	Molecular geometry-dependent atomic charge calculation with modified charge equilibration method. <i>Chem-Bio Informatics Journal</i> , 2009, 9, 30-40.	0.1	3
4662	Construction of basis sets for time-dependent studies. <i>Journal of Chemical Physics</i> , 2009, 131, 064104.	1.2	3

#	ARTICLE	IF	CITATIONS
4663	Antioxidant Properties of Pterocarpan through Their Copper(II) Coordination Ability. A DFT Study in Vacuo and in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 15206-15216.	1.1	48
4664	How long are the ends of polyene chains?. Journal of Chemical Physics, 2009, 131, 224301.	1.2	10
4665	Nested Markov chain Monte Carlo sampling of a density functional theory potential: Equilibrium thermodynamics of dense fluid nitrogen. Journal of Chemical Physics, 2009, 131, 074105.	1.2	16
4666	Damping functions in the effective fragment potential method. Molecular Physics, 2009, 107, 999-1016.	0.8	98
4667	New Red Phosphorescent Heteroleptic Tris-Cyclometalated Iridium Complex with 1-phenylisoquinoline and 2,4-diphenylquinoline. Molecular Crystals and Liquid Crystals, 2009, 513, 236-245.	0.4	1
4668	THEORETICAL STUDY ON THE INTERACTION SCHEMES OF β -CYCLODEXTRIN WITH ACETOVANILLONE. Journal of Theoretical and Computational Chemistry, 2009, 08, 57-69.	1.8	2
4669	Synthesis, Bioactivity and SAR study of <i>N</i> -(5-substituted-1,3,4-thiadiazol-2-yl)- <i>N</i> -cyclopropylformyl-thioureas as ketol-acid reductoisomerase Inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 545-552.	2.5	16
4670	A relook at the compliance constants in redundant internal coordinates and some new insights. Journal of Chemical Physics, 2009, 131, 174112.	1.2	25
4671	THE INFLUENCES OF OXIDATION AND CATIONIZATION ON THE N-GLYCOSIDIC BOND STABILITY OF 8-OXO-2-DEOXYADENOSINE – A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2009, 08, 1253-1264.	1.8	6
4672	Cross sections and photoelectron angular distributions in photodetachment from negative ions using equation-of-motion coupled-cluster Dyson orbitals. Journal of Chemical Physics, 2009, 131, 124114.	1.2	165
4673	A quantum chemistry study of Diels-Alder dimerizations in benzene and anthracene. Journal of Chemical Physics, 2009, 131, 024313.	1.2	16
4674	Thermodynamic Properties of the Gaseous Gallium Molybdates and Tungstates. Journal of Physical Chemistry A, 2009, 113, 13469-13474.	1.1	10
4675	Generating functionals based formulation of the method of moments of coupled cluster equations. Journal of Chemical Physics, 2009, 130, 084112.	1.2	16
4676	On reversible bonding of hydrogen molecules on platinum clusters. Journal of Chemical Physics, 2009, 130, 084111.	1.2	26
4677	An <i>ab initio</i> study of the reaction of HOCO radicals with NO ₂ : Addition/elimination mechanism. Journal of Chemical Physics, 2009, 130, 124306.	1.2	10
4678	Two- and three-photon absorption of organic ionic pyrylium based materials. Journal of Chemical Physics, 2009, 130, 174312.	1.2	7
4679	Nested variant of the method of moments of coupled cluster equations for vertical excitation energies and excited-state potential energy surfaces. Journal of Chemical Physics, 2009, 130, 194110.	1.2	18
4680	Electronic structure and molecular dynamics of breaking the RO-NO ₂ bond. Journal of Chemical Physics, 2009, 130, 244110.	1.2	14

#	ARTICLE	IF	CITATIONS
4681	Divide-and-conquer-based linear-scaling approach for traditional and renormalized coupled cluster methods with single, double, and noniterative triple excitations. <i>Journal of Chemical Physics</i> , 2009, 131, 114108.	1.2	126
4682	Perturbative triples correction for the equation-of-motion coupled-cluster wave functions with single and double substitutions for ionized states: Theory, implementation, and examples. <i>Journal of Chemical Physics</i> , 2009, 131, 114112.	1.2	50
4683	Altering the electronic properties of diamondoids through encapsulating small particles. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 215303.	0.7	12
4684	Hydrogen Bonding Character Between the Glycine and BF ₄ ⁻ . <i>Chinese Journal of Chemical Physics</i> , 2009, 22, 517-522.	0.6	4
4685	Theoretical Study on Reactions of Triplet Excited State Thioxanthone with Indole. <i>International Journal of Molecular Sciences</i> , 2009, 10, 4284-4289.	1.8	9
4686	DFT investigation of the "quasi-living" propene polymerisation with Cp*TiMe ₃ /B(C ₆ F ₅) ₃ : the "naked cation" approach. <i>Dalton Transactions</i> , 2009, , 8993.	1.6	8
4687	Reaction of dialkyl carbonates with alcohols: Defining a scale of the best leaving and entering groups. <i>Pure and Applied Chemistry</i> , 2009, 81, 1971-1979.	0.9	27
4688	Linear-scaling atomic orbital-based second-order Møller-Plesset perturbation theory by rigorous integral screening criteria. <i>Journal of Chemical Physics</i> , 2009, 130, 064107.	1.2	135
4689	Optimization of selected molecular orbitals in group basis sets. <i>Journal of Chemical Physics</i> , 2009, 130, 134108.	1.2	6
4690	A new electronic structure method for doublet states: Configuration interaction in the space of ionized 1h and 2h1p determinants. <i>Journal of Chemical Physics</i> , 2009, 130, 124113.	1.2	32
4691	The reaction of N ₂ O with phenylium ions C ₆ (H,D) ₅ ⁺ : An integrated experimental and theoretical mechanistic study. <i>Journal of Chemical Physics</i> , 2009, 131, 024304.	1.2	8
4692	Vertical electronic excitation with a dielectric continuum model of solvation including volume polarization. II. Implementation and applications. <i>Journal of Chemical Physics</i> , 2009, 131, 014104.	1.2	10
4693	Electronic structure of poly(azomethine) thin films. <i>Journal of Chemical Physics</i> , 2009, 131, 024901.	1.2	5
4694	A thermal self-consistent field theory for the calculation of molecular vibrational partition functions. <i>Journal of Chemical Physics</i> , 2009, 131, 114102.	1.2	20
4695	Local correlation calculations using standard and renormalized coupled-cluster approaches. <i>Journal of Chemical Physics</i> , 2009, 131, 114109.	1.2	199
4696	Electronic and geometric structures of the blue copper site of azurin investigated by QM/MM hybrid calculations. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 064235.	0.7	12
4697	Metal Ions-Stimulated Iron Oxidation in Hydroxylases Facilitates Stabilization of HIF-1 α Protein. <i>Toxicological Sciences</i> , 2009, 107, 394-403.	1.4	35
4698	Mechanism of CB1954 reduction by <i>Escherichia coli</i> nitroreductase. <i>Biochemical Society Transactions</i> , 2009, 37, 413-418.	1.6	27

#	ARTICLE	IF	CITATIONS
4699	New Blue Phosphorescent Iridium Complexes with Various Ancillary Ligands Based on Fluorinated 2-Phenyl-4-Methylpyridine. <i>Molecular Crystals and Liquid Crystals</i> , 2009, 505, 87/[325]-96/[334].	0.4	0
4700	Effects of π -stacking interactions on the near carbon K-edge x-ray absorption fine structure: A theoretical study of the ethylene pentamer and the phthalocyanine dimer. <i>Journal of Chemical Physics</i> , 2009, 130, 104305.	1.2	13
4701	Nuclear Quantum Tunneling in the Light-activated Enzyme Protochlorophyllide Oxidoreductase. <i>Journal of Biological Chemistry</i> , 2009, 284, 3762-3767.	1.6	80
4702	A DFT study of the reactions of O ₃ with Hg ^{Å°} or Br ^Å . <i>Atmospheric Environment</i> , 2009, 43, 5708-5711.	1.9	12
4703	Quantumâ€Chemical Characterization of the Origin of Dipole Formation at Molecular Organic/Organic Interfaces. <i>Advanced Functional Materials</i> , 2009, 19, 624-633.	7.8	63
4704	On the â€œCluingâ€Effect of Lithium: The Lithiumâ€Driven Assembly of Circumâ€Arranged, Edgeâ€Fused Cyclopentadienyl Lithium Compounds and Aza Analogues. <i>Chemistry - A European Journal</i> , 2009, 15, 3123-3129.	1.7	4
4705	The Effect of a Complexed Lithium Cation on a Norcaraneâ€Based Radical Clock. <i>Chemistry - A European Journal</i> , 2009, 15, 2425-2433.	1.7	7
4706	Oxidation of Ethers, Alcohols, and Unfunctionalized Hydrocarbons by the Methyltrioxorhenium/H ₂ O ₂ System: A Computational Study on Catalytic C-H Bond Activation. <i>Chemistry - A European Journal</i> , 2009, 15, 1862-1869.	1.7	15
4707	How Does the Axial Ligand of Cytochrome P450 Biomimetics Influence the Regioselectivity of Aliphatic versus Aromatic Hydroxylation?. <i>Chemistry - A European Journal</i> , 2009, 15, 5577-5587.	1.7	82
4708	Determination of the Catalytic Pathway of a Manganese Arginase Enzyme Through Density Functional Investigation. <i>Chemistry - A European Journal</i> , 2009, 15, 8026-8036.	1.7	23
4709	Ion Pairing and Salt Structure in Organic Salts through Diffusion, Overhauser, DFT and X-ray Methods. <i>Chemistry - A European Journal</i> , 2009, 15, 6848-6862.	1.7	18
4710	Structural and Reactivity Studies of â€œPincerâ€Pyridine Dicarbene Complexes of Fe ⁰ : Experimental and Computational Comparison of the Phosphine and NHC Donors. <i>Chemistry - A European Journal</i> , 2009, 15, 5491-5502.	1.7	102
4711	Synthesis and Properties of Salenâ€Aluminum Complexes as a Novel Class of Colorâ€Tunable Luminophores. <i>Chemistry - A European Journal</i> , 2009, 15, 6478-6487.	1.7	56
4712	A New Generation of Anticancer Drugs: Mesoporous Materials Modified with Titanocene Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 5588-5597.	1.7	79
4713	Fast Rutheniumâ€Catalysed Allylation of Thiols by Using Allyl Alcohols as Substrates. <i>Chemistry - A European Journal</i> , 2009, 15, 6468-6477.	1.7	51
4714	Origin of the Correlation of the Rate Constant of Substrate Hydroxylation by Nonheme Iron(IV)â€oxo Complexes with the Bondâ€Dissociation Energy of the C-H Bond of the Substrate. <i>Chemistry - A European Journal</i> , 2009, 15, 6651-6662.	1.7	98
4715	Racemization of Alcohols Catalyzed by [RuCl(CO) ₂ (I ⁵ -pentaphenylcyclopentadienyl)]â€Mechanistic Insights from Theoretical Modeling. <i>Chemistry - A European Journal</i> , 2009, 15, 5220-5229.	1.7	36
4716	Intramolecular Spin Alignment within Monoâ€Oxidized and Photoexcited Anthraceneâ€Based $\dot{\pi}$ Radicals as Prototypical Photomagnetic Molecular Devices: Relationships Between Electrochemical, Photophysical, and Photochemical Control Pathways. <i>Chemistry - A European Journal</i> , 2009, 15, 11210-11220.	1.7	20

#	ARTICLE	IF	CITATIONS
4717	Design and Synthesis of Calixarene-Based Bisalkynyl-Bridged Dinuclear Au ^I Isonitrile Complexes as Luminescent Ion Probes by the Modulation of Au...Au Interactions. Chemistry - A European Journal, 2009, 15, 8842-8851.	1.7	77
4718	Dirhodium(II) Compounds with Bridging Thienylphosphines: Studies on Reversible P,C/P,S Coordination. Chemistry - A European Journal, 2009, 15, 7706-7716.	1.7	15
4719	Metal-Catalyzed Cyclization of ¹² C- and ¹³ C-Allenols Derived from D-Glyceraldehyde" Synthesis of Enantiopure Dihydropyrans and Tetrahydrooxepines: An Experimental and Theoretical Study. Chemistry - A European Journal, 2009, 15, 9127-9138.	1.7	47
4720	Enhanced Reactivities of Iron(IV)-Oxo Porphyrin Cation Radicals in Oxygenation Reactions by Electron-Donating Axial Ligands. Chemistry - A European Journal, 2009, 15, 10039-10046.	1.7	110
4721	Gold-Catalyzed Intermolecular Addition of Carbonyl Compounds to 1,6-Enynes: Reactivity, Scope, and Mechanistic Aspects. Chemistry - A European Journal, 2009, 15, 10888-10900.	1.7	53
4722	The Influence of N-Heterocyclic Carbenes (NHC) on the Reactivity of [Ru(NHC) ₄ H] ⁺ With H ₂ , N ₂ , CO and O ₂ . Chemistry - A European Journal, 2009, 15, 10912-10923.	1.7	41
4723	The ³ [<i>n</i> (<i>n</i> +1) <i>p</i>] Emissions of Linear Silver(I) and Gold(I) Chains with Bridging Phosphine Ligands. Chemistry - A European Journal, 2009, 15, 10777-10789.	1.7	73
4724	Cycloaddition Reactions of Butadiene and 1,3-Dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. Chemistry - A European Journal, 2009, 15, 13219-13231.	1.7	92
4725	Theoretical Studies on the Reaction Mechanisms of C ₃ H ₂ (cyclopropenylidene) and O(³ P) Radicals. Chinese Journal of Chemistry, 2009, 27, 49-55.	2.6	1
4726			

#	ARTICLE	IF	CITATIONS
4735	Fluoride-Free Hiyama and Copper-Free Sonogashira Coupling in Air in a Mixed Aqueous Medium by a Series of PEPPSI-Themed Precatalysts. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 1608-1618.	1.0	108
4736	The Role of Amine-B(C ₆ F ₅) ₃ Adducts in the Catalytic Reduction of Imines with H ₂ : A Computational Study. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2229-2237.	1.0	38
4737	Frustation of Orbital Interactions in Lewis Base/Lewis Acid Adducts: A Computational Study of H ₂ Uptake by Phosphanylboranes R ₂ P=BR ₂ . <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2759-2764.	1.0	28
4738	Bis(oxazolinylmethyl) Derivatives of C ₄ H ₄ E Heterocycles (E = NH, O, S) as C ₂ -Chiral Meridionally Coordinating Ligands for Nickel and Chromium. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 4950-4961.	1.0	24
4739	Quantum-chemical treatment of the linoleic acid molecule and two of its conjugated isomers. <i>European Journal of Lipid Science and Technology</i> , 2009, 111, 1035-1041.	1.0	2
4740	Application of the Octacarbonyldicobalt-Catalyzed Carbonylation of Ethyl Diazoacetate for the One-Pot Synthesis of <i>N</i> -tert-Butyl- <i>trans</i> - α -ethoxycarbonyl- β -phenyl- γ -lactam. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1994-2002.	1.2	28
4741	Lessons of 3-Alkoxy-4-(<i>p</i> -chlorophenyl)-1,3-thiazole-2(3 <i>H</i>)-thione Chemistry Learned from Structural Investigations. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 4135-4142.	1.2	8
4742	New Options for the Reactivity of the Burgess Reagent with Epoxides in Both Racemic and Chiral Auxiliary Modes – Structural and Mechanistic Revisions, Computational Studies, and Application to Synthesis. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 2806-2819.	1.2	11
4743	On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C ₆₀ . <i>European Journal of Organic Chemistry</i> , 2009, 2009, 6231-6238.	1.2	16
4744	Implementation of dynamical nucleation theory with quantum potentials. <i>Journal of Computational Chemistry</i> , 2009, 30, 743-749.	1.5	4
4745	Theoretical study of electronic properties of organic photovoltaic materials. <i>Journal of Computational Chemistry</i> , 2009, 30, 1027-1037.	1.5	18
4746	The importance of aromatic-type interactions in serotonin synthesis: Protein-ligand interactions in tryptophan hydroxylase and aromatic amino acid decarboxylase. <i>Journal of Computational Chemistry</i> , 2009, 30, 1111-1115.	1.5	5
4747	Vibrational Raman optical activity of π -conjugated helical systems: Hexahelicene and heterohelicenes. <i>Journal of Computational Chemistry</i> , 2009, 30, 1261-1278.	1.5	34
4748	A multicore QM/MM approach for the geometry optimization of chromophore aggregate in protein. <i>Journal of Computational Chemistry</i> , 2009, 30, 1351-1359.	1.5	10
4749	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of <i>N</i> -formylglycine amide and <i>N</i> -formylalanine amide radical cations. <i>Journal of Computational Chemistry</i> , 2009, 30, 1771-1784.	1.5	8
4750	Conformational analysis of hydroxymatairesinol in aqueous solution with molecular dynamics. <i>Journal of Computational Chemistry</i> , 2009, 30, 2666-2673.	1.5	5
4751	Gas-phase dissociation of 1,4-naphthoquinone derivative anions by electrospray ionization tandem mass spectrometry. <i>Journal of Mass Spectrometry</i> , 2009, 44, 1224-1233.	0.7	21
4752	Molecular complexes between π -excedent heterocycles (indoles and carbazole) and π -deficient polynitrobenzenes. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 917-924.	1.1	5

#	ARTICLE	IF	CITATIONS
4753	Measurement and calculation of the rate constant for the reaction of isopropyl isocyanate with hydroxyl radical. <i>International Journal of Chemical Kinetics</i> , 2009, 41, 187-197.	1.0	4
4754	Rotational disorder in 2- <i>piperidyl</i> -5-nitro- <i>methylpyridine</i> : structural phase transition and its vibrational characteristics. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 323-334.	1.2	2
4756	Hydrogen-Bonding Catalysts Based on Fluorinated Alcohol Derivatives for Living Polymerization. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 5170-5173.	7.2	107
4757	DFT and electrochemical studies on nortriptyline oxidation sites. <i>Journal of Molecular Modeling</i> , 2009, 15, 945-952.	0.8	12
4758	Performance of Becke's half-and-half functional for non-covalent interactions: energetics, geometries and electron densities. <i>Journal of Molecular Modeling</i> , 2009, 15, 1051-1060.	0.8	17
4759	An ab initio quantum mechanical drug designing procedure: application to the design of balanced dual ACE/NEP inhibitors. <i>Journal of Molecular Modeling</i> , 2009, 15, 1447-1462.	0.8	2
4760	Silabenzene through divalent precursors at theoretical levels. <i>Monatshefte für Chemie</i> , 2009, 140, 33-38.	0.9	8
4761	Hindered rotation in N-acyloxy-4-methylthiazole-2(3H)-thiones. <i>Tetrahedron</i> , 2009, 65, 7527-7532.	1.0	4
4762	Broken symmetry approach and density functional theory investigation on hetero-spin system consisting of copper(II) and aminoxyl radicals: Comparison and reliability of different basis sets approaches. <i>Computational and Theoretical Chemistry</i> , 2009, 896, 54-62.	1.5	5
4763	Computational study of the structures and properties of aminonitroethane molecules. <i>Computational and Theoretical Chemistry</i> , 2009, 902, 15-20.	1.5	5
4764	¹³ C and ¹⁹ F NMR chemical shifts of the iron carbene complex (CO) ₄ FeCF ₂ – A case study at DFT level. <i>Computational and Theoretical Chemistry</i> , 2009, 905, 40-43.	1.5	3
4765	Microsolvation of sodium ion in acetonitrile clusters: Structure and energetic trend by first principle study. <i>Computational and Theoretical Chemistry</i> , 2009, 907, 22-28.	1.5	6
4766	Time-dependent closed and open-shell density functional theory from the perspective of partitioning techniques and projections. <i>Computational and Theoretical Chemistry</i> , 2009, 914, 50-59.	1.5	1
4767	A full conformational space analysis of bilirubin. <i>Computational and Theoretical Chemistry</i> , 2009, 911, 24-29.	1.5	8
4768	A detailed theoretical study of the interaction of thiourea with cis-diaqua(ethylenediamine) platinum(II). <i>Computational and Theoretical Chemistry</i> , 2009, 913, 97-106.	1.5	12
4769	A B3LYP study on counterpoise-corrected geometry optimizations for hydrated complexes of [K(H ₂ O) _n] ⁺ and [Na(H ₂ O) _n] ⁺ . <i>Computational and Theoretical Chemistry</i> , 2009, 915, 160-169.	1.5	9
4770	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. <i>Chemical Physics</i> , 2009, 358, 245-257.	0.9	73
4771	Theoretical calculation of pK _a s of phosphoric (V) acid in the polarisable continuum and cluster-continuum models. <i>Journal of Molecular Structure</i> , 2009, 924-926, 170-174.	1.8	15

#	ARTICLE	IF	CITATIONS
4772	Planarity of triphenylamine moieties of a typical hole-transport material for OLEDs, N,N'-diphenyl-N,N'-di(m-tolyl)benzidine (TPD), in the amorphous state. <i>Journal of Molecular Structure</i> , 2009, 927, 82-87.	1.8	7
4773	Perspectives in designing anti aggregation agents as Alzheimer disease drugs. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 3866-3873.	2.6	10
4774	Survey on ionic liquids effect based on metal anions over the thermal stability of heavy oil. <i>Journal of Thermal Analysis and Calorimetry</i> , 2009, 95, 173-179.	2.0	11
4775	Coordination of 2-phosphorylalkyl-substituted 1,8-naphthyridines in complexes with lanthanide nitrates. <i>Russian Chemical Bulletin</i> , 2009, 58, 1416-1422.	0.4	5
4776	A computational study of the endohedral fullerene GeH ₄ @C ₆₀ . <i>Structural Chemistry</i> , 2009, 20, 789-794.	1.0	10
4777	Synthesis, spectroscopic characterization, X-ray structure and DFT calculations of [ReOCl ₂ (8-Sqn)(OPPh ₃)]. <i>Structural Chemistry</i> , 2009, 20, 911-918.	1.0	1
4778	Molecular structure and reactivity of antituberculosis drug molecules isoniazid, pyrazinamide, and 2-methylheptylisonicotinate: a density functional approach. <i>Structural Chemistry</i> , 2009, 20, 1079-1085.	1.0	78
4779	The Role of Bridging Group of Cyclopentadienyl Ligands for the Ziegler-Natta Catalysis: Theoretical Study. <i>Topics in Catalysis</i> , 2009, 52, 772-778.	1.3	3
4780	Molecular structures and thermochemistry of the derivatives of C ₂₄ fullerene by attaching a variety of chemical groups. <i>Journal of Structural Chemistry</i> , 2009, 50, 1046-1052.	0.3	3
4781	A multi-reference coupled-cluster study on the potential energy surface of N ₂ including ground and excited states: spin projections and wavefunction overlaps. <i>Theoretical Chemistry Accounts</i> , 2009, 122, 197-206.	0.5	12
4782	DNA bindings of a novel anticancer drug, trans-[PtCl ₂ (isopropylamine)(3-picoline)], and kinetic competition of purine bases with protein residues in the bifunctional substitutions: a theoretical DFT study. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 455-468.	0.5	10
4783	A theoretical study of diborenes HLB=BLH for L=CO, NH ₃ , OH ₂ , PH ₃ , SH ₂ , ClH: structures, energies, and spin-spin coupling constants. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 187-195.	0.5	10
4784	On the origin of the catalytic power of carboxypeptidase A and other metalloenzymes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 536-550.	1.5	17
4785	What governs nitrogen configuration in substituted aminophosphines?. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 101-109.	0.9	8
4786	What can the geometry tell about the charge distribution in the mesoionic heterocycles? A DFT study on the SCN ⁻ R ²⁺ system. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 67-74.	0.9	1
4787	Synthesis of N-alkoxybenzimidoyl azides and their reactions in electrophilic media. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 227-237.	0.9	6
4788	Models for the enzymatically active state of cytochrome p-450. <i>International Journal of Quantum Chemistry</i> , 1977, 12, 225-244.	1.0	0
4789	Ab initio valence bond calculations. IX. Ionization potentials of ethylene, allyl radical, trans-, and cis-butadiene. <i>International Journal of Quantum Chemistry</i> , 2009, 14, 131-141.	1.0	0

#	ARTICLE	IF	CITATIONS
4790	Effective core potential calculations for some hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 1978, 14, 323-328.	1.0	0
4791	Ab initio study of catalyzed and uncatalyzed amide bond formation as a model for peptide bond formation: Ammonia-formic acid and ammonia-glycine reactions. <i>International Journal of Quantum Chemistry</i> , 1982, 22, 223-245.	1.0	2
4792	Ab Initio calculations relevant to the mechanism of chemical carcinogenesis II: The nitrous acidium ion-a powerful nitrosating agent. <i>International Journal of Quantum Chemistry</i> , 2009, 28, 263-279.	1.0	0
4793	Theoretical studies of the interaction of H ₂ O with small clusters of beryllium atoms. <i>International Journal of Quantum Chemistry</i> , 1985, 28, 613-628.	1.0	0
4794	A theoretical study of alanine dipeptide and analogs. <i>International Journal of Quantum Chemistry</i> , 1989, 36, 311-322.	1.0	7
4795	Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 160-170.	1.0	2
4796	A theoretical and experimental study on manipulating the structure and properties of carbon nanotubes using substitutional dopants. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 97-118.	1.0	70
4797	Delocalization in valence bond Hyperconjugation. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2426-2429.	1.0	6
4798	Efficient parallel algorithm of second-order Møller-Plesset perturbation theory with resolution of identity approximation (RI-MP2). <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2121-2130.	1.0	66
4799	Quantitative approach to the understanding of catalytic effect of metal oxides on the desorption reaction of MgH ₂ . <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2793-2800.	1.0	10
4800	Mechanism of hydrogen activation by frustrated Lewis pairs: A molecular orbital approach. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2416-2425.	1.0	124
4801	Electronic temperature in divide-and-conquer electronic structure calculation revisited: Assessment and improvement of self-consistent field convergence. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2706-2713.	1.0	31
4802	Optimal even-tempered gaussian atomic orbital bases: First-row atoms. <i>International Journal of Quantum Chemistry</i> , 1975, 9, 289-295.	1.0	22
4803	Multiphysics Coupling Simulation of Silicon Nitride CVD Using an RLSA Source. <i>Plasma Processes and Polymers</i> , 2009, 6, S776.	1.6	4
4804	Methyl β -D-galactopyranoside [methyl β -D-galactopyranosyl-(1 \rightarrow 6)- β -D-glucopyranoside] monohydrate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2009, 65, o601-o606.	0.4	0
4805	electronic Ligand Builder and Optimization Workbench (eLBOW): a tool for ligand coordinate and restraint generation. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 1074-1080.	2.5	1,035
4806	Quantum mechanical calculation of aqueous uranium complexes: carbonate, phosphate, organic and biomolecular species. <i>Chemistry Central Journal</i> , 2009, 3, 10.	2.6	64
4807	Amination of aryl chlorides and fluorides toward the synthesis of aromatic amines by palladium-catalyzed route or transition metal free way: Scopes and limitations. <i>Journal of Molecular Catalysis A</i> , 2009, 303, 15-22.	4.8	18

#	ARTICLE	IF	CITATIONS
4808	Rhodamine 6G interaction with solvents studied by vibrational spectroscopy and density functional theory. <i>Journal of Molecular Structure</i> , 2009, 931, 10-19.	1.8	35
4809	Highly efficient, orange-red organic light-emitting diodes using a series of green-emission iridium complexes as hosts. <i>Organic Electronics</i> , 2009, 10, 247-255.	1.4	41
4810	Theoretical investigation of the structure and nature of the interaction in metal-alkane η^2 -complexes of the type $[M(CO)_5(C_2H_6)]$ (M = Cr, Mo, and W). <i>Chemical Physics</i> , 2009, 365, 85-93.	0.9	12
4811	Reactions of triphenylphosphane-substituted ethoxycarbonylcarbene-bridged dicobalt carbonyl complexes with carbon monoxide or ^{13}CO : An experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2009, 362, 1333-1342.	1.2	12
4812	η^4 - and η^2 coordination of A_2H_2 (A=C, Si, Ge, Sn and Pb) ligands with transition metals. <i>Inorganica Chimica Acta</i> , 2009, 362, 2172-2176.	1.2	5
4813	Theoretical studies of the magnetic couplings and the chemical indices of the biomimetic models of oxyhemocyanin and oxytyrosinase. <i>Inorganica Chimica Acta</i> , 2009, 362, 4578-4584.	1.2	15
4814	Photocyclization of 2,4,6-triethylbenzophenones in the solid state. <i>Tetrahedron</i> , 2009, 65, 677-689.	1.0	23
4815	Electron affinities of a homologous series of tertiary alkyl radicals and their C-H bond dissociation energies (BDEs). <i>Tetrahedron</i> , 2009, 65, 1655-1659.	1.0	2
4816	Efficient preparation of N^2, N^3 -1H-isoindole-1,3-diyldenedicarbohydrazides via 1,1,3-trichloro-1H-isoindole, and their characterization. <i>Tetrahedron</i> , 2009, 65, 6218-6225.	1.0	10
4817	Thermodynamic and kinetic factors in the aza-Cope rearrangement of a series of iminium cations. <i>Tetrahedron</i> , 2009, 65, 10311-10316.	1.0	11
4818	$Co_2(CO)_8$ -induced domino reactions of ethyl diazoacetate, carbon monoxide and ferrocenylimines leading to 2-(1-ferrocenyl-methylidene)-malonic acid derivatives. <i>Tetrahedron Letters</i> , 2009, 50, 4727-4730.	0.7	16
4819	Linear fully conjugated meso-aryl pentapyrrins. <i>Tetrahedron Letters</i> , 2009, 50, 6909-6912.	0.7	8
4820	The oxyheme complexes of P450cam: A QM/MM study. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 90-96.	1.5	23
4821	The smallest borazine-fused cyclacenes: Novel C-H conformations in cyclo-BN-anthracene and cyclo-BN-tetracene from Hartree-Fock and density functional calculations. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 9-16.	1.5	7
4822	On electronic structure of tris(dimethylamino)sulphonium heptafluoro-oxocyclo-tetraphosphazenate. <i>Computational and Theoretical Chemistry</i> , 2009, 894, 32-35.	1.5	4
4823	Rhombohedral graphite: Comparative study of the electronic properties. <i>Computational and Theoretical Chemistry</i> , 2009, 897, 118-128.	1.5	11
4824	Single or double hydrogen atom transfer in the reaction of metal-associated phenolic acids with $\dot{C}OH$ radical: DFT study. <i>Computational and Theoretical Chemistry</i> , 2009, 901, 49-55.	1.5	17
4825	Ab initio study of the reactions: Ethylene $\dot{C}H$ +vinyl, propylene $\dot{C}H$ +methyl+vinyl, and propylene $\dot{C}H$ +propen-2-yl. <i>Computational and Theoretical Chemistry</i> , 2009, 904, 43-48.	1.5	0

#	ARTICLE	IF	CITATIONS
4826	Uncharged analogues of the phenalenyl cation: Hartree-Fock, Møller-Plesset, and density functional computational investigations of the isomers of boraphenalene. <i>Computational and Theoretical Chemistry</i> , 2009, 904, 49-56.	1.5	12
4827	Ab initio studies of BN-acenes and cyclo BN-acenes electronic properties and their dependence on the molecular size and the number of electrons. <i>Computational and Theoretical Chemistry</i> , 2009, 905, 1-7.	1.5	2
4828	The structure, electronic property and infrared spectroscopy of the endohedral fullerene SnH ₄ @C ₆₀ . <i>Computational and Theoretical Chemistry</i> , 2009, 906, 41-45.	1.5	12
4829	Structure, electronic and vibrational spectra and aromaticity of hemiporphyrine and its hydrates: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2009, 906, 56-62.	1.5	14
4830	Linear regression analysis of molecular energy properties for poly heterocyclic compounds. <i>Computational and Theoretical Chemistry</i> , 2009, 906, 35-40.	1.5	1
4831	Helix formation in $\hat{\mu}$ -amino acid oligomers. <i>Computational and Theoretical Chemistry</i> , 2009, 907, 109-114.	1.5	9
4832	First-principles studies of internal rotation in protonated trans-N-benzylideneaniline. <i>Computational and Theoretical Chemistry</i> , 2009, 908, 122-124.	1.5	4
4833	An ab initio study of 5,6-disubstituted 1,3-cyclohexadienes. <i>Computational and Theoretical Chemistry</i> , 2009, 909, 66-74.	1.5	4
4834	Comparative study on metal-encapsulated TM@C ₂₄ and TM@C ₂₄ H ₁₂ (TM=Ti, Zr and Hf). <i>Computational and Theoretical Chemistry</i> , 2009, 913, 265-269.	1.5	15
4835	A screened hybrid density functional study on energetic complexes: Alkaline-earth metal carbonyl perchlorates. <i>Computational and Theoretical Chemistry</i> , 2009, 915, 43-46.	1.5	5
4836	Highly nitrated cyclopropanes as new high energy materials: DFT calculations on the properties of C ₃ H ₆ n(NO ₂) _n (n=3-6). <i>Computational and Theoretical Chemistry</i> , 2009, 916, 33-36.	1.5	9
4837	Theoretical calculations of the substituent effect on molecular properties of the RCN \cdot HF hydrogen-bonded complexes with R=NH ₂ , CH ₃ O, CH ₃ , OH, SH, H, Cl, F, CF ₃ , CN and NO ₂ . <i>Vibrational Spectroscopy</i> , 2009, 49, 133-141.	1.2	3
4838	Molecular simulation studies on chemical reactivity of methylcyclopentadiene. <i>Journal of Hazardous Materials</i> , 2009, 165, 141-147.	6.5	14
4839	Theoretical studies of stereoselectivities in the direct organocatalytic Mannich reactions involving ketimine. <i>Journal of Molecular Catalysis A</i> , 2009, 303, 1-8.	4.8	11
4840	Theoretical study of the interactions of $\hat{\beta}$ -cyclodextrin with 2-hydroxy-5-methoxyacetophenone and two of its isomers. <i>Journal of Molecular Liquids</i> , 2009, 146, 15-22.	2.3	26
4841	Additivity of ring geometry distortion effects in unsaturated five-membered heterocyclic rings. <i>Journal of Molecular Structure</i> , 2009, 922, 103-108.	1.8	7
4842	Experimental and computational studies of the macrocyclic effect of an auxiliary ligand on electron and proton transfers within ternary copper(II)-Histidine complexes. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 972-984.	1.2	6
4843	Kinetics for tautomerizations and dissociations of triglycine radical cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 996-1005.	1.2	25

#	ARTICLE	IF	CITATIONS
4844	Opto-electronic properties of adamantane and hydrogen-terminated sila- and germa-adamantane: A comparative study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2009, 41, 1151-1156.	1.3	30
4845	A new χ -acidity scale for several N-donor heterocycles as ligands in neutral gold(III) complexes. <i>Polyhedron</i> , 2009, 28, 1079-1084.	1.0	10
4846	Synthesis, spectroscopic characterization, X-ray structure and DFT calculations of $[\text{Re}(\text{CO})_3\text{L}_2\text{Cl}]$ (L=1,2,4-triazolo-[1,5-a]pyrimidine). <i>Polyhedron</i> , 2009, 28, 2571-2578.	1.0	10
4847	Novel rhenium(III) complexes with the picolinate ligand: Synthesis, spectroscopic investigations, X-ray structures and DFT calculations for $[\text{ReX}_2(\text{pic})(\text{PPh}_3)_2]$ complexes. <i>Polyhedron</i> , 2009, 28, 2377-2384.	1.0	8
4848	Coordination chemistry of di-2-pyridylketone. Synthesis, spectroscopic investigations, X-ray studies and DFT calculations of Re(III) and Re(V) complexes. <i>Polyhedron</i> , 2009, 28, 2821-2830.	1.0	8
4849	Reactivity of $[\text{ReOX}_3(\text{PPh}_3)_2]$ and $[\text{ReOX}_3(\text{AsPh}_3)_2]$ towards 2-(2-hydroxyphenyl)-1H-benzimidazole: Synthesis, X-ray studies, spectroscopic characterization and DFT calculations for $[\text{ReOX}_2(\text{hpb})(\text{EPh}_3)]$ and $[\text{ReO}(\text{OMe})(\text{hpb})_2] \cdot \text{MeCN}$. <i>Polyhedron</i> , 2009, 28, 2949-2964.	1.0	23
4850	Mono- and di-nuclear oxorhenium(V) complexes of 4,7-diphenyl-1,10-phenanthroline. <i>Polyhedron</i> , 2009, 28, 3999-4009.	1.0	6
4851	Molecular dynamics simulation of mixed matrix nanocomposites containing polyimide and polyhedral oligomeric silsesquioxane (POSS). <i>Polymer</i> , 2009, 50, 1324-1332.	1.8	65
4852	Anticancer drugs based on alkenyl and boryl substituted titanocene complexes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 1981-1987.	0.8	23
4853	Design of nickel chelates of tetradentate N-heterocyclic carbenes with subdued cytotoxicity. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 2328-2335.	0.8	54
4854	Theoretical studies on the role of bridging group of CGC type ligands for the Ziegler-Natta catalysis. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3276-3280.	0.8	2
4855	Copper-free and amine-free Sonogashira coupling in air in a mixed aqueous medium by palladium complexes of N/O-functionalized N-heterocyclic carbenes. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3477-3486.	0.8	67
4856	Synthesis, ring transformations, IR-, NMR and DFT study of heterocycles with two ferrocenyl units. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 3732-3741.	0.8	20
4857	Aminosilylene-bridged ansa-zirconocenes for branched polyethylenes with bimodal molecular weight distributions. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 4216-4222.	0.8	7
4858	Palladium complexes of amido-functionalized N-heterocyclic carbenes as effective precatalysts for the Suzuki-Miyaura C-C cross-coupling reactions of aryl bromides and iodides. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 4162-4169.	0.8	40
4859	Theoretical study of different speciation of mercury adsorption on CaO (0 0 1) surface. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 2693-2699.	2.4	55
4860	DFT study of structural, electronic, and spectroscopic properties of D6d endohedral fullerenes: $\text{X}@\text{C}_{24}\text{H}_{12}$ (X=Li+, Na+, K+). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 73, 67-71.	2.0	17
4861	DFT calculations on the structural stability and infrared spectroscopy of endohedral metallofullerenes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 74, 553-557.	2.0	13

#	ARTICLE	IF	CITATIONS
4862	Cyanometalate-bridged oligonuclear transition metal complexes—Possibilities for a rational design of SMMs. <i>Coordination Chemistry Reviews</i> , 2009, 253, 2306-2314.	9.5	104
4863	Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings. <i>Chemical Physics</i> , 2009, 356, 147-152.	0.9	106
4864	Evaluation of core and core—valence correlation contributions using the incremental scheme. <i>Chemical Physics</i> , 2009, 356, 47-53.	0.9	20
4865	Photoexcitation of 11-Z-cis-7,8-dihydro retinal and 11-Z-cis retinal: A comparative computational study. <i>Chemical Physics Letters</i> , 2009, 469, 224-228.	1.2	20
4866	The inelastic neutron scattering spectrum of nicotinic acid and its assignment by solid-state density functional theory. <i>Chemical Physics Letters</i> , 2009, 473, 81-87.	1.2	14
4867	Using the Source Function descriptor to dampen the multipole model bias in charge density studies from X-ray structure factors refinements. <i>Chemical Physics Letters</i> , 2009, 476, 308-316.	1.2	25
4868	Charge-resonance excitations in symmetric molecules — Comparison of linear response DFT with CC3 for the excited states of a model dimer. <i>Chemical Physics Letters</i> , 2009, 478, 127-131.	1.2	11
4869	Terahertz absorption spectrum of triacetone triperoxide (TATP). <i>Chemical Physics Letters</i> , 2009, 478, 172-174.	1.2	30
4870	A theoretical study of the kinetics of OH radical addition to halogen substituted propenes. <i>Chemical Physics Letters</i> , 2009, 481, 29-33.	1.2	14
4871	Classification of Raman active modes of platinum(II) acetylides: A combined experimental and theoretical study. <i>Chemical Physics Letters</i> , 2009, 481, 209-213.	1.2	9
4872	Mechanistic aspects of benzothiazepines: A class of antiarrhythmic drugs. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 1-6.	2.6	12
4873	Large ring 1,3-bridged 2-azetidinones: Experimental and theoretical studies. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 2071-2080.	2.6	20
4874	Nucleophilic addition of water to 1-isoquinolinyl phenyl ketone. The synthesis, spectroscopic investigation, crystal and molecular structure and DFT calculations of [ReOBr ₂ (iquinpk-OH)(PPh ₃)]. <i>Inorganic Chemistry Communication</i> , 2009, 12, 789-792.	1.8	4
4875	Synthesis and characterization of a homoleptic titanium dihydrobis(pyrazol-1-yl)borate complex. <i>Inorganic Chemistry Communication</i> , 2009, 12, 1001-1003.	1.8	3
4876	Glucose-based spiro-isoxazolines: A new family of potent glycogen phosphorylase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 7368-7380.	1.4	59
4877	Spin-Hamiltonian Parameters from First Principle Calculations: Theory and Application. <i>Biological Magnetic Resonance</i> , 2009, , 175-229.	0.4	21
4878	Nitroxyl Radical Plus Hydroxylamine Pseudo Self-Exchange Reactions: Tunneling in Hydrogen Atom Transfer. <i>Journal of the American Chemical Society</i> , 2009, 131, 11985-11997.	6.6	81
4879	Diels—Alder Reaction between Cyclopentadiene and C ₆₀ : An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9721-9726.	1.1	63

#	ARTICLE	IF	CITATIONS
4880	Water and Alanine: From Puddles(32) to Ponds(49). <i>Journal of Physical Chemistry B</i> , 2009, 113, 14413-14420.	1.2	31
4881	Systematic Fragmentation Method and the Effective Fragment Potential: An Efficient Method for Capturing Molecular Energies. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10040-10049.	1.1	65
4882	Accurate Methods for Large Molecular Systems. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9646-9663.	1.2	188
4883	Alanine: Then There Was Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 8657-8669.	1.2	59
4884	Water~Benzene Interactions: An Effective Fragment Potential and Correlated Quantum Chemistry Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2092-2102.	1.1	96
4885	Oxidation Unzipping of Stable Nanographenes into Joint Spin-Rich Fragments. <i>Journal of the American Chemical Society</i> , 2009, 131, 9663-9669.	6.6	46
4886	The empirical valence bond as an effective strategy for computer~aided enzyme design. <i>Biotechnology Journal</i> , 2009, 4, 495-500.	1.8	11
4887	The Role of Water in Platinum~Catalyzed Cycloisomerization of 1,6~Enynes: A Combined Experimental and Theoretical Gas Phase Study. <i>ChemCatChem</i> , 2009, 1, 138-143.	1.8	33
4888	Computation of accurate excitation energies for large organic molecules with double-hybrid density functionals. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4611.	1.3	252
4889	Calculation of Exchange Coupling Constants of Transition Metal Complexes with DFT. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6751-6755.	1.1	80
4890	Tautomeric forms study of 1H-(2~pyridyl)-3-methyl-5-hydroxypyrazole and 1H-(2~pyridyl)-3-phenyl-5-hydroxypyrazole. Synthesis, structure, and cytotoxic activity of their complexes with palladium(II) ions. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009, 24, 1257-1268.	2.5	11
4891	Diels~Alder Exo Selectivity in Terminal-Substituted Dienes and Dienophiles: Experimental Discoveries and Computational Explanations. <i>Journal of the American Chemical Society</i> , 2009, 131, 1947-1957.	6.6	103
4892	Effect of Porphyrin Ligands on the Regioselective Dehydrogenation versus Epoxidation of Olefins by Oxoiron(IV) Mimics of Cytochrome P450. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11713-11722.	1.1	78
4893	Conductance of a conjugated molecule with carbon nanotube contacts. <i>Physical Review B</i> , 2009, 80, .	1.1	20
4894	Intramolecular MLOH/~ and MLNH/~ interactions in crystal structures of metal complexes. <i>Chemical Papers</i> , 2009, 63, .	1.0	6
4895	Electronic structure of products of interaction between Fe3O4 cluster and water and its association with the corrosion behavior of magnetite. <i>Russian Journal of Electrochemistry</i> , 2009, 45, 941-945.	0.3	1
4896	Hydrolysis of 8-Quinoyl Phosphate Monoester: Kinetic and Theoretical Studies of the Effect of Lanthanide Ions. <i>Journal of Organic Chemistry</i> , 2009, 74, 1042-1053.	1.7	14
4897	Time-Dependent Density Functional Theory Study of the Electronic Excitation Spectra of Chlorophyllide a and Pheophorbide a in Solvents. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4817-4825.	1.2	29

#	ARTICLE	IF	CITATIONS
4898	Why Is the Suzuki-Miyaura Cross-Coupling of sp^3 Carbons in β -Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. <i>Journal of Organic Chemistry</i> , 2009, 74, 4049-4054.	1.7	54
4899	Fully Automated Incremental Evaluation of MP2 and CCSD(T) Energies: Application to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 287-294.	2.3	109
4900	Proton-Regulated Electron Transfers from Tyrosine to Tryptophan in Proteins: Through-Bond Mechanism versus Long-Range Hopping Mechanism. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16681-16688.	1.2	23
4901	Gosteli's Claisen Rearrangement: DFT Study of Substituent Rate Effects. <i>Journal of Organic Chemistry</i> , 2009, 74, 4336-4342.	1.7	30
4902	Comparison of the Blue-Shifted $C-D$ Stretching Vibrations for DMSO- d_6 in Imidazolium-Based Room Temperature Ionic Liquids and in Water. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5978-5984.	1.2	71
4903	Accommodation of an N -(Deoxyguanosin-8-yl)-2-acetylaminofluorene Adduct in the Active Site of Human DNA Polymerase β : Hoogsteen or Watson-Crick Base Pairing?. <i>Biochemistry</i> , 2009, 48, 7-18.	1.2	20
4904	On the Organizing Role of Water Molecules in the Assembly of Boronic Acids and 4,4'-Bipyridine: 1D, 2D and 3D Hydrogen-Bonded Architectures Containing Cyclophane-Type Motifs. <i>Crystal Growth and Design</i> , 2009, 9, 1575-1583.	1.4	66
4905	Thermodynamic Functions of Molecular Conformations of (2-Fluoro-2-phenyl-1-ethyl)ammonium Ion and (2-Hydroxy-2-phenyl-1-ethyl)ammonium Ion as Models for Protonated Noradrenaline and Adrenaline: First-Principles Computational Study of Conformations and Thermodynamic Functions for the Noradrenaline and Adrenaline Models. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2507-2515.	1.1	2
4906	Platinum(II)-Complexed Tetrahydroimidazo[1,2-b][1,2,4]oxadiazoles Derived from Metal-Mediated 1,3-Dipolar Cycloaddition. Novel Type of Heterocycles, Which Do Not Exist without the Metal Center. <i>Organometallics</i> , 2009, 28, 1406-1413.	1.1	34
4907	Mono- and Bis- Methyltrioxorhenium(VII) Complexes with Salen Ligands: Synthesis, Properties, Applications. <i>Inorganic Chemistry</i> , 2009, 48, 6812-6822.	1.9	22
4908	How to Stabilize σ -Silapropargyl/Alkynylsilyl Complex of $[CpL_2M]_2$ ($L = CO, PMe_3$, or PF_3 and $M = Ti, Zr, Hf, Nb, Ta, Mo, W, Re, Os, Ir, Pt, Au, Ag, Cu, Ni, Pd, Rh, Ru, Rh, Ir, Pt, Au, Ag, Cu, Ni, Pd, Rh, Ru$) Overl	1.1	25
4909	Computational Study of $C-C$ Coupling on Diruthenium Bis(η^4 -vinyl) Ethylene π -Complex. <i>Organometallics</i> , 2009, 28, 3029-3039.	1.1	7
4910	The Binding of Ag and Au to Ethene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7474-7481.	1.1	28
4911	Palladium $N(CH_2CH_2)_2P(CH_2CH_2)_2$ -Dialkylamides: Synthesis, Structural Characterization, and Reactivity. <i>Inorganic Chemistry</i> , 2009, 48, 3699-3709.	1.9	31
4912	Characterizing Complexes with $F-Li-N$, $H-Li-N$, and CH_3Li-N Lithium Bonds: Structures, Binding Energies, and Spin-Spin Coupling Constants. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10327-10334.	1.1	18
4913	Ruthenium Acetylide Complexes Supported by Trithiacyclononane and Aromatic Diimine: Structural, Spectroscopic, and Theoretical Studies. <i>Organometallics</i> , 2009, 28, 5656-5660.	1.1	19
4914	51V NMR Chemical Shifts Calculated from QM/MM Models of Peroxo Forms of Vanadium Haloperoxidases. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4456-4465.	1.2	52
4915	Structure and Magnetic Interactions in the Organic-Based Ferromagnet Decamethylferrocenium Tetracyanoethenide, $[FeCp^*_2]^{+}[TCNE]^{-}$. <i>Inorganic Chemistry</i> , 2009, 48, 3296-3307.	1.9	34

#	ARTICLE	IF	CITATIONS
4916	Computational and synthetic studies on the cyclometallation reaction of dimethylbenzylamine with [IrCl ₂ Cp*] ₂ : role of the chelating base. Dalton Transactions, 2009, , 5887.	1.6	91
4917	Is Thorium a d Transition Metal or an Actinide? An Answer from a DFT Study of the Reaction between Pyridine <i>N</i> -Oxide and Cp ₂ M(CH ₃) ₂ with M = Zr, Th, and U. Organometallics, 2009, 28, 672-679.	1.1	64
4918	Hybrid-DFT Study on Electronic Structures of the Active Site of Sweet Potato Purple Acid Phosphatase: The Origin of Stronger Antiferromagnetic Couplings than Other Purple Acid Phosphatases. Journal of Physical Chemistry A, 2009, 113, 5099-5104.	1.1	8
4919	Gas-Phase Reactivity of Protonated 2-, 3-, and 4-Dehydropyridine Radicals Toward Organic Reagents. Journal of Physical Chemistry A, 2009, 113, 13663-13674.	1.1	22
4920	Crystal Structure and Conformational Analysis of 4-[(<i>p</i> -N,N-Dimethylamino)benzylidene]-2-(3,5-dinitrophenyl)oxazole-5-one. Spectroscopy Letters, 2009, 42, 1-6.	0.5	5
4921	Stereoselective Formation of Helical Binuclear Metal Complexes: Synthesis, Characterization, and Crystal Structures of Chiral Bis-Rhenium(I) Quaterpyridine Complexes. Inorganic Chemistry, 2009, 48, 4108-4117.	1.9	21
4922	Concerning the Reaction Pathway of the Metathesis Reaction involving WW and CN Triple Bonds: A Theoretical Study. Inorganic Chemistry, 2009, 48, 10358-10363.	1.9	4
4923	Dichlorocarbene Addition to C ₆₀ from the Trichloromethyl Anion: Carbene Mechanism or Bingel Mechanism?. Journal of Physical Chemistry A, 2009, 113, 3673-3676.	1.1	24
4924	Effects of Terminal Functional Groups on the Stability of the Polyproline II Structure: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2009, 131, 15474-15482.	6.6	122
4925	Ruthenium(II) Isocyanide Complexes Supported by Triazacyclononane/Trithiacyclononane and Aromatic Diimine: Structural, Spectroscopic, and Theoretical Studies. Organometallics, 2009, 28, 3537-3545.	1.1	26
4926	Bond Activations of PhSiH ₃ by Cp ₂ SmH: A Mechanistic Investigation by the DFT Method. Organometallics, 2009, 28, 3767-3775.	1.1	32
4927	Rationalizing the Reactivity of Frustrated Lewis Pairs: Thermodynamics of H ₂ Activation and the Role of Acid-Base Properties. Journal of the American Chemical Society, 2009, 131, 10701-10710.	6.6	303
4928	On the Mechanism of B(C ₆ F ₅) ₃ -Catalyzed Direct Hydrogenation of Imines: Inherent and Thermally Induced Frustration. Journal of the American Chemical Society, 2009, 131, 2029-2036.	6.6	247
4929	Imidazole-Containing (N ₃ S)-Ni ^{II} Complexes Relating to Nickel Containing Biomolecules. Inorganic Chemistry, 2009, 48, 7280-7293.	1.9	44
4930	Rare [(NHC) ₂ Ni-OH]-Type Terminal Nickel Hydroxo and [(NHC) ₂ Ni]-Type Complexes of <i>N</i> / <i>O</i> -Functionalized N-Heterocyclic Carbenes as Precatalysts for Highly Desirable Base-Free Michael Reactions in Air at Ambient Temperature. Organometallics, 2009, 28, 2267-2275.	1.1	80
4931	Primary Phosphines Studied by Gas-Phase Electron Diffraction and Quantum Chemical Calculations. Are They Different from Amines?. Inorganic Chemistry, 2009, 48, 8603-8612.	1.9	19
4932	QM/MM Study of the Second Proton Transfer in the Catalytic Cycle of the D251N Mutant of Cytochrome P450cam. Journal of Physical Chemistry B, 2009, 113, 9577-9588.	1.2	15
4933	Quantum Tunneling in Testosterone 6 β -Hydroxylation by Cytochrome P450: Reaction Dynamics Calculations Employing Multiconfiguration Molecular-Mechanical Potential Energy Surfaces. Journal of Physical Chemistry A, 2009, 113, 11501-11508.	1.1	13

#	ARTICLE	IF	CITATIONS
4934	Rapid, Selective Ru-Sulfonate-Catalyzed Allylation of Indoles Using Alcohols as Substrates. <i>Organometallics</i> , 2009, 28, 3437-3448.	1.1	32
4935	Chemical Bonding in the N ₂ Molecule and the Role of the Quantum Mechanical Interference Effect. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12541-12548.	1.1	23
4936	Asymmetric Allylboration Reactions with Soderquist's Chiral 10-Substituted-9-borabicyclo[3.3.2]decanes: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2009, 74, 3562-3565.	1.7	9
4937	Theoretical Study on the Reaction Mechanism for the Formation of 2-Methylpyridine Cobalt(I) Complex from Cobaltacyclopentadiene and Acetonitrile. <i>Organometallics</i> , 2009, 28, 3636-3649.	1.1	46
4938	Role of Dimethyl Sulfoxide in the Hydrolytic Peeling of Boron Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15565-15568.	1.5	8
4939	Mechanistic Aspects of the Formation of Guanidinohydantoin from Spiroiminodihydantoin under Acidic Conditions. <i>Chemical Research in Toxicology</i> , 2009, 22, 526-535.	1.7	27
4940	Study of the Mechanism of the N ⁺ CO Photodissociation in N,N-Dimethylformamide by Direct Trajectory Surface Hopping Simulations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12582-12590.	1.1	19
4941	Reactions of Titanium Hydrazinediido Complexes with Unsaturated Organic Substrates. <i>Organometallics</i> , 2009, 28, 4747-4757.	1.1	27
4942	Synthesis and Reactivity of Titanium and Zirconium Complexes Supported by a Multidentate Monoanionic [N ₂ P ₂] Ligand. <i>Organometallics</i> , 2009, 28, 3338-3349.	1.1	27
4943	Missing Metallofullerene with C ₈₀ Cage. <i>Journal of the American Chemical Society</i> , 2009, 131, 10950-10954.	6.6	95
4944	DFT and In-Situ Spectroelectrochemical Study of the Adsorption of Fluoroacetate Anions at Gold Electrodes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 989-1000.	1.5	26
4945	How is the Reactivity of Cytochrome P450cam Affected by Thr252X Mutation? A QM/MM Study for X = Serine, Valine, Alanine, Glycine. <i>Journal of the American Chemical Society</i> , 2009, 131, 4755-4763.	6.6	53
4946	Excited States and Photochemistry of Bicyclo[1.1.0]butane. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1686-1695.	1.1	7
4947	What Makes the Huge ³¹ P- ³¹ P Coupling Constants in S(PF ₂) ₂ and Se(PF ₂) ₂ Vary So Much with Temperature?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 938-942.	1.1	2
4948	Influence of Guest-Host Interactions on the Structural, Energetic, and Mössbauer Spectroscopy Properties of Iron(II)tris(2,2'-bipyridine) in the Low-Spin and High-Spin States: A Density-Functional Theory Study of the Zeolite-Y Embedded Complex. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 97-115.	2.3	23
4949	A Single Reference Perturbation Theory beyond the Møller-Plesset Partition. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 931-936.	2.3	16
4950	The Isomerization Barrier in Cyanocyclobutadienes: An ab Initio Multireference Average Quadratic Coupled Cluster Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8351-8358.	1.1	11
4951	High- and Low-Temperature Modifications of Sc ₃ RuC ₄ and Sc ₃ OsC ₄ : Relativistic Effects, Structure, and Chemical Bonding. <i>Inorganic Chemistry</i> , 2009, 48, 6436-6451.	1.9	31

#	ARTICLE	IF	CITATIONS
4952	Monocationic Trihydride and Dicationic Dihydrider ² Dihydrogen and Bis(dihydrogen) Osmium Complexes Containing Cyclic and Acyclic Triamine Ligands: Influence of the N ⁺ O ⁺ N Angles on the Hydrogen ⁺ Hydrogen Interactions. <i>Inorganic Chemistry</i> , 2009, 48, 2677-2686.	1.9	17
4953	Abundant Dipositively Charged Protonated a ₂ and a ₃ Ions from Diproline and Triproline. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4963-4969.	1.2	5
4954	Mechanism of Helix Induction in Poly(4-carboxyphenyl isocyanide) with Chiral Amines and Memory of the Macromolecular Helicity and Its Helical Structures. <i>Journal of the American Chemical Society</i> , 2009, 131, 10719-10732.	6.6	104
4955	Behavior of P ⁺ Pt and P ⁺ Pd Bonds in Phosphido Complexes toward Electrophilic Fragments. <i>Inorganic Chemistry</i> , 2009, 48, 7679-7690.	1.9	23
4956	Excitation and Emission Properties of Platinum(II) Acetylides at High and Low Concentrations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11242-11249.	1.1	11
4957	Study on the Reaction Mechanism and Kinetics of the Thermal Decomposition of Nitroethane. <i>Industrial & Engineering Chemistry Research</i> , 2009, 48, 8745-8751.	1.8	39
4958	Proximity and Cooperativity Effects in Binuclear d ⁰ Olefin Polymerization Catalysis. Theoretical Analysis of Structure and Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 3974-3984.	6.6	66
4959	Potential for C ⁺ H Activation in CH ₄ Utilizing a CuMFI-Type Zeolite as a Catalyst. <i>Journal of Physical Chemistry C</i> , 2009, 113, 7213-7222.	1.5	32
4960	Mechanism and Dynamic Correlation Effects in Cycloaddition Reactions of Singlet Difluorocarbene to Alkenes and Disilene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9852-9860.	1.1	12
4961	Why Do Cysteine Dioxygenase Enzymes Contain a 3-His Ligand Motif Rather than a 2His/1Asp Motif Like Most Nonheme Dioxygenases?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1835-1846.	1.1	54
4962	An Accurate Calculation of Electronic Contribution to Static Permittivity Tensor for Organic Molecular Crystals on the Basis of the Charge Response Kernel Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9207-9212.	1.1	14
4963	Stable and Highly Persistent Quinoxaline-Centered Metalloorganic Radical Anions: Preparation, Structural, Spectroscopic, and Computational Investigations. <i>Inorganic Chemistry</i> , 2009, 48, 149-163.	1.9	17
4964	Endohedral Metalloborofullerenes La ₂ @B ₈₀ and Sc ₃ N@B ₈₀ : A Density Functional Theory Prediction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11613-11618.	1.1	29
4965	Application of Dispersion-Corrected Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10321-10326.	1.1	35
4966	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5786-5799.	1.1	114
4967	Radical Anions of Metallo-organic Diazines: Structural, Spectroscopic, and Theoretical Investigation of a Pyrazyl Radical Anion. <i>Organometallics</i> , 2009, 28, 6194-6200.	1.1	6
4968	Roles of Conformational Restrictions of a Bismalonate in the Interactions with a Carbon Nanotube. <i>Journal of Physical Chemistry C</i> , 2009, 113, 14184-14194.	1.5	16
4969	Highly Conserved Histidine Plays a Dual Catalytic Role in Protein Splicing: A p <i>K</i> / <i>a</i> Shift Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 11581-11589.	6.6	62

#	ARTICLE	IF	CITATIONS
4970	Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spin ² Spin Coupling Constants for Molecules with C, N, and O Double and Triple Bonds and Selected F-Substituted Derivatives. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 208-216.	2.3	41
4971	Quantum Chemical Calculations of the Cl ⁺ + CH ₃ I ⁺ CH ₃ Cl + I ⁺ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1976-1984.	1.1	29
4972	New Palladium(II) Complex of P,S-Containing Hybrid Calixphyrin. Theoretical Study of Electronic Structure and Reactivity for Oxidative Addition. <i>Journal of the American Chemical Society</i> , 2009, 131, 10955-10963.	6.6	32
4973	Probing the Mechanism of O ₂ Activation by a Copper(I) Biomimetic Complex of a C ⁶⁰ H Hydroxylating Copper Monooxygenase. <i>Inorganic Chemistry</i> , 2009, 48, 4062-4066.	1.9	42
4974	Is the Photoinduced Isomerization in Retinal Protonated Schiff Bases a Single- or Double-Torsional Process?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11907-11918.	1.1	39
4975	Effects of ZSM-5 Zeolite Confinement on Reaction Intermediates during Dioxygen Activation by Enclosed Dicopper Cations. <i>Inorganic Chemistry</i> , 2009, 48, 508-517.	1.9	68
4976	Palladium Motion in Cyclomeric Compounds: A Theoretical Study. <i>Inorganic Chemistry</i> , 2009, 48, 11131-11141.	1.9	1
4977	Electronic Structure and Spectroscopy of [Ru(tpy) ₂] ²⁺ , [Ru(tpy)(bpy)(H ₂ O)] ²⁺ , and [Ru(tpy)(bpy)(Cl)] ⁺ . <i>Inorganic Chemistry</i> , 2009, 48, 10720-10725.	1.9	91
4978	Theoretical studies on electronic structures, spectra and charge transporting properties of a series of Pt(C ₆ N) ₂ complexes. <i>Synthetic Metals</i> , 2009, 159, 1090-1098.	2.1	7
4979	Crocetane: A potential marker of photic zone euxinia in thermally mature sediments and crude oils of Devonian age. <i>Organic Geochemistry</i> , 2009, 40, 1-11.	0.9	45
4980	Structure-activity relationships of a caged thrombin binding DNA aptamer: Insight gained from molecular dynamics simulation studies. <i>Journal of Structural Biology</i> , 2009, 166, 241-250.	1.3	31
4981	Fundamental Differences of Substrate Hydroxylation by High-Valent Iron(IV)-Oxo Models of Cytochrome P450. <i>Inorganic Chemistry</i> , 2009, 48, 6661-6669.	1.9	37
4982	Conformational and color polymorphism of achiral 2-methyl-3-(2-naphthalenylthio)-1,4-naphthalenedione. <i>CrystEngComm</i> , 2009, 11, 1223.	1.3	17
4983	Influence of local sequence context on damaged base conformation in human DNA polymerase β : molecular dynamics studies of nucleotide incorporation opposite a benzo[a]pyrene-derived adenine lesion. <i>Nucleic Acids Research</i> , 2009, 37, 7095-7109.	6.5	16
4984	Theoretical Study of Structure, Bonding, and Electronic Behavior of Low-Valent Bismuth Cyclopentadienyl and Pentamethylcyclopentadienyl Half-Sandwich Compounds. <i>Inorganic Chemistry</i> , 2009, 48, 6986-6996.	1.9	8
4985	Switchable Molecular Conductivity. <i>Journal of the American Chemical Society</i> , 2009, 131, 10447-10451.	6.6	23
4986	Predicting Raman Spectra Using Density Functional Theory. <i>Applied Spectroscopy</i> , 2009, 63, 733-741.	1.2	29
4987	On the accurate calculation of polarizabilities and second hyperpolarizabilities of polyacetylene oligomer chains using the CAM-B3LYP density functional. <i>Journal of Chemical Physics</i> , 2009, 130, 194114.	1.2	256

#	ARTICLE	IF	CITATIONS
4988	Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6041-6043.	1.1	60
4989	Palladium complexes of abnormal N-heterocyclic carbenes as precatalysts for the much preferred Cu-free and amine-free Sonogashira coupling in air in a mixed-aqueous medium. <i>Dalton Transactions</i> , 2009, , 10581.	1.6	126
4990	Novel Bispidine Ligands and Their First-Row Transition Metal Complexes: Trigonal Bipyramidal and Trigonal Prismatic Geometries. <i>Inorganic Chemistry</i> , 2009, 48, 6604-6614.	1.9	33
4991	A Systematic Comparison of Second-Order Polarization Propagator Approximation and Equation-of-Motion Coupled Cluster Singles and Doubles $C\hat{a}^{\sim}C$, $C\hat{a}^{\sim}N$, $N\hat{a}^{\sim}N$, $C\hat{a}^{\sim}H$, and $N\hat{a}^{\sim}H$ Spin \hat{a}^{\sim} Spin Coupling Constants. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12411-12420.	1.1	29
4992	Spontaneous Self-Assembly of Silica Nanocages into Inorganic Framework Materials. <i>Journal of Physical Chemistry C</i> , 2009, 113, 518-523.	1.5	16
4993	Inelastic neutron scattering and Raman spectroscopic investigation of l-alanine alaninium nitrate, a homologue of a ferroelectric material. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9474.	1.3	11
4994	Plicatin B conformational landscape and affinity to copper (I and II) metal cations. A DFT study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 776-790.	1.3	51
4995	Counterintuitive Absence of an Excited-State Intramolecular Charge Transfer Reaction with 2,4,6-Tricyanoanilines. Experimental and Computational Results. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2693-2710.	1.1	23
4996	Photodynamics Simulations of Thymine: Relaxation into the First Excited Singlet State. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12686-12693.	1.1	85
4997	The lithiation and acyl transfer reactions of phosphine oxides, sulfides and boranes in the synthesis of cyclopropanes. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1329.	1.5	11
4998	Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods. <i>Journal of Chemical Physics</i> , 2009, 131, 224315.	1.2	32
4999	A Study of the Interactions between $I\hat{a}^{\sim}/I3\hat{a}^{\sim}$ Redox Mediators and Organometallic Sensitizing Dyes in Solar Cells. <i>Journal of Physical Chemistry C</i> , 2009, 113, 783-790.	1.5	101
5000	Periodic Trends and Index of Boron Lewis Acidity. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5985-5992.	1.1	79
5001	Through-Space Effects of Substituents Dominate Molecular Electrostatic Potentials of Substituted Arenes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2301-2312.	2.3	201
5002	First-principles semiclassical initial value representation molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3861.	1.3	70
5003	ZnO Nanoparticles Functionalized with Organic Acids: An Experimental and Quantum-Chemical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17332-17341.	1.5	54
5004	Cyclopentadienyl Ligands as Perfect Anion Receptors: Teamwork between $\text{I}\hat{\epsilon}$ -Anion Interaction and $C\hat{a}^{\sim}H\hat{A}:\hat{A}:\hat{A}$ -Anion Hydrogen Bonds. <i>Crystal Growth and Design</i> , 2009, 9, 5304-5310.	1.4	4
5005	Paramagnetic Perturbation of the $19F$ NMR Chemical Shift in Fluorinated Cysteine by $O2$: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10916-10922.	1.2	4

#	ARTICLE	IF	CITATIONS
5006	Rate Limiting Step Precedes C ^α -C Bond Formation in the Archetypical Proline-Catalyzed Intramolecular Aldol Reaction. <i>Journal of the American Chemical Society</i> , 2009, 131, 1632-1633.	6.6	63
5007	Experimental and DFT Studies on Competitive Heterocyclic Rearrangements. 3. A Cascade Isoxazole ^{1,2,4} -Oxadiazole ^{1,2,4} -Oxazole Rearrangement. <i>Journal of Organic Chemistry</i> , 2009, 74, 351-358.	1.7	36
5008	Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1237-1244.	2.3	30
5010	Antihypertensive Drug Valsartan in Solution and at the AT ₁ Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, <i>in Silico</i> Docking, and Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 726-739.	2.5	39
5011	Transformations and Reactions of Re ₂ (CO) ₈ (¹ / ₄ -SbPh ₂)(¹ / ₄ -H) Induced by the Addition of a Platinum(tri- <i>t</i> -butylphosphine) Group. <i>Inorganic Chemistry</i> , 2009, 48, 652-662.	1.9	15
5012	Restricted active space spin-flip configuration interaction approach: theory, implementation and examples. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9779.	1.3	202
5013	Theoretical Study of the Neutral Hydrolysis of Hydrogen Isocyanate in Aqueous Solution via Assisted-Concerted Mechanisms. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1858-1863.	1.1	15
5014	Unexpected Regioselectivity in the Synthesis of Pyranonaphthoquinone via the Diels-Alder Reaction. <i>Organic Letters</i> , 2009, 11, 4628-4631.	2.4	13
5015	Extensive regularization of the coupled cluster methods based on the generating functional formalism: Application to gas-phase benchmarks and to the S _N 2 reaction of CHCl ₃ and OH ⁻ in water. <i>Journal of Chemical Physics</i> , 2009, 131, 234107.	1.2	15
5016	Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals. <i>Journal of the American Chemical Society</i> , 2009, 131, 1502-1512.	6.6	174
5017	Dissociating N ₂ : a multi-reference coupled cluster study on the potential energy surfaces of ground and excited states. <i>Molecular Physics</i> , 2009, 107, 143-155.	0.8	38
5018	Origin of Stereoselectivity in the Imidazolidinone-Catalyzed Reductions of Cyclic ^{1,2} -Unsaturated Ketones. <i>Organic Letters</i> , 2009, 11, 4298-4301.	2.4	40
5019	Generation and Trapping of Cyclopentenylidene Gold Species: Four Pathways to Polycyclic Compounds. <i>Journal of the American Chemical Society</i> , 2009, 131, 2993-3006.	6.6	226
5020	H-Bond-Assisted Regioselective (<i>cis</i> -1) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. <i>Journal of Organic Chemistry</i> , 2009, 74, 1480-1487.	1.7	37
5021	Kinetics of the Gas-Phase Reactions of OH and NO ₃ Radicals and O ₃ with Allyl Alcohol and Allyl Isocyanate. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9814-9824.	1.1	17
5022	A Theoretical Study of Nickel(0)-Catalyzed Phenylcyanation of Alkynes. Reaction Mechanism and Regioselectivity. <i>Organometallics</i> , 2009, 28, 2583-2594.	1.1	60
5023	Concomitant Polymorphs of the Antihyperlipoproteinemic Bezafibrate. <i>Crystal Growth and Design</i> , 2009, 9, 2646-2655.	1.4	27
5024	Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. <i>Journal of Organic Chemistry</i> , 2009, 74, 8174-8180.	1.7	25

#	ARTICLE	IF	CITATIONS
5025	MoO ₂ Cl ₂ as a Novel Catalyst for C~P Bond Formation and for Hydrophosphonylation of Aldehydes. <i>Organometallics</i> , 2009, 28, 6206-6212.	1.1	74
5026	Synthesis and C-Alkylation of Hindered Aldehyde Enamines. <i>Journal of Organic Chemistry</i> , 2009, 74, 1019-1028.	1.7	38
5027	Monomeric and Oligomeric Amine~Borane f-Complexes of Rhodium. Intermediates in the Catalytic Dehydrogenation of Amine~Boranes. <i>Journal of the American Chemical Society</i> , 2009, 131, 15440-15456.	6.6	183
5028	Structures and Aggregation of the Methylamine~Borane Molecules, MenH3~nNBH3 (n = 1~3), Studied by X-ray Diffraction, Gas-Phase Electron Diffraction, and Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2009, 131, 2231-2243.	6.6	75
5029	Tuning Electronic Properties of Functionalized Polyhedral Oligomeric Silsesquioxanes: A DFT and TDDFT Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9707-9714.	1.1	46
5030	Regioselective Intramolecular Nucleophilic Addition of Alcohols to C ₆₀ : One-Step Formation of a cis-1 Bicyclic-Fused Fullerene. <i>Journal of Organic Chemistry</i> , 2009, 74, 6253-6259.	1.7	33
5031	Color Tuning in Short Wavelength-Sensitive Human and Mouse Visual Pigments: Ab initio Quantum Mechanics/Molecular Mechanics Studies. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11685-11692.	1.1	41
5032	Molecular recognition in Mn-catalyzed C~H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. <i>Dalton Transactions</i> , 2009, , 5989.	1.6	27
5033	Silicon~Hydrogen Bond Activation and Hydrosilylation of Alkenes Mediated by CpCo Complexes: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 3007-3015.	6.6	29
5034	Interfacial Electron Transfer in TiO ₂ Surfaces Sensitized with Ru(II)~Polypyridine Complexes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12532-12540.	1.1	80
5035	A combined effective fragment potential~fragment molecular orbital method. I. The energy expression and initial applications. <i>Journal of Chemical Physics</i> , 2009, 131, 024101.	1.2	46
5036	Density Functional Analysis of Ancillary Ligand Electronic Contributions to Metal-Mediated Eneidyne Cyclization. <i>Inorganic Chemistry</i> , 2009, 48, 3926-3933.	1.9	8
5037	Non-Covalent Interactions with Dual-Basis Methods: Pairings for Augmented Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1560-1572.	2.3	39
5038	A Convergence Study of QM/MM Isomerization Energies with the Selected Size of the QM Region for Peptidic Systems. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11734-11741.	1.1	99
5039	Ion Pairing and Allyl Dynamics in a Series of [Pd(η -allyl)(N,N-chelate)](anion) Salts. On the Influence of the BPh ₄ ⁻ Anion. <i>Organometallics</i> , 2009, 28, 6489-6506.	1.1	20
5040	A Comparison of 4f vs 5f Metal~Metal Bonds in (CpSiMe ₃) ₃ M~ECp* (M = Nd, U; E = Al, Ga; Cp* = C ₅ Me ₅): Synthesis, Thermodynamics, Magnetism, and Electronic Structure. <i>Journal of the American Chemical Society</i> , 2009, 131, 13767-13783.	6.6	131
5041	Investigation of the [Cp*Mo(PMe ₃) ₃ H] ⁿ⁺ (n = 0, 1) Redox Pair: Dynamic Processes on Very Different Time Scales. <i>Inorganic Chemistry</i> , 2009, 48, 209-220.	1.9	26
5042	Chiral and Achiral Fundamental Conformational Building Units of f ² -Peptides: A Matrix Isolation Conformational Study on Ac-f ² -HGly-NHMe and Ac-f ² -HAla-NHMe. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7918-7926.	1.2	15

#	ARTICLE	IF	CITATIONS
5043	Investigation of the Ligand-Field States of the Hexaammine Cobalt(III) Ion with Quantum Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1061-1067.	2.3	9
5044	Unusual chalcogen-boron ring compounds: the gas-phase structures of 1,4-B4S2(NMe2)4 and related molecules. <i>Dalton Transactions</i> , 2009, , 1446.	1.6	4
5045	Synthesis and characterization of a germanium bismethanediide complex. <i>Chemical Communications</i> , 2009, , 6816.	2.2	36
5047	On the possibility of catalytic reduction of carbonyl moieties with tris(pentafluorophenyl)borane and H2: a computational study. <i>Dalton Transactions</i> , 2009, , 5780.	1.6	49
5048	Oxidative dehydrogenation of an amine group of a macrocyclic ligand in the coordination sphere of a CuII complex. <i>Dalton Transactions</i> , 2009, , 6013.	1.6	17
5049	DFT 2H quadrupolar coupling constants of ruthenium complexes: a good probe of the coordination of hydrides in conjunction with experiments. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5657.	1.3	24
5050	Synthesis and structural studies of amido, hydrazido and imido zirconium(IV) complexes incorporating a diamido/diamine cyclam-based ligand. <i>Dalton Transactions</i> , 2009, , 7494.	1.6	34
5051	Asymmetric synthesis of trans-disubstituted cyclopropanes using phosphine oxides and phosphine boranes. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1323-1328.	1.5	25
5052	The 559-to-600 nm shift observed in red fluorescent protein eqFP611 is attributed to cis \leftrightarrow trans isomerization of the chromophore in an anionic protein pocket. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6042.	1.3	3
5053	Role of vibrational anharmonicity in atmospheric radical hydrogen-bonded complexes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6377.	1.3	12
5054	Jahn-Teller distortions in the electronically excited states of <i>sym</i> -triazine. <i>Molecular Physics</i> , 2009, 107, 929-938.	0.8	12
5055	Structural characterization of a highly active superoxide-dismutase mimic. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6778.	1.3	26
5056	The effect of π -stacking and H-bonding on ionization energies of a nucleobase: uracil dimer cation. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1303.	1.3	47
5057	Cationic and dicationic zirconocene compounds as initiators of carbocationic isobutene polymerisation. <i>Dalton Transactions</i> , 2009, , 9026.	1.6	17
5058	Ruthenium based catalysts for olefin hydrosilylation: dichloro(<i>p</i> -cymene)ruthenium and related complexes. <i>Dalton Transactions</i> , 2009, , 5894.	1.6	20
5059	Stereochemistry of free boranes and heteroboranes from electron scattering and model chemistries. <i>Dalton Transactions</i> , 2009, , 585-599.	1.6	21
5060	Ultrafast internal conversion pathway and mechanism in 2-(2-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1406.	1.3	174
5061	A theoretical and experimental study of non-linear absorption properties of substituted 2,5-di-(phenylethynyl)thiophenes and structurally related compounds. <i>Molecular Physics</i> , 2009, 107, 629-641.	0.8	13

#	ARTICLE	IF	CITATIONS
5062	Theoretical prediction of O–H, Si–H, and Si–C σ -bond activation reactions by titanium(IV)-imido complex. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1415-1424.	0.6	6
5063	An evaluation of the modified 6-31G* basis set for the atoms Ga-Kr using the Gaussian-3 and Gaussian-4 composite methods. <i>Molecular Physics</i> , 2009, 107, 1027-1034.	0.8	1
5064	Aromatic C–F activation by complexes containing the {Pt ₂ S ₂ } core via nucleophilic substitution: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2009, , 5980.	1.6	24
5065	Substituent effects on ⁶¹ Ni NMR chemical shifts. <i>Dalton Transactions</i> , 2009, , 6037.	1.6	11
5066	Hydrogenation of imines by phosphonium borate zwitterions: a theoretical study. <i>Dalton Transactions</i> , 2009, , 1321.	1.6	39
5067	The gas-phase structure of the decasilsesquioxane Si ₁₀ O ₁₅ H ₁₀ . <i>Dalton Transactions</i> , 2009, , 6843.	1.6	6
5068	Expanding the role of oxo-molybdenum(vi) catalysts: a DFT interpretation of X–H activation leading to reduction or oxidation. <i>Dalton Transactions</i> , 2009, , 8155.	1.6	33
5069	Adducts of the supraicosahedral stannacarborane 1,6-Me ₂ -4,1,6-closo-SnC ₂ B ₁₀ H ₁₀ ; synthetic, structural and computational studies. <i>Dalton Transactions</i> , 2009, , 2345.	1.6	12
5070	Quantum-chemistry calculations of hydrogen adsorption in MOF-5. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9250.	1.3	27
5071	Protonation of O ₂ adsorbed on a Pt ₃ island supported on transition metal surfaces. <i>Journal of Chemical Physics</i> , 2009, 131, 044709.	1.2	2
5072	UV excitation and radiationless deactivation of imidazole. <i>Journal of Chemical Physics</i> , 2009, 130, 034305.	1.2	58
5073	Bis(oxazolinylmethyl)pyrrole Derivatives and Their Coordination as Chiral π -Pincer-Ligands to Rhodium. <i>Inorganic Chemistry</i> , 2009, 48, 8523-8535.	1.9	31
5074	Tautomerism in Cytosine and Uracil: An Experimental and Theoretical Core Level Spectroscopic Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5736-5742.	1.1	113
5075	Hydrotrioxides Rather than Cyclic Tetraoxides (Tetraoxolanes) as the Primary Reaction Intermediates in the Low-Temperature Ozonation of Aldehydes. The Case of Benzaldehyde. <i>Journal of Organic Chemistry</i> , 2009, 74, 96-101.	1.7	14
5076	A Density Functional Theory Study of the Magnetic Exchange Coupling in Dinuclear Manganese(II) Inverse Crown Structures. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14008-14013.	1.1	17
5077	A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly π -Conjugated Systems. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 506-514.	2.3	28
5078	Ferrous Iron Reduction of Superoxide, A Proton-Coupled Electron-Transfer Four-Point Test. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1020-1025.	1.1	7
5079	The Accuracy of Geometries for Iron Porphyrin Complexes from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11949-11953.	1.1	53

#	ARTICLE	IF	CITATIONS
5080	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11297.	1.3	134
5081	Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 726-735.	1.1	111
5082	Synergistic activation of the Diels-Alder reaction by an organic catalyst and substituents: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1304.	1.5	18
5083	An Experimental and Theoretical Core-Level Study of Tautomerism in Guanine. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9376-9385.	1.1	64
5084	Two Regioisomers of Endohedral Pyrrolidinodimetallofullerenes $M_{2@C_{80}}(CH_2)_2NTrt$ (M=La, Ce). <i>Journal of Physical Chemistry A</i> , 2009, 113, 10533-10542.	1.7	44
5085	Quantum Chemical Investigation of Thermal Cis-to-Trans Isomerization of Azobenzene Derivatives: Substituent Effects, Solvent Effects, and Comparison to Experimental Data. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6763-6773.	1.1	217
5086	DFT Study on N ₂ Activation by a Hydride-Bridged Diniobium Complex. N ₂ Bond Cleavage Accompanied by H ₂ Evolution. <i>Inorganic Chemistry</i> , 2009, 48, 3875-3881.	1.9	29
5087	R-matrix calculation of low-energy electron collisions with uracil. <i>Journal of Chemical Physics</i> , 2009, 130, 164307.	1.2	68
5088	Studies on bis(halogeno) dioxomolybdenum(VI)-bipyridine complexes: Synthesis and catalytic activity. <i>Dalton Transactions</i> , 2009, , 8746.	1.6	24
5089	Thiadiazole-containing expanded heteroazaporphyrinoids: a gas-phase electron diffraction and computational structural study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8570.	1.3	23
5090	In silico study of MMP inhibition. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 3817.	1.5	10
5091	Ancillary Ligand and Ketone Substituent Effects on the Rate of Ketone Insertion into Zr-C Bonds of Zirconocene-1-Aza-1,3-diene Complexes. <i>Organometallics</i> , 2009, 28, 2938-2946.	1.1	9
5092	Experimental Equilibrium Structures: Application of Molecular Dynamics Simulations to Vibrational Corrections for Gas Electron Diffraction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9511-9520.	1.1	25
5093	Classification of OH Bonds and Infrared Spectra of the Topology-Distinct Protonated Water Clusters $H_3O^+(H_2O)_n$ ($n=1-7$). <i>Journal of Physical Chemistry A</i> , 2009, 113, 1586-1594.	1.1	30
5094	Tuning the Binding Energy of Surfactant to CdSe Nanocrystal: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3116-3119.	1.5	13
5095	Experimental and Theoretical Investigation Into Hydrogen Storage via Spillover in IRMOF-8. <i>Journal of Physical Chemistry C</i> , 2009, 113, 3222-3231.	1.5	68
5096	A density functional theory study of the correlation between analyte basicity, ZnPc adsorption strength, and sensor response. <i>Journal of Chemical Physics</i> , 2009, 130, 204307.	1.2	20
5097	Water-Chloride and Water-Bromide Hydrogen-Bonded Networks: Influence of the Nature of the Halide Ions on the Stability of the Supramolecular Assemblies. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8626-8634.	1.1	19

#	ARTICLE	IF	CITATIONS
5098	Isomerism in dihalogenometal porphyrins and phthalocyanines: a theoretical study of dihalogenotitanium complexes. <i>Molecular Physics</i> , 2009, 107, 2493-2501.	0.8	0
5099	Formation and Reactivity of [(tacn)-N-CO-Re ^{III} Br(CO) ₂] ⁺ in Water: a Theoretical and Experimental Study. <i>Inorganic Chemistry</i> , 2009, 48, 4963-4970.	1.9	16
5100	Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8712-8723.	1.1	34
5101	Theoretical and Experimental Study of Valence-Shell Ionization Spectra of Guanine. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15142-15149.	1.1	34
5102	Performance of the major semiempirical, ab initio, and density functional theory methods in evaluating isomerization enthalpies for linear to branched heptanes. <i>Nature Precedings</i> , 2010, , .	0.1	6
5103	Application of Real-time Time-dependent Density Functional Theory with the CVB3LYP Functional to Core Excitations. <i>Chemistry Letters</i> , 2010, 39, 407-409.	0.7	19
5104	Synthesis and Structures of Lithium Salts of Stannole Anions. <i>Bulletin of the Chemical Society of Japan</i> , 2010, 83, 825-827.	2.0	20
5105	Large scale Hartree-Fock calculations with conventional SCF algorithm. Influence of integral and index compression on Fock matrix construction. <i>Russian Journal of Physical Chemistry A</i> , 2010, 84, 812-819.	0.1	1
5106	Possible criterion for the balance of basis sets in quantum-chemical calculations. <i>Russian Journal of Physical Chemistry A</i> , 2010, 84, 1921-1929.	0.1	1
5107	The comparison of addition of molecules possessing P(V)-H bond to alkynes catalyzed with Pd and Ni complexes. <i>Russian Journal of Organic Chemistry</i> , 2010, 46, 1269-1276.	0.3	23
5108	Comparison of the directional characteristics of swift ion excitation for two small biomolecules: glycine and alanine. <i>European Physical Journal D</i> , 2010, 60, 71-76.	0.6	11
5109	Olefin Epoxidation Catalyzed by $\hat{\text{I}}^{\text{V}}$ -Cyclopentadienyl Molybdenum Compounds: A Computational Study. <i>Organometallics</i> , 2010, 29, 303-311.	1.1	84
5110	Mechanism of Enantioselective C-C Bond Formation with Bifunctional Chiral Ru Catalysts: NMR and DFT Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 16637-16650.	6.6	37
5111	Ab Initio EOM-CCSD Investigation of One-Bond C-C, N-C, and N-N Spin-Spin Coupling Constants in Fluoroazines. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5205-5210.	1.1	7
5112	Cyclopentadienyl Molybdenum(II/VI) N-Heterocyclic Carbene Complexes: Synthesis, Structure, and Reactivity under Oxidative Conditions. <i>Organometallics</i> , 2010, 29, 1924-1933.	1.1	60
5113	On the applicability of local softness and hardness. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1072-1080.	1.3	98
5114	The gas-phase structure of octaphenyloctasilsesquioxane Si ₈ O ₁₂ Ph ₈ and the crystal structures of Si ₈ O ₁₂ (p-tolyl) ₈ and Si ₈ O ₁₂ (p-ClCH ₂ C ₆ H ₄) ₈ . <i>Dalton Transactions</i> , 2010, 39, 6960.	1.6	21
5115	Accelerating self-consistent field convergence with the augmented Roothaan-Hall energy function. <i>Journal of Chemical Physics</i> , 2010, 132, 054109.	1.2	69

#	ARTICLE	IF	CITATIONS
5116	Hydrazine and Thermal Reduction of Graphene Oxide: Reaction Mechanisms, Product Structures, and Reaction Design. <i>Journal of Physical Chemistry C</i> , 2010, 114, 832-842.	1.5	1,002
5117	Parametrization of the two-electron reduced density matrix for its direct calculation without the many-electron wave function: Generalizations and applications. <i>Physical Review A</i> , 2010, 81, .	1.0	47
5118	Theoretical characterization of photoinduced electron transfer in rigidly linked donor-acceptor molecules: the fragment charge difference and the generalized Mulliken-Hush schemes. <i>Molecular Physics</i> , 2010, 108, 2775-2789.	0.8	19
5119	Synthesis and Properties of N_7O_+ . <i>Inorganic Chemistry</i> , 2010, 49, 1245-1251.	1.9	15
5120	Alternative perturbation theories for triple excitations in coupled-cluster theory. <i>Molecular Physics</i> , 2010, 108, 2951-2960.	0.8	16
5121	Quantitative structure-activity relationships for estimating the aryl hydrocarbon receptor binding affinities of resveratrol derivatives and the antioxidant activities of hydroxystilbenes. <i>Medicinal Chemistry Research</i> , 2010, 19, 864-901.	1.1	8
5122	Charge transfer between DNA and proteins in the nucleosomes. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 185-191.	0.5	4
5123	Exchange repulsion between effective fragment potentials and ab initio molecules. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 481-491.	0.5	26
5124	Intramolecular ferromagnetic coupling in bis-oxoverdazyl and bis-thioxoverdazyl diradicals with polyacene spacers. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 57-67.	0.5	40
5125	Simple avoidance of Pauli repulsion errors in the generalized hybrid orbital (GHO) method. <i>Chemical Physics Letters</i> , 2010, 484, 344-348.	1.2	6
5126	The importance of anharmonicity in predicting the IR spectra of low coordinated organoarsenic compounds. <i>Chemical Physics Letters</i> , 2010, 493, 24-26.	1.2	6
5127	Glycolate adsorption at gold and platinum electrodes: A theoretical and in situ spectroelectrochemical study. <i>Electrochimica Acta</i> , 2010, 55, 2055-2064.	2.6	23
5128	Hydrogen/deuterium exchange of phenylalanine analogs studied with infrared multiple photon dissociation. <i>International Journal of Mass Spectrometry</i> , 2010, 297, 162-169.	0.7	4
5129	Synthesis and non-linear optical properties of some novel nickel derivatives. <i>Chemical Physics</i> , 2010, 372, 33-45.	0.9	21
5130	The effect of hydration on the photo-deactivation pathways of 4-aminopyrimidine. <i>Chemical Physics</i> , 2010, 375, 110-117.	0.9	14
5131	A DFT study on the mechanism of Wolff Rearrangement in a five-membered Iridacycle. <i>Procedia Computer Science</i> , 2010, 1, 2659-2667.	1.2	2
5132	Water as the reaction medium for multicomponent reactions based on boronic acids. <i>Tetrahedron</i> , 2010, 66, 2736-2745.	1.0	91
5133	Synthesis and computational studies of diphenylamine donor-carbazole linker-based donor-acceptor compounds. <i>Tetrahedron</i> , 2010, 66, 9641-9649.	1.0	14

#	ARTICLE	IF	CITATIONS
5134	Asymmetric catalysis with 7-ring chelate diphosphines: DIOP, BINAP and conformational mobility. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 1737-1744.	1.8	14
5135	Relative stability of complexes of six-carbon-rings with variable numbers of double bonds: DFT and ab initio results. <i>Computational and Theoretical Chemistry</i> , 2010, 941, 78-84.	1.5	2
5136	Comparative semiempirical, ab initio, and density functional theory study on the thermodynamic properties of linear and branched perfluoroalkyl sulfonic acids/sulfonyl fluorides, perfluoroalkyl carboxylic acid/acyl fluorides, and perhydroalkyl sulfonic acids, alkanes, and alcohols. <i>Computational and Theoretical Chemistry</i> , 2010, 941, 107-118.	1.5	22
5137	DFT approach to reaction mechanisms through molecular complexes. The case of an organo-catalysed nucleosidation reaction. <i>Computational and Theoretical Chemistry</i> , 2010, 944, 43-52.	1.5	4
5138	The electronic properties of a homoleptic bisphosphine Cu(I) complex: A joint theoretical and experimental insight. <i>Computational and Theoretical Chemistry</i> , 2010, 962, 7-14.	1.5	16
5139	DFT and experimental study of N,N-bis(3-carboxy,4-aminophenyl)-1,4-quinonediimine, a carboxyl substituted aniline trimer. <i>Journal of Molecular Structure</i> , 2010, 977, 220-229.	1.8	8
5140	Control of relationship between conformational and color polymorphs of achiral 2-methyl-3-arythio-1,4-naphthalenediones. <i>Journal of Molecular Structure</i> , 2010, 982, 16-21.	1.8	5
5141	Coupling and uncoupling mechanisms in the methoxythreonine mutant of cytochrome P450cam: a quantum mechanical/molecular mechanical study. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 361-372.	1.1	13
5142	Quantum chemical studies on substitution effects within silyl group in the silylative coupling of olefins. <i>Journal of Molecular Modeling</i> , 2010, 16, 395-400.	0.8	3
5143	DFT calculations on nitrodiborane compounds as new potential high energy materials. <i>Journal of Molecular Modeling</i> , 2010, 16, 915-918.	0.8	4
5144	Photodimerizations of hydroxy- and benzoylated 4-azachalcones and quantum chemical investigation of the reactions. <i>Journal of Molecular Modeling</i> , 2010, 16, 1347-1355.	0.8	1
5145	Incorporation of 2,3-Disubstituted-1,4-Naphthoquinones into the A1 Binding Site of Photosystem I Studied by EPR and ENDOR Spectroscopy. <i>Applied Magnetic Resonance</i> , 2010, 37, 65-83.	0.6	17
5146	A Pulsed EPR and DFT Investigation of the Stabilization of Coordinated Phenoxyl Radicals in a Series of Cobalt Schiff-Base Complexes. <i>Applied Magnetic Resonance</i> , 2010, 37, 289-303.	0.6	6
5147	Quantum chemical investigation of nitrotyrosine (3-nitro-l-tyrosine) and 8-nitroguanine. <i>Amino Acids</i> , 2010, 38, 319-327.	1.2	3
5148	How the energy evaluation method used in the geometry optimization step affect the quality of the subsequent QSAR/QSPR models. <i>Journal of Computer-Aided Molecular Design</i> , 2010, 24, 17-22.	1.3	9
5149	Molecular geometries, electronic properties, and vibrational spectroscopic studies of endohedral metallofullerenes TM@C ₂₄ and TM@C ₂₄ H ₁₂ (TM=Cr, Mo, and W). <i>Structural Chemistry</i> , 2010, 21, 673-680.	1.0	14
5150	Synthesis, X-ray studies, spectroscopic investigation, and DFT calculations of [ReBr ₃ (dppt)(OPPh ₃)]. <i>Structural Chemistry</i> , 2010, 21, 761-769.	1.0	10
5151	Structure, stability and dissociation of silanitriles RSiN (R=H ₂ B, H ₂ N, H ₂ P). <i>Structural Chemistry</i> , 2010, 21, 947-954.	1.0	3

#	ARTICLE	IF	CITATIONS
5152	The Role of Oxazolidinones in L-Proline-Assisted Aldol-Type Reactions. Topics in Catalysis, 2010, 53, 1031-1038.	1.3	4
5153	Dechlorination pathways of diverse chlorinated aromatic pollutants conducted by Dehalococcoides sp. strain CBDB1. Science of the Total Environment, 2010, 408, 2549-2554.	3.9	14
5154	DFT study of nitrated zeolites: Mechanism of nitrogen substitution in HY and silicalite. Journal of Catalysis, 2010, 269, 53-63.	3.1	27
5155	<i>Ab initio</i> theoretical studies on N_{28} , $B_{4N_{24}}$, $B_{12N_{16}}$, and $B_{16N_{12}}$ with <i>Td</i> symmetry. Chinese Journal of Chemistry, 1996, 14, 490-496.	2.6	0
5156	Thermodynamic Estimate of pK_a Values of the Carboxylic Acids in Aqueous Solution with the Density Functional Theory. Chinese Journal of Chemistry, 2010, 28, 727-733.	2.6	13
5157	Synthesis and Biological Evaluation of 9-oxo- <i>H</i> -indeno[1,2- <i>b</i>]pyrazine-2,3-dicarbonitrile Analogues as Potential Inhibitors of Deubiquitinating Enzymes. ChemMedChem, 2010, 5, 552-558.	1.6	96
5158	Oriented Electric Fields Accelerate Diels-Alder Reactions and Control the <i>endo/exo</i> Selectivity. ChemPhysChem, 2010, 11, 301-310.	1.0	208
5159	Theoretical Study of the Reactions $M^{+} + CH_3F$ ($M=Ge, As, Se, Sb$). ChemPhysChem, 2010, 11, 1909-1917.	1.0	2
5160	On the Reliability of the AMBER Force Field and its Empirical Dispersion Contribution for the Description of Noncovalent Complexes. ChemPhysChem, 2010, 11, 2399-2408.	1.0	30
5161	The Propensity of \pm -Aminoisobutyric Acid (=Methylalanine; Aib) to Induce Helical Secondary Structure in an \pm -Heptapeptide: A Computational Study. Helvetica Chimica Acta, 2010, 93, 1513-1531.	1.0	4
5162	Exploration of density functional methods for one-electron reduction potential of nitrobenzenes. Journal of Computational Chemistry, 2010, 31, 144-150.	1.5	25
5163	DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic $HPt(SnCl_3)(PH_3)_2$ model catalyst. Journal of Computational Chemistry, 2010, 31, 1986-2000.	1.5	13
5164	<i>Ab Initio</i> and Quantum Chemical Topology studies on the isomerization of HONO to HNO_2 . Effect of the basis set in QCT. Journal of Computational Chemistry, 2010, 31, 2555-2567.	1.5	6
5165	meta-Terphenyl Phosphaalkenes Bearing Electron-Donating and -Accepting Groups. European Journal of Inorganic Chemistry, 2010, 2010, 854-865.	1.0	33
5166	$[2,6-(Me_2NCH_2)_2C_6H_3(H_2O)Sn]W(CO)_5$ Aqua Complex of a Transition-Metal-Bound Organotin(II) Cation versus an Ammonium-Type Structure. European Journal of Inorganic Chemistry, 2010, 2010, 902-908.	1.0	36
5167	Protonation of $Cp^*M(dppe)H$ Hydrides: Peculiarities of the Osmium Congener. European Journal of Inorganic Chemistry, 2010, 2010, 1489-1500.	1.0	16
5168	The Preparation and Structure of $[Pt(S_2N_2)\{P(OR)_n\}_2]$ and $[Pt(SeSN_2)\{P(OMe)_n\}_2]$ ($n=0, 3$). European Journal of Inorganic Chemistry, 2010, 2010, 3185-3194.	1.0	3
5169	Functionalization of Dinitrogen Using a Historically Significant Ru Complex: A New Life for an Old Complex. European Journal of Inorganic Chemistry, 2010, 2010, 4716-4719.	1.0	5

#	ARTICLE	IF	CITATIONS
5170	Epoxidation of Alkenes with H_2O_2 Catalyzed by Ditungstenium-Containing Tungstodarsenate(III): Experimental and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5312-5317.	1.0	42
5171	Density Functional Theory Studies of $[Fe(O)2L]_2^{2+}$: What is the Role of the Spectator Ligand L with Different Coordination Numbers?. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5113-5123.	1.0	4
5172	Bridged μ_2 -Tricarbonylrhenium(I)-Biscarbene Complexes: Synthesis, Characterization, and Molecular Dynamics. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5284-5293.	1.0	28
5173	Rearrangements of N-Heterocyclic Carbenes of Pyrazole to 4-Aminoquinolines and Benzoquinolines. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 4296-4305.	1.2	31
5174	Asymmetric Lithiation of Boron Trifluoride-Activated Aminoferrocenes: An Experimental and Computational Investigation. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 1967-1982.	2.1	27
5175	Acid-Free Nickel Catalyst for Stereo- and Regioselective Hydrophosphorylation of Alkynes: Synthetic Procedure and Combined Experimental and Theoretical Mechanistic Study. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 2979-2992.	2.1	71
5176	Brønsted Base-Catalyzed Tandem Isomerization-Michael Reactions of Alkynes: Synthesis of Oxacycles and Azacycles. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 3373-3379.	2.1	61
5177	Molecular dynamics simulation of desulfurization by ionic liquids. <i>AIChE Journal</i> , 2010, 56, 2983-2996.	1.8	47
5179	Pincer-Type Heck Catalysts and Mechanisms Based on Pd^{IV} Intermediates: A Computational Study. <i>Chemistry - A European Journal</i> , 2010, 16, 1521-1531.	1.7	44
5180	Modulation of Stacking Interactions by Transition-Metal Coordination: Ab Initio Benchmark Studies. <i>Chemistry - A European Journal</i> , 2010, 16, 5391-5399.	1.7	19
5181	The Effect of the Equatorial Environment on Oxo-Group Silylation of the Uranyl Dication: A Computational Study. <i>Chemistry - A European Journal</i> , 2010, 16, 4881-4888.	1.7	25
5182	Chemoselectivity as a Delineator of Cuprate Structure in Catalytic 1,4-Addition of Diorganozinc Reagents to Michael Acceptors. <i>Chemistry - A European Journal</i> , 2010, 16, 5620-5629.	1.7	19
5183	Iridium-Catalysed Asymmetric Allylic Substitutions with Cyclometalated (Phosphoramidite)Ir Complexes as Resting States, Catalytically Active (η^5 -Allyl)Ir Complexes and Computational Exploration. <i>Chemistry - A European Journal</i> , 2010, 16, 6601-6615.	1.7	82
5184	DFT Mechanistic Study on Diene Metathesis Catalyzed by Ru-Based Grubbs-Hoveyda-Type Carbenes: The Key Role of π -Electron Delocalization in the Hoveyda Ligand. <i>Chemistry - A European Journal</i> , 2010, 16, 7331-7343.	1.7	78
5185	Transition States and Origins of 1,4-Asymmetric Induction in Alkylations of 2,2,6-Trialkylpiperidine Enamines. <i>Chemistry - A European Journal</i> , 2010, 16, 6310-6316.	1.7	7
5186	Cobalt-Mediated Linear 2:1 Co-oligomerization of Alkynes with Enol Ethers to Give 1-Alkoxy-1,3,5-Trienes: A Missing Mode of Reactivity. <i>Chemistry - A European Journal</i> , 2010, 16, 8904-8913.	1.7	29
5187	Reactivity of the Latent 12-Electron Fragment $[Rh(P(i)Bu)_3]^{2+}$ with Aryl Bromides: Aryl-Br and Phosphine Ligand C-H Activation. <i>Chemistry - A European Journal</i> , 2010, 16, 8376-8389.	1.7	16
5188	Hole-Transfer Dyads and Triads Based on Perylene Monoimide, Quaterthiophene, and Extended Tetrathiafulvalene. <i>Chemistry - A European Journal</i> , 2010, 16, 9140-9153.	1.7	17

#	ARTICLE	IF	CITATIONS
5189	High-Yielding Synthesis of the Anti-Influenza Neuraminidase Inhibitor (α -Oseltamivir by Two α -One-Pot α -Sequences. <i>Chemistry - A European Journal</i> , 2010, 16, 12616-12626.	1.7	138
5190	Competitive and Selective $Csp^{3}Br$ versus $Csp^{2}Br$ Bond Activation in Palladium-Catalysed Suzuki Cross-Coupling: An Experimental and Theoretical Study of the Role of Phosphine Ligands. <i>Chemistry - A European Journal</i> , 2010, 16, 13390-13397.	1.7	65
5191	Functionalized Alkynylplatinum(II) Polypyridyl Complexes for Use as Sensitizers in Dye-Sensitized Solar Cells. <i>Chemistry - A European Journal</i> , 2010, 16, 12244-12254.	1.7	61
5192	A Simple Approach to Coordination Compounds of the Pentacyanocyclopentadienide Anion. <i>Chemistry - A European Journal</i> , 2010, 16, 13723-13728.	1.7	30
5193	Étude de l'influence des Bases sur le Calcul de Grandeurs Moléculaires. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1975, 84, 1105-1118.	0.0	1
5194	Étude Théorique Des Liaisons Intermoléculaires Par le Transfert De Charge. V. Les Complexes $NH_3^+Cl_2^-$, $H_2O^+Cl_2^-$ et $HF^+Cl_2^-$. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1977, 86, 241-254.	0.0	8
5195	Contribution to the Theoretical Study of the Onno Dimer. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1982, 91, 663-675.	0.0	2
5196	Theoretical Study of the Electronic Structure of Ketene, Ketenimine, Keteniminium Ion and Related Cumulenes. Evaluation of a 1,2 Dipolar Model. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1985, 94, 831-847.	0.0	12
5197	Le Transfert du Proton Entre Molécules d'Eau. <i>Bulletin Des Sociétés Chimiques Belges</i> , 1988, 97, 931-940.	0.0	3
5200	Tuning the <i>cis/trans</i> Conformer Ratio of Xaa-Pro Amide Bonds by Intramolecular Hydrogen Bonds: The Effect on PPII Helix Stability. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6324-6327.	7.2	98
5201	Dichlorophenyl Derivatives of $La@C_{82}$: Endohedral Metal Induced Localization of Pyramidalization and Spin on a Triple-Hexagon Junction. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 9715-9719.	7.2	57
5202	Synthesis, characterization and biological studies of alkenyl-substituted titanocene(IV) carboxylate complexes. <i>Applied Organometallic Chemistry</i> , 2010, 24, 656-662.	1.7	19
5203	XRD studies, vibrational spectra, and molecular structure of 1H-imidazo [4,5-b]pyridine based on DFT quantum chemical calculations. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 1021-1029.	1.2	16
5204	Synthesis Characterization Molecular Modeling of a Pharmaceutical Co-Crystal: (2-Chloro-4-Nitrobenzoic Acid):(Nicotinamide). <i>Journal of Pharmaceutical Sciences</i> , 2010, 99, 4054-4071.	1.6	47
5205	Density-functional computation of ^{93}Nb NMR chemical shifts. <i>Magnetic Resonance in Chemistry</i> , 2010, 48, S61-S68.	1.1	17
5206	Ab initio Hartree-Fock and density functional theory study on characterization of 3-(5-methylthiazol-2-yl-diazenyl)-2-phenyl-1H-indole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 1362-1369.	2.0	52
5207	Asymmetric induction in thia-Diels-Alder reactions of chiral polyfluoroalkylthionocarboxylates. <i>Journal of Fluorine Chemistry</i> , 2010, 131, 172-183.	0.9	26
5208	Rules of thumb for assessing reductive dechlorination pathways of PCDDs in specific systems. <i>Journal of Hazardous Materials</i> , 2010, 177, 1145-1149.	6.5	16

#	ARTICLE	IF	CITATIONS
5209	A screened hybrid density functional study on energetic complexes: Cobalt, nickel and copper carbonyl perchlorates. <i>Journal of Hazardous Materials</i> , 2010, 179, 21-27.	6.5	25
5210	Structure of duplex DNA containing the cisplatin 1,2-{Pt(NH ₃) ₂ } ₂ +d(GpG) cross-link at 1.77Å... resolution. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 902-908.	1.5	101
5211	Octamethylporphyrin copper, C ₂₈ H ₂₈ N ₄ Cu – A first experimental structure determination of porphyrins in gas phase. <i>Journal of Molecular Structure</i> , 2010, 978, 163-169.	1.8	16
5212	Theoretical and experimental study on the reactions between 3,5-di-O-p-toluoyl-d-2-deoxyribose chloride and alcohols. <i>Journal of Molecular Structure</i> , 2010, 977, 1-5.	1.8	2
5213	Optical absorption and emission properties of end-capped oligothienoacenes: A joint theoretical and experimental study. <i>Organic Electronics</i> , 2010, 11, 1701-1712.	1.4	19
5214	Synthesis, crystal structure, and physical property of radical cation salt of 2-(thiopyran-4-ylidene)-4,5-ethylenedithio-1,3-dithiole (TP-EDTT): (TP-EDTT) ₂ SbF ₆ . <i>Physica B: Condensed Matter</i> , 2010, 405, S49-S54.	1.3	3
5215	The roles of ligands proton affinity, π -back donation and metal fragment hardness on the Au–N bond in N-donor heterocycles gold(III) complexes. <i>Polyhedron</i> , 2010, 29, 767-772.	1.0	8
5216	Novel rhenium oxocomplexes of 2-hydroxymethylbenzimidazole – Synthesis, X-ray studies, spectroscopic characterization and DFT calculations. <i>Polyhedron</i> , 2010, 29, 1619-1629.	1.0	9
5217	Synthesis of neutral gold(III) pyrimidine-complexes and theoretical studies on the proton affinity of the coordinated ligands. <i>Polyhedron</i> , 2010, 29, 1833-1836.	1.0	3
5218	Novel rhenium oxocomplexes of indazole-3-carboxylic acid – Synthesis, X-ray studies, spectroscopic characterization and DFT calculations. <i>Polyhedron</i> , 2010, 29, 2061-2069.	1.0	8
5219	Evaluation of dispersion-corrected density functional theory (B3LYP-DCP) for compounds of biochemical interest. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 178-187.	1.3	19
5220	Hierarchical approach to conformational search and selection of computational method in modeling the mechanism of ester ammonolysis. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 246-255.	1.3	5
5221	Theoretical study of formation of pyridines by interaction of a cobaltacyclopentadiene with model nitriles (hydrogen cyanide or trifluoroacetonitrile): Electronic effects of nitriles on the reaction mechanism. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2240-2250.	0.8	31
5222	C–C coupling reaction of pyridine derivatives at the dimethyl rare-earth metal cation [YMe ₂ (THF) ₅] ⁺ : A DFT investigation. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2789-2793.	0.8	14
5223	The role of cyclopentadienyl versus indenyl in Mo(II) spirodiene complexes reactivity: A DFT mechanistic study. <i>Inorganica Chimica Acta</i> , 2010, 363, 555-561.	1.2	8
5224	Mechanism of the cobalt-catalyzed carbonylation of ethyl diazoacetate. <i>Inorganica Chimica Acta</i> , 2010, 363, 2016-2028.	1.2	16
5225	Investigation of the UV–Vis absorption of bis(N-methylthiosemicarbazono) zinc Zn[ATSM]. <i>Inorganica Chimica Acta</i> , 2010, 363, 1133-1139.	1.2	4
5226	Stereoselective non-equivalent bis-dimine coordination to Co(II) ion: Structure, luminescence and density functional theory calculations. <i>Inorganica Chimica Acta</i> , 2010, 363, 2874-2880.	1.2	2

#	ARTICLE	IF	CITATIONS
5227	Suzuki–Miyaura cross-coupling of aryl chlorides catalyzed by palladium precatalysts of N/O-functionalized pyrazolyl ligands. <i>Inorganica Chimica Acta</i> , 2010, 363, 3113-3121.	1.2	15
5228	A new blue luminescent dichlorido-bridged dinuclear copper(II) complex with DNA binding and cytotoxic activities: Synthesis, structure and DFT studies. <i>Inorganica Chimica Acta</i> , 2010, 363, 2752-2761.	1.2	43
5229	Ruthenium(II) thiocrown complexes: Synthetic, spectroscopic, electrochemical, DFT, and single crystal X-ray structural studies of [Ru([15]aneS5)Cl](PF6). <i>Inorganica Chimica Acta</i> , 2010, 364, 55-60.	1.2	6
5230	Charge disproportionation in a semiconducting \hat{I} -type salt of BTM-TTP. <i>Physica B: Condensed Matter</i> , 2010, 405, S198-S201.	1.3	0
5231	Hydrogenation of carbon-heteroatom unsaturated bonds: An assessment of consistency of density functional methods. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 97-103.	4.8	3
5232	Binding energy of d10 transition metals to alkenes by wave function theory and density functional theory. <i>Journal of Molecular Catalysis A</i> , 2010, 324, 80-88.	4.8	50
5233	Molecular structures of vinylarsine, vinyldichloroarsine and arsine studied by gas-phase electron diffraction and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2010, 978, 26-34.	1.8	4
5234	Structural analysis of nanocrystalline BaTiO3. <i>Journal of Molecular Structure</i> , 2010, 984, 131-136.	1.8	52
5235	Synthesis and crystal structures of iron(II) dichloride complexes with \hat{I}^{\pm} -isosparteine, \hat{I}^2 -isosparteine and 2-methylsparteine. <i>Journal of Molecular Structure</i> , 2010, 984, 176-181.	1.8	1
5236	Influence of 8-aminoquinoline on the corrosion behaviour of copper in 0.1M NaCl. <i>Electrochimica Acta</i> , 2010, 55, 2782-2792.	2.6	16
5237	Facile structural elucidation of imidazoles and oxazoles based on NMR spectroscopy and quantum mechanical calculations. <i>Tetrahedron</i> , 2010, 66, 1465-1471.	1.0	12
5238	The origin of diastereoselectivity in the Michael addition reaction: a computational study of the interaction between CH-acidic Schiff base and \hat{I}^{\pm} , \hat{I}^2 -unsaturated ketones. <i>Tetrahedron</i> , 2010, 66, 5168-5172.	1.0	6
5239	Selective arylation of aldehydes with di-rhodium(II)/NHC catalysts. <i>Tetrahedron</i> , 2010, 66, 8494-8502.	1.0	30
5240	Electronic effects of ruthenium-catalyzed [3+2]-cycloaddition of alkynes and azides. <i>Tetrahedron</i> , 2010, 66, 9415-9420.	1.0	34
5241	Experimental and theoretical studies on Mannich-type reactions of chiral non-racemic N-(benzyloxyethyl) nitrones. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2934-2943.	1.8	13
5242	Impact of substitution on the reorganization energy of bis-triarylamine derivatives. <i>Computational and Theoretical Chemistry</i> , 2010, 940, 1-5.	1.5	4
5243	Tin tetrachloride adducts with phosphoryl ligands: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2010, 942, 110-114.	1.5	11
5244	Computational studies of the stability of the (H2O)100 nanodrop. <i>Computational and Theoretical Chemistry</i> , 2010, 944, 163-167.	1.5	14

#	ARTICLE	IF	CITATIONS
5245	Structural stability, electronegativity and electronic property of endohedral TM@C ₂₄ and exohedral TMC ₂₄ (TM=Sc, Y and La) metallofullerene complexes: Density-functional theory investigations. Computational and Theoretical Chemistry, 2010, 947, 16-21.	1.5	12
5246	Computational study of structure of a catalyst for Darzens asymmetric synthesis. Computational and Theoretical Chemistry, 2010, 947, 101-106.	1.5	3
5247	Gas phase isomerization enthalpies of organic compounds: A semiempirical, density functional theory, and ab initio post-Hartree-Fock theoretical study. Computational and Theoretical Chemistry, 2010, 948, 102-107.	1.5	50
5248	A DFT and TD-DFT study on intermolecular charge transfer complexes of pyrene with phenothiazine and promazine. Computational and Theoretical Chemistry, 2010, 949, 36-40.	1.5	13
5249	Quantum chemical studies on chameleonic ligand and its grid-type copper(I) and zinc(II) complexes. Computational and Theoretical Chemistry, 2010, 949, 82-87.	1.5	2
5250	Adsorption of di-, tri- and polyatomic gases on the anatase TiO ₂ (001) and (101) surfaces and their adsorption abilities. Computational and Theoretical Chemistry, 2010, 952, 103-108.	1.5	36
5251	Strong ligand field effects of blue phosphorescent mono-cyclometalated iridium(III) complexes. Thin Solid Films, 2010, 518, 6199-6204.	0.8	7
5252	Entropy-driven adsorption of carbon nanotubes on (0 0 1) and (1 1 1) surfaces of CeO ₂ islands grown on sapphire substrate. Surface Science, 2010, 604, 654-659.	0.8	12
5253	Key observations of cumene hydroperoxide concentration on runaway reaction parameters. Thermochemica Acta, 2010, 501, 65-71.	1.2	17
5254	Ab initio, DFT calculation and vibrational analysis of 2,4,6-trinitrotoluene. Vibrational Spectroscopy, 2010, 53, 248-259.	1.2	10
5255	Quantum chemical insights into the initiation mechanism of transition metal catalysed polymerisation of isobutene. Applied Catalysis A: General, 2010, 384, 154-164.	2.2	7
5256	Quantum chemical interpretation of redox properties of ruthenium complexes with vinyl and TCNX type non-innocent ligands. Coordination Chemistry Reviews, 2010, 254, 1383-1396.	9.5	93
5257	Order-disorder phase transitions and their influence on the structure and vibrational properties of new hybrid material: 2-Amino-4-methyl-3-nitropyridinium trifluoroacetate. Chemical Physics, 2010, 374, 1-14.	0.9	20
5258	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
5259	1-(3-Deoxy-3-fluoro- ¹² -d-glucopyranosyl) pyrimidine derivatives as inhibitors of glycogen phosphorylase b: Kinetic, crystallographic and modelling studies. Bioorganic and Medicinal Chemistry, 2010, 18, 3413-3425.	1.4	35
5260	Synthesis, antiproliferative activity in cancer cells and theoretical studies of novel 6 ^{1±} ,7 ^{1±} -dihydroxyvouacapan-17 ^{1±} -oic acid Mannich base derivatives. Bioorganic and Medicinal Chemistry, 2010, 18, 8172-8177.	1.4	15
5261	Oxo-bridged isomers of aza-trishomocubane sigma (σ) receptor ligands: Synthesis, in vitro binding, and molecular modeling. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 145-148.	1.0	27
5262	Time-dependent Hartree-Fock frequency-dependent polarizability calculation applied to divide-and-conquer electronic structure method. Chemical Physics Letters, 2010, 485, 247-252.	1.2	35

#	ARTICLE	IF	CITATIONS
5263	Theoretical study of the gas phase reaction of methyl acetate with the hydroxyl radical: Structures, mechanisms, rates and temperature dependencies. <i>Chemical Physics Letters</i> , 2010, 490, 116-122.	1.2	26
5264	Ability of a coupled electron pair approximation to treat single bond breakings. <i>Chemical Physics Letters</i> , 2010, 493, 179-184.	1.2	10
5265	Possibility of multi-conformational structure of mismatch DNA nucleobase in the presence of silver(I) ions. <i>Chemical Physics Letters</i> , 2010, 495, 125-130.	1.2	13
5266	EPR spin trapping and DFT studies on structure of active antioxidants in bioglycerol. <i>Chemical Physics Letters</i> , 2010, 497, 135-141.	1.2	14
5267	Electron Momentum Spectroscopy of pyrimidine at the benchmark ADC(3) level. <i>Chemical Physics Letters</i> , 2010, 498, 45-51.	1.2	13
5268	First-principles study of structural, electronic and vibrational properties of aluminum-doped silica nanotubes. <i>Chemical Physics Letters</i> , 2010, 498, 172-177.	1.2	13
5269	Divide-and-conquer self-consistent field calculation for open-shell systems: Implementation and application. <i>Chemical Physics Letters</i> , 2010, 500, 172-177.	1.2	43
5270	A DFT study of the reactivity of Cp ₂ AnMe ₂ with pyridine N-oxide: Towards a predicted different reactivity of U/Pu and Np. <i>Comptes Rendus Chimie</i> , 2010, 13, 870-875.	0.2	10
5271	Synthesis, structures, optical and electrochemical properties, and complexation of 2,5-bis(pyrrol-2-yl)phospholes. <i>Comptes Rendus Chimie</i> , 2010, 13, 1035-1047.	0.2	20
5272	Synthesis, characterization and molecular structure of Re(III) complexes containing 2-benzoylpyridine. <i>Inorganic Chemistry Communication</i> , 2010, 13, 231-235.	1.8	2
5273	Novel rhenium(II) complex of 2,3,5,6-tetra(2-pyridyl)pyrazine – Synthesis, X-ray studies, spectroscopic characterization and DFT calculations. <i>Inorganic Chemistry Communication</i> , 2010, 13, 904-908.	1.8	5
5274	2-Amino-5-(3,4-dimethoxybenzylidene)-1-methylimidazol-4(5 <i>H</i>)-one <i>N,N</i> -dimethylformamide monosolvate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2010, 66, o101-o103.	0.4	1
5275	X-ray constrained unrestricted Hartree-Fock and Douglas-Kroll-Hess wavefunctions. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, 78-92.	0.3	44
5276	Solid solution of two diastereomers of [3a(<i>R,S</i>),7a(<i>R,S</i>)]-3-[(1-phenylethyl)perhydro-1,3-benzothiazol-2-iminium]chloride. <i>Acta Crystallographica Section B: Structural Science</i> , 2010, 66, 678-686.	1.8	9
5277	Synthesis and properties of new aromatic polyisophthalamides with adamantylamide pendent groups. <i>Journal of Polymer Science Part A</i> , 2010, 48, 1743-1751.	2.5	45
5278	A DFT-based exploration augmented by X-ray and NMR of the stereoselectivity in the 1,3-dipolar cycloaddition of 1-pyrroline oxide to methyl cinnamate and benzylidene acetophenone. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 1187-1195.	0.9	11
5279	New perspectives on polyhedral molecules and their crystal structures. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 1080-1087.	0.9	9
5280	Approach to potential energy surfaces by neural networks. A review of recent work. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 432-445.	1.0	10

#	ARTICLE	IF	CITATIONS
5281	Models for the adsorption and self-assembly of ethanol and 1-decanethiol on Au(111) surfaces. A comparative study by computer simulation. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 293-306.	1.0	0
5282	Elongation cutoff technique at Kohn-Sham level of theory. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2130-2139.	1.0	19
5283	Electrospray tandem quadrupole fragmentation of quinolone drugs and related ions. On the reversibility of water loss from protonated molecules. <i>Rapid Communications in Mass Spectrometry</i> , 2010, 24, 3271-3278.	0.7	26
5284	A comparison of the fragmentation pathways of $[Cu^{II}(M_a)(M_b)]^{2+}$ complexes where M_a and M_b are peptides containing either a tryptophan or a tyrosine residue. <i>Rapid Communications in Mass Spectrometry</i> , 2010, 24, 3485-3492.	0.7	6
5285	Unusual Energy Balance Between Atoms in Postperovskite $MgSiO_3$. <i>Journal of the American Ceramic Society</i> , 2010, 93, 3449-3454.	1.9	1
5286	Thermodynamic analysis of protein kinase A δ activation. <i>Biochemistry (Moscow)</i> , 2010, 75, 233-241.	0.7	0
5287	Polarization of amino acids and their interaction in biomolecules. <i>JETP Letters</i> , 2010, 92, 360-364.	0.4	0
5288	Gas phase carbon acidity and correlations with aqueous pK_a values: A comparison of B3LYP/6-311++G(d,p), Gaussian-4 (G4), and experimental approaches. <i>Nature Precedings</i> , 2010, , .	0.1	0
5289	Aqueous phase hydration and hydrate acidity of perfluoroalkyl and n:2 fluorotelomer aldehydes. <i>Nature Precedings</i> , 2010, , .	0.1	1
5290	Gas phase constant pressure heat capacities ($C_{p,gas}$) for the C-1- through C-10- straight chain alkanes, isobutane, hydrogen atom, hydroxyl and methyl radicals, and water between 298.15 and 1500 K: A comparison of theoretical values against experimental data. <i>Nature Precedings</i> , 2010, , .	0.1	2
5291	Theoretical studies on the all-anti zigzag geometries of perfluoro-n-alkyl chains. <i>Nature Precedings</i> , 0, , .	0.1	5
5292	Performance of the M062X density functional against the ISOL set of benchmark isomerization energies for large organic molecules. <i>Nature Precedings</i> , 0, , .	0.1	7
5293	Comparative density functional theory study on the relative gas phase enthalpies and free energies of formation for the mono- through hepta-halogenated (X=F, Cl, Br) anthraquinones. <i>Nature Precedings</i> , 2010, , .	0.1	0
5295	Theoretical Studies of Substitutionally Doped Single-Walled Nanotubes. <i>Journal of Nanotechnology</i> , 2010, 2010, 1-42.	1.5	12
5296	A Critical Evaluation of the Dynamical Thresholding Algorithm in Coupled Cluster Calculations. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 293-309.	1.4	2
5297	Barrier-free proton transfer induced by electron attachment to the complexes between 1-methylcytosine and formic acid. <i>Molecular Physics</i> , 2010, 108, 2621-2631.	0.8	7
5298	Strong Ligand Field Effects of Blue Phosphorescent Iridium(III) Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2010, 520, 97/[373]-107/[383].	0.4	1
5299	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. <i>Journal of Chemical Physics</i> , 2010, 132, 194105.	1.2	40

#	ARTICLE	IF	CITATIONS
5300	Unexpected $\hat{1}/4$ -oxo five-member ring intermediates for oxygen atom transfer between osmium complexes. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2846-2853.	0.8	0
5301	Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism. <i>Journal of Chemical Physics</i> , 2010, 132, 014109.	1.2	103
5302	Theoretical investigation of the interaction of CH ₄ with Al ₂ and Al ₃ neutral and charged clusters. <i>Journal of Chemical Physics</i> , 2010, 132, 154701.	1.2	12
5303	Strongly contracted canonical transformation theory. <i>Journal of Chemical Physics</i> , 2010, 132, 024106.	1.2	75
5304	Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer. <i>Journal of Chemical Physics</i> , 2010, 132, 154103.	1.2	59
5305	Applications of QM/MM in inorganic chemistry. <i>Spectroscopic Properties of Inorganic and Organometallic Compounds</i> , 0, , 87-110.	0.4	1
5306	X-ray structure analysis and DFT study of a chiral (salen)Mn(III) complex toward understanding of inversion of enantioselection in epoxidation catalysts. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2868-2878.	0.8	7
5307	Vibrational properties of ferroelectric $\hat{1}^2$ -vinylidene fluoride polymers and oligomers. <i>Physical Review B</i> , 2010, 81, .	1.1	30
5308	Trypsin-Catalyzed Cross-Linking of $\hat{1}^2$ -Triethoxysilyl-Terminated Polydimethylsiloxane: An Experimental and Computational Approach. <i>ACS Symposium Series</i> , 2010, , 47-57.	0.5	2
5309	Multireference quantum chemistry through a joint density matrix renormalization group and canonical transformation theory. <i>Journal of Chemical Physics</i> , 2010, 132, 024105.	1.2	148
5310	Molecular dynamics study of solvation differences between cis- and transplatin molecules in water. <i>Journal of Chemical Physics</i> , 2010, 132, 174507.	1.2	15
5311	Excited states and electronic spectra of extended tetraazaporphyrins. <i>Journal of Chemical Physics</i> , 2010, 133, 144316.	1.2	37
5312	QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIPS ON DISSOLVABILITY OF PCDD/Fs USING QUANTUM CHEMICAL DESCRIPTORS AND PARTIAL LEAST SQUARES. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 9-22.	1.8	3
5313	Crystal Structure of Histamine Dehydrogenase from <i>Nocardioides</i> simplex. <i>Journal of Biological Chemistry</i> , 2010, 285, 25782-25791.	1.6	16
5314	Communication: Bond length alternation of conjugated oligomers: Another step on the fifth rung of Perdew's ladder of functional. <i>Journal of Chemical Physics</i> , 2010, 133, 151104.	1.2	23
5315	A linked electron pair functional. <i>Journal of Chemical Physics</i> , 2010, 133, 224106.	1.2	15
5316	Charge-Transfer Interactions in Organic Functional Materials. <i>Materials</i> , 2010, 3, 4214-4251.	1.3	18
5318	Structures and Encapsulation Motifs of Functional Molecules Probed by Laser Spectroscopic and Theoretical Methods. <i>Sensors</i> , 2010, 10, 3519-3548.	2.1	16

#	ARTICLE	IF	CITATIONS
5319	Supramolecular main-chain liquid crystalline polymers and networks with competitive hydrogen bonding. <i>Liquid Crystals</i> , 2010, 37, 1127-1131.	0.9	13
5320	The Variety of Carbon-Metal Bonds inside Cu-ZSM-5 Zeolites: A Density Functional Theory Study. <i>Materials</i> , 2010, 3, 2516-2535.	1.3	15
5321	Fluorescence of the perylene radical cation and an inaccessible D/D1 conical intersection: An MMVB, RASSCF, and TD-DFT computational study. <i>Journal of Chemical Physics</i> , 2010, 132, 044306.	1.2	22
5322	The effect of oxidation on the electronic structure of the green fluorescent protein chromophore. <i>Journal of Chemical Physics</i> , 2010, 132, 115104.	1.2	32
5323	Quantum mechanics based force field for carbon (QMFF-Cx) validated to reproduce the mechanical and thermodynamics properties of graphite. <i>Journal of Chemical Physics</i> , 2010, 133, 134114.	1.2	18
5324	pCCSD: Parameterized coupled-cluster theory with single and double excitations. <i>Journal of Chemical Physics</i> , 2010, 133, 184109.	1.2	54
5325	Roles of radical characters of pristine and nitrogen-substituted hydrographene in dioxygen bindings. <i>Journal of Chemical Physics</i> , 2010, 133, 174703.	1.2	6
5326	Local Dielectric Property of Hafnium and Lanthanum Atoms in HfLaO _x . <i>Japanese Journal of Applied Physics</i> , 2010, 49, 121504.	0.8	18
5327	Local Dielectric Property of Cubic Hafnia. <i>Japanese Journal of Applied Physics</i> , 2010, 49, 111504.	0.8	15
5328	<i>R</i> -matrix calculation of low-energy electron collisions with phosphoric acid. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2010, 43, 235203.	0.6	14
5329	The Cobalt-Catalyzed Ketene Formation from Diazoalkanes. <i>Letters in Organic Chemistry</i> , 2010, 7, 634-644.	0.2	11
5330	Method and basis set dependence of anharmonic ground state nuclear wave functions and zero-point energies: Application to SSSH. <i>Journal of Chemical Physics</i> , 2010, 132, 054105.	1.2	8
5331	Improved version of a local contracted configuration interaction of singles and doubles with partial inclusion of triples and quadruples. <i>Journal of Chemical Physics</i> , 2010, 132, 034108.	1.2	11
5332	Application of second-order Møller-Plesset perturbation theory with resolution-of-identity approximation to periodic systems. <i>Journal of Chemical Physics</i> , 2010, 133, 184103.	1.2	26
5333	Electronic Structure and Spectroscopy of Nucleic Acid Bases: Ionization Energies, Ionization-Induced Structural Changes, and Photoelectron Spectra. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12305-12317.	1.1	91
5334	Transition State Models for Probing Stereoinduction in Evans Chiral Auxiliary-Based Asymmetric Aldol Reactions. <i>Journal of the American Chemical Society</i> , 2010, 132, 12319-12330.	6.6	54
5335	Ab initio transition state theory for polar reactions in solution. <i>Faraday Discussions</i> , 2010, 145, 487-505.	1.6	93
5336	Computational Study of Promising Organic Dyes for High-Performance Sensitized Solar Cells. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1219-1227.	2.3	68

#	ARTICLE	IF	CITATIONS
5337	Design of Energetic Ionic Liquids. , 2010, , .		1
5338	Scrutinizing the Chemical Nature and Photophysics of an Expanded Hemiporphyrine: The Special Case of [30]Trithia-2,3,5,10,12,13,15,20,22,23,25,30-dodecaazahexaphyrin. <i>Journal of the American Chemical Society</i> , 2010, 132, 12991-12999.	6.6	42
5339	Alcohol Binding to the Odorant Binding Protein LUSH: Multiple Factors Affecting Binding Affinities. <i>Biochemistry</i> , 2010, 49, 6136-6142.	1.2	6
5340	Excited States of Fluorescent Proteins, mKO and DsRed: Chromophore-Protein Electrostatic Interaction Behind the Color Variations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2971-2979.	1.2	43
5341	Mild and Expedient Asymmetric Reductions of α,β -Unsaturated Alkenyl and Alkynyl Ketones by TarB-NO ₂ and Mechanistic Investigations of Ketone Reduction. <i>Journal of Organic Chemistry</i> , 2010, 75, 7717-7725.	1.7	28
5342	Understanding the NMR chemical shifts for 6-halopurines: role of structure, solvent and relativistic effects. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5126.	1.3	44
5343	Novel Acyclic Diaminocarbene Ligands with Increased Steric Demand and Their Application in Gold Catalysis. <i>Organic Letters</i> , 2010, 12, 4860-4863.	2.4	70
5344	Synthesis and Characterization of Magnesium and Aluminum Bis(phosphoranyl)methanediide Complexes. <i>Organometallics</i> , 2010, 29, 939-944.	1.1	22
5345	Steric Control in the Synthesis of Phosphinous Acid-Coordinated Mono- and Binuclear Platinum(II) Complexes. <i>Organometallics</i> , 2010, 29, 3936-3950.	1.1	66
5346	Highly Convenient Regioselective Intermolecular Hydroamination of Alkynes Yielding Ketimines Catalyzed by Gold(I) Complexes of 1,2,4-triazole Based N-heterocyclic Carbenes. <i>Inorganic Chemistry</i> , 2010, 49, 4972-4983.	1.9	92
5347	Assessment of TD-DFT methods and of various spin scaled CIS(D) and CC2 versions for the treatment of low-lying valence excitations of large organic dyes. <i>Journal of Chemical Physics</i> , 2010, 132, .	1.2	313
5348	Synthesis, Light-Emitting, and Two-Photon Absorption Properties of Platinum-Containing Poly(arylene-ethynylene)s Linked by 1,3,4-Oxadiazole Units. <i>Macromolecules</i> , 2010, 43, 7936-7949.	2.2	59
5349	Adsorption of small aromatic molecules on the (111) surfaces of noble metals: A density functional theory study with semiempirical corrections for dispersion effects. <i>Journal of Chemical Physics</i> , 2010, 132, 224701.	1.2	210
5350	What Factors Influence the Rate Constant of Substrate Epoxidation by Compound I of Cytochrome P450 and Analogous Iron(IV)-Oxo Oxidants?. <i>Journal of the American Chemical Society</i> , 2010, 132, 7656-7667.	6.6	163
5351	Ruthenium Complexes with Cooperative PNP-Pincer Amine, Amido, Imine, and Enamido Ligands: Facile Ligand Backbone Functionalization Processes. <i>Inorganic Chemistry</i> , 2010, 49, 5482-5494.	1.9	94
5352	Silicon Nanosheets and Their Self-Assembled Regular Stacking Structure. <i>Journal of the American Chemical Society</i> , 2010, 132, 2710-2718.	6.6	197
5353	The effect of orbital type and active space size on valence bond structure weights and bond dissociation energies. <i>Molecular Physics</i> , 2010, 108, 2551-2558.	0.8	1
5354	Capsule Formation, Carboxylate Exchange, and DFT Exploration of Cadmium Cluster Metallocavitands: Highly Dynamic Supramolecules. <i>Journal of the American Chemical Society</i> , 2010, 132, 3893-3908.	6.6	75

#	ARTICLE	IF	CITATIONS
5355	Theoretical study of the opsin shift of deprotonated retinal schiff base in the M state of bacteriorhodopsin. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13107.	1.3	16
5356	The inactivation of lipid peroxide radical by quercetin. A theoretical insight. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7662.	1.3	92
5357	Synthesis and Mechanistic Studies of Organic Chromophores with Different Energy Levels for p-Type Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4738-4748.	1.5	174
5358	Do Traditional, Chlorine-shared, and Ion-pair Halogen Bonds Exist? An ab Initio Investigation of FCl:CNX Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12958-12962.	1.1	81
5360	Initial Steps of the SolâGel Process: Modeling Silicate Condensation in Basic Medium. <i>Chemistry of Materials</i> , 2010, 22, 5105-5111.	3.2	37
5361	Accuracy of computational solvation free energies for neutral and ionic compounds: Dependence on level of theory and solvent model. <i>Nature Precedings</i> , 0, , .	0.1	12
5362	Probing $\langle J \rangle$ and $\langle J^2 \rangle$ SpinâSpin Coupling Constants for Fluoroazines: An Ab Initio Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2637-2643.	1.1	19
5363	Water-stable, hydroxamate anchors for functionalization of TiO ₂ surfaces with ultrafast interfacial electron transfer. <i>Energy and Environmental Science</i> , 2010, 3, 917.	15.6	99
5364	Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. <i>Journal of the American Chemical Society</i> , 2010, 132, 16017-16029.	6.6	507
5365	Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation. <i>Journal of the American Chemical Society</i> , 2010, 132, 3375-3387.	6.6	320
5366	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2872-2887.	2.3	1,183
5367	Systematic Study of Modifications to Ruthenium(II) Polypyridine Dyads for Electron Injection Enhancement. <i>Inorganic Chemistry</i> , 2010, 49, 2975-2982.	1.9	31
5368	On the factors affecting tautomerism: consequences of N-substituents (Me/NR ₂) in structures derived from salicylaldehydes. <i>Molecular Simulation</i> , 2010, 36, 41-52.	0.9	3
5369	Stereocontrolled Syntheses of (â)-Cubebol and (â)-10-Epicubebol Involving Intramolecular Cyclopropanation of β -Lithiated Epoxides. <i>Journal of Organic Chemistry</i> , 2010, 75, 2157-2168.	1.7	39
5370	SMARTCyp: A 2D Method for Prediction of Cytochrome P450-Mediated Drug Metabolism. <i>ACS Medicinal Chemistry Letters</i> , 2010, 1, 96-100.	1.3	233
5371	Hydrolysis of cisplatinâa first-principles metadynamics study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10348.	1.3	56
5372	Computational and Experimental Study of the Structure, Binding Preferences, and Spectroscopy of Nickel(II) and Vanadyl Porphyrins in Petroleum. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2180-2188.	1.2	55
5373	Reactivity of Bis(2,2,5,5-tetramethyl-2,5-disila-1-azacyclopent-1-yl)tin with CO ₂ , OCS, and CS ₂ and Comparison to That of Bis[bis(trimethylsilyl)amido]tin. <i>Inorganic Chemistry</i> , 2010, 49, 11133-11141.	1.9	30

#	ARTICLE	IF	CITATIONS
5374	First-Principles Study of Field Emission Properties of Graphene-ZnO Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2010, 114, 19284-19288.	1.5	51
5375	Synthesis, Characterization, and Photophysical Properties of Three Platinum(II) Complexes Bearing Fluorescent Analogues of the Di-2-pyridylmethane Ligand. <i>Inorganic Chemistry</i> , 2010, 49, 5303-5315.	1.9	24
5376	Quantum chemical treatment of β -sitosterol molecule. <i>Pharmaceutical Biology</i> , 2010, 48, 637-642.	1.3	7
5377	Combined Experimental and Simulation Study of the Cure Kinetics of DCPD. <i>Journal of Composite Materials</i> , 2010, 44, 2605-2618.	1.2	12
5378	Ab Initio Study of the Pathways and Barriers of Tricyclo[4.1.0.0 ^{2,6}]heptene Isomerization. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11798-11806.	1.1	5
5379	Experimental and Computational Investigation of C [≡] N Bond Activation in Ruthenium N-Heterocyclic Carbene Complexes. <i>Journal of the American Chemical Society</i> , 2010, 132, 18408-18416.	6.6	78
5380	Influence of Hydrogen Bonding on Hydrogen-Atom Abstraction Reactions of Dehydropyridinium Cations in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12851-12857.	1.1	4
5381	Zooming into π -Stacked Manifolds of Nucleobases: Ionized States of Dimethylated Uracil Dimers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2001-2009.	1.1	19
5382	Theoretical Study on Activation and Protonation of Dinitrogen on Cubane-Type M ₃ S ₄ Clusters (M = V, Cr, Mn, Fe, Co, Ni, Cu, Mo, Ru, and W). <i>Inorganic Chemistry</i> , 2010, 49, 2464-2470.	1.9	13
5383	Quantum Chemical Study of Conformational Fingerprints in the Photoelectron Spectra and (e, 2e) Electron Momentum Distributions of <i>n</i> -Hexane. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4400-4417.	1.1	33
5384	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20870-20876.	1.5	15
5385	Phenanthrene-Tethered Furan-Containing Cyclophenes: Synthesis and Photophysical Properties. <i>Journal of Organic Chemistry</i> , 2010, 75, 4591-4595.	1.7	20
5386	Mechanism and Regioselectivity of the Osmium-Catalyzed Aminohydroxylation of Olefins. <i>Journal of Organic Chemistry</i> , 2010, 75, 1491-1497.	1.7	16
5387	Shutting Down Secondary Reaction Pathways: The Essential Role of the Pyrrolyl Ligand in Improving Silica Supported d ⁰ -ML ₄ Alkene Metathesis Catalysts from DFT Calculations. <i>Journal of the American Chemical Society</i> , 2010, 132, 7750-7757.	6.6	121
5388	Transformation of Triclosan by Fe(III)-Saturated Montmorillonite. <i>Environmental Science & Technology</i> , 2010, 44, 668-674.	4.6	41
5389	Mean Excitation Energies and Their Directional Characteristics for Energy Deposition by Swift Ions on the DNA and RNA Nucleobases. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20335-20341.	1.5	14
5390	Hydrido-Ruthenium Cluster Complexes as Models for Reactive Surface Hydrogen Species of Ruthenium Nanoparticles. Solid-State ² H NMR and Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2010, 132, 11759-11767.	6.6	44
5391	Experimental and Theoretical Study of a Tungsten Dihydride Silyl Complex: New Insight into Its Bonding Nature and Fluxional Behavior. <i>Organometallics</i> , 2010, 29, 6267-6281.	1.1	23

#	ARTICLE	IF	CITATIONS
5392	Synthesis, Structures, and Properties of Plumboles. Phosphorus, Sulfur and Silicon and the Related Elements, 2010, 185, 1068-1076.	0.8	17
5393	Bonding Structure of Phenylacetylene on Hydrogen-Terminated Si(111) and Si(100): Surface Photoelectron Spectroscopy Analysis and Ab Initio Calculations. Langmuir, 2010, 26, 17000-17012.	1.6	22
5394	Does Stacking Restrain the Photodynamics of Individual Nucleobases?. Journal of the American Chemical Society, 2010, 132, 8261-8263.	6.6	67
5395	Diffusion of Atomic Oxygen on the Si(100) Surface. Journal of Physical Chemistry C, 2010, 114, 12649-12658.	1.5	18
5396	Structure and Reactivity of Neutral and Cationic <i>trans</i> - <i>N,N'</i> -Dibenzylcyclam Zirconium Alkyl Complexes. Organometallics, 2010, 29, 3753-3764.	1.1	30
5397	Formation of a Cobalt(III) π -Phenoxy Radical Complex by Acetic Acid Promoted Aerobic Oxidation of a Co(II)salen Complex. Inorganic Chemistry, 2010, 49, 2083-2092.	1.9	37
5398	Role of Substitution on the Photophysical Properties of 5,5'-Diaryl-2,2'-bipyridine (bpy*) in [Ir(ppy) ₂ (bpy*)]PF ₆ Complexes: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2010, 49, 5625-5641.	1.9	155
5399	Cyanide-Bridged Fe(III) π -Mn(III) Bimetallic Systems Assembled from the <i>fac</i> -Fe Tricyanide and Mn Schiff bases: Structures, Magnetic Properties, and Density Functional Theory Calculations. Inorganic Chemistry, 2010, 49, 4632-4642.	1.9	44
5400	Ultrafast Energy Transfer in a Regioregular Silylene-Spaced Copolymer. Journal of Physical Chemistry C, 2010, 114, 13909-13916.	1.5	9
5401	Total Synthesis of the <i>N,C</i> -Coupled Naphthylisoquinoline Alkaloids Ancistrocladinium A and B and Related Analogues. Journal of the American Chemical Society, 2010, 132, 1151-1158.	6.6	53
5402	C π -CN Bond Activation of Aromatic Nitriles and Fluxionality of the π -Arene Intermediates: Experimental and Theoretical Investigations. Organometallics, 2010, 29, 2430-2445.	1.1	87
5403	Carbonate Formation from CO ₂ via Oxo versus Oxalate Pathway: Theoretical Investigations into the Mechanism of Uranium-Mediated Carbonate Formation. Organometallics, 2010, 29, 5504-5510.	1.1	73
5404	Theoretical Insights into Branched and Fused Expanded Pyridiniums by the Means of Density Functional Theory. Journal of Physical Chemistry A, 2010, 114, 8434-8443.	1.1	27
5405	Copper(I) π -Olefin Complexes: The Effect of the Trispyrazolylborate Ancillary Ligand in Structure and Reactivity. Organometallics, 2010, 29, 3481-3489.	1.1	32
5406	Thermal Decomposition Pathways of Hydroxylamine: Theoretical Investigation on the Initial Steps. Journal of Physical Chemistry A, 2010, 114, 9262-9269.	1.1	52
5407	Conformational Sampling of Macrocyclic Alkenes Using a Kennard π Stone-Based Algorithm. Journal of Physical Chemistry A, 2010, 114, 6879-6887.	1.1	17
5408	Amide <i>Cis</i> π - <i>Trans</i> Isomerization in Aqueous Solutions of Methyl <i>N</i> -Formyl- <i>D</i> -glucosaminides and Methyl <i>N</i> -Acetyl- <i>D</i> -glucosaminides: Chemical Equilibria and Exchange Kinetics. Journal of the American Chemical Society, 2010, 132, 4641-4652.	6.6	38
5409	Highly Efficient Reduction of Sulfoxides with the System Borane/Oxo-rhenium Complexes. Organometallics, 2010, 29, 5517-5525.	1.1	63

#	ARTICLE	IF	CITATIONS
5410	Neutral <i>cis</i> -Alkyl Olefin Rhodium(I) Complexes: Models of Intermediates in Late Transition Metal Olefin Polymerization with Surprising Structure. <i>Organometallics</i> , 2010, 29, 5496-5503.	1.1	21
5411	Microwave spectrum and structural parameters for the formamide-formic acid dimer. <i>Journal of Chemical Physics</i> , 2010, 133, 174304.	1.2	27
5412	Synthetic and Computational Studies on Factors Controlling Structures of Molecular Triangles and Squares and Their Equilibrium in Solutions. <i>Inorganic Chemistry</i> , 2010, 49, 2008-2015.	1.9	45
5413	Carbon-Oxygen Bond Forming Mechanisms in Rhenium Oxo-Alkyl Complexes. <i>Organometallics</i> , 2010, 29, 2026-2033.	1.1	9
5414	Experimental Evidence for Magnetic Exchange in Di- and Trinuclear Uranium(IV) Ethynylbenzene Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 1595-1606.	1.9	66
5415	Modeling Photoelectron Spectra of Conjugated Oligomers with Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10997-11007.	1.1	16
5416	Nonadiabatic ab Initio Dynamics of a Model Protonated Schiff Base of 9-cis Retinal. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8190-8201.	1.1	30
5417	Mechanism Insight into the Cyanide-Catalyzed Benzoin Condensation: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9222-9230.	1.1	24
5418	Quantum Chemical Characterization of Low-Lying Excited States of an Aryl Peroxycarbonate: Mechanistic Implications for Photodissociation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4289-4295.	1.1	2
5419	Thermal Carbosilylation of Endohedral Dimetallofullerene La ₂ @Ih-C ₈₀ with Silirane. <i>Journal of the American Chemical Society</i> , 2010, 132, 17953-17960.	6.6	31
5420	Raman Spectroscopic Investigation of Tetraethylammonium Polybromides. <i>Inorganic Chemistry</i> , 2010, 49, 8684-8689.	1.9	76
5421	Low Symmetry in Molecules with Heavy Peripheral Atoms. The Gas-Phase Structure of Perfluoro(methylcyclohexane), C ₆ F ₁₁ CF ₃ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 11022-11026.	1.1	3
5422	Electron Momentum Spectroscopy of Norbornadiene at the Benchmark ADC(3) Level. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9374-9387.	1.1	9
5423	Comparative DFT Analysis of Ligand and Solvent Effects on the Mechanism of H ₂ Activation in Water Mediated by Half-Sandwich Complexes [Cp ² Ru(PTA) ₂ Cl] (Cp ² =) Tj ETQq1 1 0.784314 rBT /Overlock 10 Tf	1.1	32
5424	Two-, three-, and four-bond N ¹⁵ F spin-spin coupling constants in fluoroazines. <i>Molecular Physics</i> , 2010, 108, 1367-1373.	0.8	9
5425	Single-Molecule Interfacial Electron Transfer in Donor-Bridge-Nanoparticle Acceptor Complexes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14309-14319.	1.2	26
5426	Fluxionality of [(Ph ₃ P) ₃ M(X)] (M = Rh, Ir). The Red and Orange Forms of [(Ph ₃ P) ₃ Ir(Cl)]. Which Phosphine Dissociates Faster from Wilkinson's Catalyst?. <i>Journal of the American Chemical Society</i> , 2010, 132, 12013-12026.	6.6	50
5427	Yb@C ₂ n (<i>n</i> = 40, 41, 42): New Fullerene Allotropes with Unexplored Electrochemical Properties. <i>Journal of the American Chemical Society</i> , 2010, 132, 5896-5905.	6.6	108

#	ARTICLE	IF	CITATIONS
5428	A DFT Study on the Magnetostructural Property of Ferromagnetic Heteroverdazyl Diradicals with Phenylene Coupler. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11833-11841.	1.1	34
5429	Local Electronic Structure and Stability of Pentacene Oxyradicals. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5429-5437.	1.5	20
5430	Combined Solid-State NMR and Theoretical Calculation Studies of Brønsted Acid Properties in Anhydrous 12-Molybdophosphoric Acid. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15464-15472.	1.5	57
5431	Quantum Refinement of Protein Structures: Implementation and Application to the Red Fluorescent Protein DsRed.M1. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15413-15423.	1.2	28
5432	Holo-Ni(II)HpNikR Is an Asymmetric Tetramer Containing Two Different Nickel-Binding Sites. <i>Journal of the American Chemical Society</i> , 2010, 132, 14447-14456.	6.6	36
5433	Solid-State Density Functional Theory Investigation of the Terahertz Spectra of the Structural Isomers 1,2-Dicyanobenzene and 1,3-Dicyanobenzene. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12513-12521.	1.1	44
5434	Thorpe-Ingold Acceleration of Oxirane Formation Is Mostly a Solvent Effect. <i>Journal of the American Chemical Society</i> , 2010, 132, 8766-8773.	6.6	28
5435	Theoretical Study on the Structure and Cation-Anion Interaction of Amino Acid Cation Based Amino Acid Ionic Liquid [Pro] ⁺ [NO ₃] ⁻ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 10243-10252.	1.1	52
5436	C-H vs C-C Bond Activation of Acetonitrile and Benzonitrile via Oxidative Addition: Rhodium vs Nickel and Cp* vs Tp ² (Tp ² = Hydrotris(3,5-dimethylpyrazol-1-yl)borate, Cp* =) <i>Tj ETQqO O 0 rgBT /Overlock 10 Tf 50 422 Td (i<sup>5</sup>/su</i> 16278-16284.	6.6	85
5437	Building Self-Assembled Molecular Layers with Axially Substituted Titanium Phthalocyanines. <i>Langmuir</i> , 2010, 26, 12709-12715.	1.6	6
5438	Platinum-Mediated C-H Bond Activation of Arene Solvents and Subsequent C-C Bond Formation. <i>Organometallics</i> , 2010, 29, 4619-4627.	1.1	21
5439	Acyclic Guanidines as Organic Catalysts for Living Polymerization of Lactide. <i>Macromolecules</i> , 2010, 43, 1660-1664.	2.2	74
5440	Theoretical Study of Initial Adsorptions and Subsequent Surface Rearrangements of H ₂ O ₂ on Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14187-14192.	1.5	4
5441	Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and Møller-Plesset Perturbation Theories. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6721-6727.	1.1	107
5442	Nickel Complexes with Bis(8-quinolyl)silyl Ligands. An Unusual Ni ₃ Si ₂ Cluster Containing Six-Coordinate Silicon. <i>Organometallics</i> , 2010, 29, 5544-5550.	1.1	25
5443	Ionization-Induced Structural Changes in Uracil Dimers and Their Spectroscopic Signatures. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 705-717.	2.3	21
5444	Molecular Orientation of Individual Lu@C ₈₂ Molecules Demonstrated by Scanning Tunneling Microscopy. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14704-14709.	1.5	27
5445	Sulfur-Based Redox Reactions in Mo ₃ S ₇ ⁴⁺ and Mo ₃ S ₄ ⁴⁺ Clusters Bearing Halide and 1,2-Dithiolene Ligands: a Mass Spectrometric and Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2010, 49, 8045-8055.	1.9	11

#	ARTICLE	IF	CITATIONS
5446	Local and Global Electronic Effects in Single and Double Boron-Doped Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 1528-1533.	1.5	26
5447	The Anionic (9-Methyladenine) ⁺ (1-Methylthymine) Base Pair Solvated by Formic Acid. A Computational and Photoelectron Spectroscopy Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11353-11362.	1.2	8
5448	Unambiguous Assignment of Vibrational Spectra of Cyclosporins A and H. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9768-9773.	1.1	5
5449	Structural Determinants for the Stereoselective Hydrolysis of Chiral Substrates by Phosphotriesterase. <i>Biochemistry</i> , 2010, 49, 7988-7997.	1.2	25
5450	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. <i>Organometallics</i> , 2010, 29, 2040-2045.	1.1	28
5451	Photocatalytic Water Oxidation at the GaN (101̄...0) ⁺ Water Interface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13695-13704.	1.5	74
5452	Proton and Hydride Affinities in Excited States: Magnitude Reversals in Proton and Hydride Affinities between the Lowest Singlet and Triplet States of Annulenyl and Benzannulenyl Anions and Cations. <i>Journal of Organic Chemistry</i> , 2010, 75, 2189-2196.	1.7	8
5453	Competitive Carbon ⁺ Sulfur vs Carbon ⁺ Carbon Bond Activation of 2-Cyanothiophene with [Ni(dippe)H] ₂ . <i>Journal of the American Chemical Society</i> , 2010, 132, 12412-12421.	6.6	68
5454	Multiple Low-Lying States for Compound I of P450 _{cam} and Chloroperoxidase Revealed from Multireference Ab Initio QM/MM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 940-953.	2.3	66
5455	Theoretical Study of Excited States of Pyrazolate- and Pyridinethiolate-Bridged Dinuclear Platinum(II) Complexes: Relationship between Geometries of Excited States and Phosphorescence Spectra. <i>Inorganic Chemistry</i> , 2010, 49, 8977-8985.	1.9	25
5456	Si ⁺ X Multiple Bonding with Four-Coordinate Silicon? Insights into the Nature of the Si ⁺ O and Si ⁺ S Double Bonds in Stable Silanoic Esters and Related Thioesters: A Combined NMR Spectroscopic and Computational Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 5443-5455.	6.6	101
5457	Photophysical and Theoretical Studies of Ruthenium(II) ⁺ Acetylide and ⁺ Cyanide Complexes with Aromatic Diimine and Trithiacyclononane. <i>Organometallics</i> , 2010, 29, 6259-6266.	1.1	20
5458	What Is the Preferred Structure of the Meisenheimer ⁺ Wheland Complex Between <i>sym</i> -Triaminobenzene and 4,6-Dinitrobenzofuroxan?. <i>Journal of Organic Chemistry</i> , 2010, 75, 3761-3765.	1.7	14
5459	Water Catalysis and Anticatalysis in Photochemical Reactions: Observation of a Delayed Threshold Effect in the Reaction Quantum Yield. <i>Journal of the American Chemical Society</i> , 2010, 132, 15154-15157.	6.6	19
5460	Photoisomerization Ability of Molecular Switches Adsorbed on Au(111): Comparison between Azobenzene and Stilbene Derivatives. <i>Journal of Physical Chemistry C</i> , 2010, 114, 1231-1239.	1.5	46
5461	Influence of Explicit Hydration Waters in Calculating the Hydrolysis Constants for Geochemically Relevant Metals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1917-1925.	1.1	40
5462	Metal-Complexes As Ligands to Generate Asymmetric Homo- and Heterodinuclear M _A ^{III} M _B ^{II} Species: a Magneto-Structural and Spectroscopic Comparison of Imidazole-N versus Pyridine-N. <i>Inorganic Chemistry</i> , 2010, 49, 626-641.	1.9	21
5463	Bottom-Up Approach to Innovative Memory Devices: II. Molecular Adsorption on Electrodes and the Asymmetric Response. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21439-21443.	1.5	2

#	ARTICLE	IF	CITATIONS
5464	Direct Dynamics Implementation of the Least-Action Tunneling Transmission Coefficient. Application to the CH ₄ /CD ₃ H/CD ₄ + CF ₃ Abstraction Reactions. Journal of Chemical Theory and Computation, 2010, 6, 3015-3025.	2.3	12
5465	Global Exploration of the Enthalpy Landscape of Calcium Carbide. Journal of Physical Chemistry B, 2010, 114, 15573-15581.	1.2	33
5466	Trends in R [•] X Bond Dissociation Energies (R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). Journal of Chemical Theory and Computation, 2010, 6, 1462-1469.	2.3	39
5467	Steric Factors Override Thermodynamic Driving Force in Regioselectivity of Proline Hydroxylation by Prolyl-4-hydroxylase Enzymes. Journal of Physical Chemistry A, 2010, 114, 13234-13243.	1.1	41
5468	{2 + 2} Cycloaddition of Alkyne with Titanium [•] Imido Complex: Theoretical Study of Determining Factor of Reactivity and Regioselectivity. Journal of Physical Chemistry A, 2010, 114, 659-665.	1.1	17
5469	Theoretical and Raman Spectroscopic Studies of Phenolic Lignin Model Monomers. Journal of Physical Chemistry B, 2010, 114, 8009-8021.	1.2	86
5470	Site-specific Xe additions into Cu [•] ZSM-5 zeolite. Physical Chemistry Chemical Physics, 2010, 12, 2392.	1.3	32
5471	Azomethane: Nonadiabatic Photodynamical Simulations in Solution. Journal of Physical Chemistry A, 2010, 114, 12585-12590.	1.1	43
5472	Grafting of Lanthanide Complexes on Silica Surfaces: A Theoretical Investigation. Journal of Physical Chemistry A, 2010, 114, 6322-6330.	1.1	29
5473	Mechanistic Study of Amine to Imine Oxidation in a Dinuclear Cu(II) Complex Containing an Octaaza Dinucleating Ligand. Inorganic Chemistry, 2010, 49, 5977-5985.	1.9	29
5474	Unexpected Photoproduct Generated via the Acetone-Sensitized Photolysis of 5-Bromo-2 [•] -deoxyuridine in a Water/Isopropanol Solution: Experimental and Computational Studies. Journal of Physical Chemistry B, 2010, 114, 16902-16907.	1.2	2
5475	Effect of Hydration on the Hydrogen Abstraction Reaction by HO in DMS and its Oxidation Products. Journal of Physical Chemistry A, 2010, 114, 4857-4863.	1.1	56
5476	¹³ C-Acetyl Side-Chains in Saccharides: NMR ¹³ C-Coupling Equations Sensitive to CH [•] NH and NH [•] CO Bond Conformations in 2-Acetamido-2-deoxy-aldohexopyranosyl Rings. Journal of Organic Chemistry, 2010, 75, 4899-4910.	1.7	21
5477	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. Journal of Physical Chemistry C, 2010, 114, 3340-3345.	1.5	56
5478	Theoretical Characterization of the Air-Stable, High-Mobility Dinaphtho[2,3- <i>b</i> : <i>i</i> ':2 [•] 3 [•] - <i>f</i> : <i>i</i> ']thieno[3,2- <i>b</i> : <i>i</i> ']-thiophene Organic Semiconductor. Journal of Physical Chemistry C, 2010, 114, 2334-2340.	1.5	73
5479	Favored Reaction Mechanism of Calcium-Dependent Phospholipase A ₂ . Insights from Density Functional Exploration. Journal of Physical Chemistry B, 2010, 114, 11584-11593.	1.2	5
5480	Unusual Electronic Effects Imparted by Bridging Dinitrogen: an Experimental and Theoretical Investigation. Inorganic Chemistry, 2010, 49, 9497-9507.	1.9	17
5481	Unprecedented Near-Infrared (NIR) Emission in Diplatinum(III) (d ⁷) [•] Complexes at Room Temperature. Journal of the American Chemical Society, 2010, 132, 7094-7103.	6.6	53

#	ARTICLE	IF	CITATIONS
5482	Nonadiabatic Excited-State Dynamics with Hybrid ab Initio Quantum-Mechanical/Molecular-Mechanical Methods: Solvation of the Pentadieniminium Cation in Apolar Media. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6757-6765.	1.1	74
5483	Inclusion of Dispersion Effects Significantly Improves Accuracy of Calculated Reaction Barriers for Cytochrome P450 Catalyzed Reactions. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3232-3237.	2.1	153
5484	Understanding the Interactions of Cellulose with Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4293-4301.	1.2	299
5485	The R.E.D. tools: advances in RESP and ESP charge derivation and force field library building. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 7821.	1.3	778
5486	Theoretical study of H ₂ splitting and storage by boron–nitrogen-based systems: a bimolecular case and some qualitative aspects. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 149-155.	1.3	18
5487	Nuclear-Electronic Orbital Method within the Fragment Molecular Orbital Approach. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5582-5588.	1.5	16
5488	Rationally Designed Fluorescence Turn-On Sensors: A New Design Strategy Based on Orbital Control. <i>Inorganic Chemistry</i> , 2010, 49, 8552-8557.	1.9	115
5489	Synthesis and Reactions of Phosphaporphyrins: Reconstruction of ĩ€-Skeleton Triggered by Oxygenation of a Core Phosphorus Atom. <i>Journal of Organic Chemistry</i> , 2010, 75, 375-389.	1.7	45
5490	Effects of mercury(II) on structural properties, electronic structure and UV absorption spectra of a duplex containing thymine–mercury(II)–thymine nucleobase pairs. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 909-917.	1.3	33
5491	Interaction of Ketocyanine Dye with a Co ²⁺ Ion: An Electronic Spectroscopic Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10388-10394.	1.1	7
5492	Catalytic Role of Vicinal OH in Ester Aminolysis: Proton Shuttle versus Hydrogen Bond Stabilization. <i>Journal of Organic Chemistry</i> , 2010, 75, 6782-6792.	1.7	18
5493	Calculation of IR frequencies and intensities in electrical and mechanical anharmonicity approximations: Application to small water clusters. <i>Journal of Chemical Physics</i> , 2010, 133, 034102.	1.2	47
5494	Experimental and Theoretical Investigation of Epoxide Quebrachitol Derivatives Through Spectroscopic Analysis. <i>Organic Letters</i> , 2010, 12, 5458-5461.	2.4	25
5495	Describing Anions by Density Functional Theory: Fractional Electron Affinity. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2726-2735.	2.3	104
5496	Manganese Catalysts for C–H Activation: An Experimental/Theoretical Study Identifies the Stereoelectronic Factor That Controls the Switch between Hydroxylation and Desaturation Pathways. <i>Journal of the American Chemical Society</i> , 2010, 132, 7605-7616.	6.6	100
5497	Ring-Opening Polymerization of ϵ -Caprolactone Catalyzed by Sulfonic Acids: Computational Evidence for Bifunctional Activation. <i>Journal of Organic Chemistry</i> , 2010, 75, 6581-6587.	1.7	98
5498	Self-Assembly of Structurally Persistent Micelles Is Controlled by Specific-Ion Effects and Hydrophobic Guests. <i>Langmuir</i> , 2010, 26, 10460-10466.	1.6	22
5499	Tautomerism in Cytosine and Uracil: A Theoretical and Experimental X-ray Absorption and Resonant Auger Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10270-10276.	1.1	77

#	ARTICLE	IF	CITATIONS
5500	CO and NO complexes of Fe(II) and Co(II) porphyrins. <i>Journal of Coordination Chemistry</i> , 2010, 63, 2854-2867.	0.8	7
5501	Surface Speciation of Phosphate on Boehmite ($\text{Î}^3\text{-AlOOH}$) Determined from NMR Spectroscopy. <i>Langmuir</i> , 2010, 26, 4753-4761.	1.6	63
5502	Platinum(II) and Phosphorus MM3 Force Field Parametrization for Chromophore Absorption Spectra at Room Temperature. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4981-4987.	1.1	10
5503	Convergence in the Evolution of Nanodiamond Raman Spectra with Particle Size: A Theoretical Investigation. <i>ACS Nano</i> , 2010, 4, 4475-4486.	7.3	36
5504	Using the nitro group to induce Î^{E} -stacking in terthiophenes. <i>Canadian Journal of Chemistry</i> , 2010, 88, 309-317.	0.6	6
5505	Structure of the Calix[4]arene $\text{â}^{\text{H}}(\text{H}_{2\text{O}}$) Cluster: The World's Smallest Cup of Water. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2967-2972.	1.1	38
5506	Oriental order of a ferroelectric liquid crystal with small layer contraction. <i>Physical Review E</i> , 2010, 82, 031702.	0.8	11
5507	The mechanism of the Stevens and Sommelet â^{H} Hauser Rearrangements. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 3608-3617.	1.7	73
5508	Mechanisms of the Au- and Pt-Catalyzed Intramolecular Acetylenic Schmidt Reactions: A DFT Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 7842-7854.	1.7	57
5509	Reaction free energies in organic solvents: comparing different quantum mechanical methods. <i>Molecular Simulation</i> , 2010, 36, 1197-1207.	0.9	4
5510	Dilithioplumbole: A Lead-Bearing Aromatic Cyclopentadienyl Analog. <i>Science</i> , 2010, 328, 339-342.	6.0	112
5511	The [13]Annulene Cation Is a Stable M â^{H} bius Annulene Cation. <i>Organic Letters</i> , 2010, 12, 1708-1711.	2.4	24
5512	The Vibrational Spectrum of Parabanic Acid by Inelastic Neutron Scattering Spectroscopy and Simulation by Solid-State DFT. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3630-3641.	1.1	6
5513	Mechanistic Aspects of Nucleophilic Substitution at Half-Sandwich Metal Complexes. <i>Organometallics</i> , 2010, 29, 6209-6218.	1.1	8
5514	Computational Studies of the Isomerization and Hydration Reactions of Acetaldehyde Oxide and Methyl Vinyl Carbonyl Oxide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9192-9204.	1.1	117
5515	Vibrational spectra of corticosteroid hormones in the terahertz range. <i>Proceedings of SPIE</i> , 2010, , .	0.8	3
5516	Triphenylphosphane-Modified Cobalt Catalysts for the Selective Carbonylation of Ethyl Diazoacetate. <i>Organometallics</i> , 2010, 29, 3837-3851.	1.1	20
5517	Dissociation of copper(ii) ternary complexes containing cystine. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9017.	1.3	1

#	ARTICLE	IF	CITATIONS
5518	Mechanistic Insights into Alkene Epoxidation with H_2O_2 by Ti- and other TM-Containing Polyoxometalates: Role of the Metal Nature and Coordination Environment. <i>Journal of the American Chemical Society</i> , 2010, 132, 7488-7497.	6.6	148
5519	Ab Initio Study of Ternary Complexes $A\cdot\cdot\cdot NCH\cdot\cdot\cdot C$ with A,C = HCN, HF, HCl, ClF, and LiH: Energetics and Spin-Spin Coupling Constants across Intermolecular Bonds. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8463-8473.	1.1	26
5520	Quantum-chemical simulation of solid-state NMR spectra: the example of a molecular tweezer host-guest complex. <i>Molecular Physics</i> , 2010, 108, 333-342.	0.8	15
5521	Variational geminal-augmented multireference self-consistent field theory: Two-electron systems. <i>Journal of Chemical Physics</i> , 2010, 132, 054103.	1.2	30
5522	Orientation and Stereodynamic Paths of Planar Monodentate Ligands in Square Planar Nickel N2S Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 5503-5514.	1.9	20
5523	The binding of vitamin B12 to transcobalamin(II); structural considerations for bioconjugate design—a molecular dynamics study. <i>Molecular BioSystems</i> , 2010, 6, 1611.	2.9	15
5524	Vanadium Diaminebis(phenolate) Complexes: Syntheses, Structures, and Reactivity in Sulfoxidation Catalysis. <i>Inorganic Chemistry</i> , 2010, 49, 7452-7463.	1.9	82
5525	A comparison between nickel and palladium precatalysts of 1,2,4-triazole based N-heterocyclic carbenes in hydroamination of activated olefins. <i>Dalton Transactions</i> , 2010, 39, 2515.	1.6	57
5526	Highly efficient palladium precatalysts of homoscorpionate bispyrazolyl ligands for the more challenging Suzuki-Miyaura cross-coupling of aryl chlorides. <i>Dalton Transactions</i> , 2010, 39, 7353.	1.6	34
5527	Synthesis of <i>cis</i> - and <i>trans</i> -Diisothiocyanato-Bis(NHC) Complexes of Nickel(II) and Applications in the Kumada-Corriu Reaction. <i>Organometallics</i> , 2010, 29, 3746-3752.	1.1	38
5528	Cobalt-Porphyrin Catalyzed Electrochemical Reduction of Carbon Dioxide in Water. 1. A Density Functional Study of Intermediates. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10166-10173.	1.1	69
5529	Osmium Complexes Containing N-Heterocyclic Carbene-Based C,N,C-Pincer Ligands. <i>Organometallics</i> , 2010, 29, 2533-2539.	1.1	37
5530	Free energy calculations using dual-level Born-Oppenheimer molecular dynamics. <i>Journal of Chemical Physics</i> , 2010, 133, 064103.	1.2	22
5531	Scaling Behavior of Electronic Excitations in Assemblies of Molecules with Degenerate Ground States. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2213-2220.	1.1	3
5532	B3LYP calculations of cerium oxides. <i>Journal of Chemical Physics</i> , 2010, 132, 054110.	1.2	65
5533	A DFT periodic study on the interaction between O_2 and cation exchanged chabazite MCHA (M = H ⁺ , Na ⁺ or Cu ⁺): effects in the triplet-singlet energy gap. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 442-452.	1.3	19
5534	The importance of chain connectivity in the formation of non-covalent interactions between polymers and single-walled carbon nanotubes and its impact on dispersion. <i>Soft Matter</i> , 2010, 6, 2801.	1.2	34
5535	Sodium complexes containing 2-iminopyrrolyl ligands: the influence of steric hindrance in the formation of coordination polymers. <i>Dalton Transactions</i> , 2010, 39, 736-748.	1.6	42

#	ARTICLE	IF	CITATIONS
5536	Computational investigation on the mechanism and the stereoselectivity of Morita-Baylis-Hillman reaction and the effect of the bifunctional catalyst N-methylprolinol. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 3985.	1.5	30
5537	Molecular mechanism of acid-triggered aryl-halide reductive elimination in well-defined aryl-halide species. <i>Dalton Transactions</i> , 2010, 39, 10458.	1.6	41
5538	A DFT study of the reactivity of actinidocenes (U, Np and Pu) with pyridine and pyridine N-oxide derivatives. <i>Dalton Transactions</i> , 2010, 39, 6682.	1.6	29
5539	Computational study of ethene hydroarylation at $[\text{Ir}(\text{OAc})(\text{PMe}_3)\text{Cp}]^+$. <i>Dalton Transactions</i> , 2010, 39, 10520.	1.6	20
5540	Existence of dual species composed of Cu^+ in CuMFI being bridged by C_2H_2 . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6455.	1.3	25
5541	Development of novel thioether compound for spontaneous chiral crystallization. <i>CrystEngComm</i> , 2010, 12, 1394-1396.	1.3	2
5542	Synthesis and structures of platinum diphenylacetylene and dithiolate complexes bearing diphosphinidenecyclobutene ligands (DPCB-Y). <i>New Journal of Chemistry</i> , 2010, 34, 1713.	1.4	11
5543	Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5375.	1.3	29
5544	Theoretical study on the effect of intramolecular hydrogen bonding on OH stretching overtone decay lifetime of ethylene glycol, 1,3-propanediol, and 1,4-butanediol. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13950.	1.3	28
5545	Polychlorinated trityl radicals for dynamic nuclear polarization: the role of chlorine nuclei. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5824.	1.3	20
5546	The thermal isomerization of the GFP chromophore: A computational study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11051.	1.3	9
5547	Water and ethanol desorption in the flexible metal organic frameworks, MIL-53 (Cr, Fe), investigated by complex impedance spectroscopy and density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12478.	1.3	41
5548	Supraicosahedral indenyl cobaltacarboranes. <i>Dalton Transactions</i> , 2010, 39, 5286.	1.6	24
5549	Theoretical and Spectroelectrochemical Studies on the Adsorption and Oxidation of Glyoxylate and Hydrated Glyoxylate Anions at Gold Electrodes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12554-12564.	1.5	19
5550	On the existence of the H3 tautomer of adenine in aqueous solution. Rationalizations based on hybrid quantum mechanics/molecular mechanics predictions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 761-768.	1.3	25
5551	Structure of the hydrated Ca^{2+} and Cl^- : Combined X-ray absorption measurements and QM/MM MD simulations study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10876.	1.3	49
5552	The gas-phase structure and some reactions of the bulky primary silane $(\text{Me}_3\text{Si})_3\text{CSiH}_3$ and the solid-state structure of the bulky dialkyl disilane $[(\text{Me}_3\text{Si})_3\text{CSiH}_2]_2$. <i>Dalton Transactions</i> , 2010, 39, 9353.	1.6	4
5553	Improvement of cytotoxicity of titanocene-functionalized mesoporous materials by the increase of the titanium content. <i>Dalton Transactions</i> , 2010, 39, 2597.	1.6	47

#	ARTICLE	IF	CITATIONS
5554	Computational Studies on the Photophysical Properties and NMR Fluxionality of Dinuclear Platinum(II) A-Frame Alkynyl Diphosphine Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 10930-10939.	1.9	5
5555	Synthesis, Structural Characterization, and Photophysical Study of Luminescent Face-to-Face Dinuclear Platinum(II) Alkynyl Phosphine Complexes and Their Tetranuclear Mixed-Metal Platinum(II)-Silver(I) and -Copper(I) Complexes. <i>Organometallics</i> , 2010, 29, 5558-5569.	1.1	30
5556	Atom-Efficient Carbon-Oxygen Bond Formation Processes. DFT Analysis of the Intramolecular Hydroalkoxylation/Cyclization of Alkynyl Alcohols Mediated by Lanthanide Catalysts. <i>Organometallics</i> , 2010, 29, 2004-2012.	1.1	23
5557	Quantum Chemical Study on Ethylene Addition to $(O\hat{\cdot})_2Os(NH)_2$ and $(O\hat{\cdot})_2Os(NH)-cyclo-(NHCH_2)_2CH_2HN\hat{\cdot}$ as Model Complexes for the Osmium-Catalyzed Aminohydroxylation of Olefins. <i>Organometallics</i> , 2010, 29, 1560-1568.	1.1	7
5558	Polycyclic aromatic hydrocarbon formation mechanism in the $\hat{\cdot}$ particle phase: A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9429.	1.3	27
5559	Synthetic, structural and computational studies on adducts of the 4,1,2-SnC ₂ B ₁₀ supraicosahedral stannacarborane. <i>Dalton Transactions</i> , 2010, 39, 2412.	1.6	14
5560	The molecular structure, equilibrium conformation and barrier to internal rotation in decachloroferrocene, $Fe(\hat{\cdot}-C_5Cl_5)_2$, determined by gas electron diffraction. <i>Dalton Transactions</i> , 2010, 39, 4631.	1.6	7
5561	The digallane molecule, Ga ₂ H ₆ : experimental update giving an improved structure and estimate of the enthalpy change for the reaction $Ga_2H_6(g) \hat{\cdot} 2GaH_3(g)$. <i>Dalton Transactions</i> , 2010, 39, 5637.	1.6	9
5562	Silyl and $\hat{\cdot}$ -silane ruthenium complexes: Chloride substituent effects on the catalysed silylation of ethylene. <i>Dalton Transactions</i> , 2010, 39, 8492.	1.6	18
5563	Bipolar redox behaviour, field-effect mobility and transistor switching of the low-molecular azo glass AZOPD. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13828.	1.3	15
5564	Electric field gradients of transition metal complexes from density functional theory: assessment of functionals, geometries and basis sets. <i>Dalton Transactions</i> , 2010, 39, 5319.	1.6	21
5565	Combined experimental and theoretical investigation into C-H activation of cyclic alkanes by Cp ² Rh(CO) ₂ (Cp ² = $\hat{\cdot}$ -5-C ₅ H ₅ or $\hat{\cdot}$ -5-C ₅ Me ₅). <i>Dalton Transactions</i> , 2011, 40, 1751.	1.6	18
5566	51V NMR parameters of VOCl ₃ : static and dynamic density functional study from the gas phase to the bulk. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 619-627.	1.3	19
5567	Basic ancillary ligands promote O-O bond formation in iridium-catalyzed water oxidation: A DFT study. <i>Dalton Transactions</i> , 2011, 40, 11241.	1.6	45
5568	Existence of both blue-shifting hydrogen bond and Lewis acid-base interaction in the complexes of carbonyls and thiocarbonyls with carbon dioxide. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14033.	1.3	40
5569	On multiferroicity of TTF-CA molecular crystal. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 144-148.	1.3	15
5570	Theoretical studies on the mechanism and stereoselectivity of Rh(Phebox)-catalyzed asymmetric reductive aldol reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5845.	1.5	26
5571	Modification of the magnetic properties of a heterometallic wheel by inclusion of a Jahn-Teller distorted Cu(II) ion. <i>Dalton Transactions</i> , 2011, 40, 8533.	1.6	12

#	ARTICLE	IF	CITATIONS
5572	Chiral selection in the formation of borates from racemic binaphthols and related diols. <i>CrystEngComm</i> , 2011, 13, 2923.	1.3	8
5573	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 115-160.	0.9	116
5574	The thermal C2≡C6/[2 + 2] cyclisation of enyne-allenes: Reversible diradical formation. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 3776.	1.5	15
5575	Dinuclear silver(I) complexes for the design of metal–ligand networks based on triazolopyrimidines. <i>Dalton Transactions</i> , 2011, 40, 11845.	1.6	42
5576	Protonation and coordination ability of small peptides – theoretical and experimental approaches for elucidation. <i>Journal of Coordination Chemistry</i> , 2011, 64, 2419-2442.	0.8	15
5577	Bridge-Mediated Excitation Energy Transfer Pathways through Protein Media: a Slater Determinant-Based Electronic Coupling Calculation Combined with Localized Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10814-10822.	1.1	16
5578	Border Reactivity of Polycyclic Aromatic Hydrocarbons and Soot Platelets Toward Ozone. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 470-481.	1.1	7
5579	Methanol triggered ligand flip isomerization in a binuclear copper(I) complex and the luminescence response. <i>Chemical Communications</i> , 2011, 47, 9179.	2.2	52
5580	Regression Formulas for Density Functional Theory Calculated ¹ H and ¹³ C NMR Chemical Shifts in Toluene- <i>d</i> ₈ . <i>Journal of Physical Chemistry A</i> , 2011, 115, 12364-12372.	1.1	50
5581	Mechanism of the photochemical process of singlet oxygen production by phenalenone. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4138.	1.3	19
5582	Chemically reactive species remain alive inside carbon nanotubes: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 337-346.	1.3	17
5583	Phosphoric and phosphoramidic acids as bifunctional catalysts for the ring-opening polymerization of ϵ -caprolactone: a combined experimental and theoretical study. <i>Polymer Chemistry</i> , 2011, 2, 2249.	1.9	98
5584	DFT study of the Ring Opening Polymerization of ϵ -caprolactone by grafted lanthanide complexes: 1 st Effect of the grafting mode on the reactivity of borohydride complexes. <i>Dalton Transactions</i> , 2011, 40, 11211.	1.6	24
5585	Antiferromagnetic interactions in the quarter-filled organic conductor (EDO-TTF) ₂ PF ₆ . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 12328.	1.3	9
5586	DFT calculations of ²⁹ Si-NMR chemical shifts in Ru(II) silyl complexes: Searching for trends and accurate values. <i>Dalton Transactions</i> , 2011, 40, 11321.	1.6	12
5587	Pseudo Jahn–Teller origin of cis–trans and other conformational changes. The role of double bonds. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 3502.	1.3	21
5588	DFT study of the Ring Opening Polymerization of ϵ -caprolactone by grafted lanthanide complexes: 2 nd Effect of the initiator ligand. <i>Dalton Transactions</i> , 2011, 40, 11228.	1.6	23
5589	Agostic or not? Detailed Density Functional Theory studies of the compounds [LRh(CO)Cl], [LRh(COD)Cl] and [LRhCl] (L = cyclic (alkyl)(amino)carbene, COD = cyclooctadiene). <i>Dalton Transactions</i> , 2011, 40, 136-141.	1.6	24

#	ARTICLE	IF	CITATIONS
5590	O–O Bond activation in H ₂ O ₂ and (CH ₃) ₃ C-OOH mediated by [Ni(cyclam)(CH ₃ CN) ₂](ClO ₄) ₂ : Different mechanisms to form the same Ni(III) product?. Dalton Transactions, 2011, 40, 6868.	1.6	15
5591	Ionization potentials of adenine along the internal conversion pathways. Physical Chemistry Chemical Physics, 2011, 13, 15492.	1.3	28
5592	Urease inhibition and anti-leishmanial assay of substituted benzoylguanidines and their copper(II) complexes. Dalton Transactions, 2011, 40, 9202.	1.6	22
5593	Simultaneous control of spectroscopic and electrochemical properties in functionalised electrochemiluminescent tris(2,2'-bipyridine)ruthenium(II) complexes. Analyst, The, 2011, 136, 1329.	1.7	60
5594	Theoretical studies on interactions between low energy electrons and protein-DNA fragments: valence anions of AT-amino acids side chain complexes. Physical Chemistry Chemical Physics, 2011, 13, 19499.	1.3	5
5595	Predicting hydration Gibbs energies of alkyl-aromatics using molecular simulation: a comparison of current force fields and the development of a new parameter set for accurate solvation data. Physical Chemistry Chemical Physics, 2011, 13, 17384.	1.3	22
5596	Pathway analysis of super-exchange electronic couplings in electron transfer reactions using a multi-configuration self-consistent field method. Physical Chemistry Chemical Physics, 2011, 13, 7043.	1.3	12
5597	Molecular dynamics effects on luminescence properties of oligothiophene derivatives: a molecular mechanics-response theory study based on the CHARMM force field and density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 17532.	1.3	22
5598	Multiple bonding versus cage formation in organophosphorus compounds: the gas-phase structures of tricyclo-P ₃ (CBut) ₂ Cl and Pt(CBut) ₂ determined by electron diffraction and computational methods. Dalton Transactions, 2011, 40, 5611.	1.6	5
5599	Brønsted-NH ₄ ⁺ mechanism versus nitrite mechanism: new insight into the selective catalytic reduction of NO by NH ₃ . Physical Chemistry Chemical Physics, 2011, 13, 453-460.	1.3	46
5600	Picosecond X-ray absorption measurements of the ligand substitution dynamics of Fe(CO) ₅ in ethanol. Physical Chemistry Chemical Physics, 2011, 13, 5590.	1.3	35
5601	Oligothiophene Tetracyanobutadienes: Alternative Donor-Acceptor Architectures for Molecular and Polymeric Materials. Chemistry of Materials, 2011, 23, 823-831.	3.2	42
5602	Empirical Correlation Methods for Temporary Anions. Journal of Physical Chemistry A, 2011, 115, 6675-6682.	1.1	28
5603	On the Unexpected Stability of the Dianion of Perylene Diimide in Water-A Computational Study. Journal of Physical Chemistry A, 2011, 115, 2047-2056.	1.1	49
5604	Dissociative Chemisorption of Trimethylgallium, Trimethylindium, and Ammonia on Gallium and Indium Nitride Substrates. A Computational Study. Journal of Physical Chemistry C, 2011, 115, 9090-9104.	1.5	12
5605	Quantum Proton Transfer in Hydrated Sulfuric Acid Clusters: A Perspective from Semiempirical Path Integral Simulations. Journal of Physical Chemistry A, 2011, 115, 11486-11494.	1.1	20
5606	Platinum(II) Complexes with Tetradentate Dianionic (O ⁻) ₂ C ⁻ (O ⁻) ₂ -Ligands. Organometallics, 2011, 30, 2980-2985.	1.1	23
5607	Application of the Quantum Cluster Equilibrium (QCE) Model for the Liquid Phase of Primary Alcohols Using B3LYP and B3LYP-D DFT Methods. Journal of Physical Chemistry B, 2011, 115, 3936-3941.	1.2	30

#	ARTICLE	IF	CITATIONS
5608	Simulating Picosecond Iron K-Edge X-ray Absorption Spectra by ab Initio Methods To Study Photoinduced Changes in the Electronic Structure of Fe(II) Spin Crossover Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10749-10761.	1.1	27
5609	Theoretical Study of Absorption and Emission Properties of Green and Yellow Emitting Iridium(III) Complexes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11861-11865.	1.1	15
5610	Molecular Orientation of Asphaltenes and PAH Model Compounds in Langmuir-Blodgett Films Using Sum Frequency Generation Spectroscopy. <i>Langmuir</i> , 2011, 27, 6049-6058.	1.6	116
5611	Ab Initio Study of Ternary Complexes X:(HCNH) ⁺ :Z with X, Z = NCH, CNH, FH, ClH, and FCl: Diminutive Cooperative Effects on Structures, Binding Energies, and Spin-Spin Coupling Constants Across Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12677-12687.	1.1	22
5612	Rearrangements and Interconversions of Heteroatom-Substituted Isocyanates, Isothiocyanates, Nitrile Oxides, and Nitrile Sulfides, RX≡NCY and RY≡CNX. <i>Journal of Organic Chemistry</i> , 2011, 76, 6024-6029.	1.7	16
5613	Radicals Formed in N-Acetylproline by Electron Attachment: Electron Spin Resonance Spectroscopy and Computational Studies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14846-14851.	1.2	6
5614	A Computational Study on the Chemical Fixation of Carbon Dioxide with Epoxide Catalyzed by LiBr Salt. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2258-2267.	1.1	46
5615	Synthesis, characterisation and mesomorphic properties of ester containing aroylhydrazones and their nickel(II) complexes. <i>Liquid Crystals</i> , 2011, 38, 1117-1129.	0.9	11
5616	o-Iminobenzosemiquinonate and p-methylbenzosemiquinonate Anion Radicals Coupled VO ₂ Stabilization. <i>Inorganic Chemistry</i> , 2011, 50, 2488-2500.	1.9	31
5617	Synthesis and Characterization of the Os ^{IV} (acac) ₂ PhCl and Study of CH Activation with Benzene. <i>Organometallics</i> , 2011, 30, 5088-5094.	1.1	6
5618	Role of four-membered rings in C ₃₂ fullerene stability and mechanisms of generalized Stone-Wales transformation: a density functional theory investigation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14629.	1.3	15
5619	Structures, Energies, and Spin-Spin Coupling Constants of Methyl-Substituted 1,3-Diborata-2,4-diphosphoniocyclobutanes: Four-member B ₂ P ₂ (CH ₃) _n H ₈ ⁿ , with n = 0, 1, 2, 4. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10502-10510.	1.1	1
5620	Synthesis, Structure, Ligand Dynamics, and Catalytic Activity of Cationic [Pd(³ -allyl)(² -E,N-EN-chelate)] ⁺ (E = P, O, S, Se) Complexes. <i>Organometallics</i> , 2011, 30, 5928-5942.	1.1	19
5621	Probing Ground-to-CT State Electronic Coupling for the System with No Apparent Charge Transfer Absorption Intensity by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2011, 115, 22557-22562.	1.5	8
5622	Topological and Electronic Influences on Magnetic Exchange Coupling in Fe(III) Ethynylbenzene Dendritic Building Blocks. <i>Journal of the American Chemical Society</i> , 2011, 133, 20823-20836.	6.6	23
5623	Gas Phase Synthesis of Au Clusters Deposited on Titanium Oxide Clusters and Their Reactivity with CO Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11479-11485.	1.1	42
5624	CO Oxidation by Lattice Oxygen on V ₂ O ₅ Nanotubes. <i>Journal of Physical Chemistry C</i> , 2011, 115, 14806-14811.	1.5	19
5625	High-level direct-dynamics variational transition state theory calculations including multidimensional tunneling of the thermal rate constants, branching ratios, and kinetic isotope effects of the hydrogen abstraction reactions from methanol by atomic hydrogen. <i>Journal of Chemical Physics</i> , 2011, 134, 094302.	1.2	66

#	ARTICLE	IF	CITATIONS
5626	Theoretical Investigations on the Photoinduced Phase Transition Mechanism of Tetrathiafulvalene-p-chloranil. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2233-2239.	2.3	7
5627	Structures, Energies, and Spin-Spin Coupling Constants of Fluoro-Substituted 1,3-Diborata-2,4-diphosphoniocyclobutanes: Four-Member B ₂ P ₂ F _n H ₈ (n = 0, 1, 2, 4). <i>Journal of Physical Chemistry A</i> , 2011, 115, 4511-4520.	1.1	5
5628	Modeling the Geometric, Electronic, and Redox Properties of Iron(III)-Containing Amphiphiles with Asymmetric [N ₂ O] Headgroups. <i>Inorganic Chemistry</i> , 2011, 50, 8356-8366.	1.9	15
5629	Electronic Structures of Group 9 Metallocorroles with Axial Amines. <i>Inorganic Chemistry</i> , 2011, 50, 764-770.	1.9	18
5630	Semiempirical UNO-CAS and UNO-CI: Method and Applications in Nanoelectronics. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11303-11312.	1.1	30
5631	On the Efficiency of Algorithms for Solving Hartree-Fock and Kohn-Sham Response Equations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1610-1630.	2.3	64
5632	Transient Innermolecular Carbene-Hemicarcerand Complex of Fluorophenylcarbene. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13799-13803.	1.1	3
5633	Investigation of the Low-Frequency Vibrations of Crystalline Tartaric Acid Using Terahertz Spectroscopy and Solid-State Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10052-10058.	1.1	23
5634	Behavior of Ag ₃ Clusters Inside a Nanometer-Sized Space of ZSM-5 Zeolite. <i>Inorganic Chemistry</i> , 2011, 50, 6533-6542.	1.9	24
5635	Pyridylamido Hafnium and Zirconium Complexes: Synthesis, Dynamic Behavior, and Ethylene/1-Octene and Propylene Polymerization Reactions. <i>Organometallics</i> , 2011, 30, 3318-3329.	1.1	73
5636	Solvent Effects on the Electronic Transitions of <i>p</i> -Nitroaniline: A QM/EFP Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 392-401.	1.1	111
5637	Electron Localization Function Study on Intramolecular Electron Transfer in the QTTFQ and DBTTFI Radical Anions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13513-13522.	1.1	12
5638	Synthesis of Imino-Enamido Hafnium and Zirconium Complexes: A New Family of Olefin Polymerization Catalysts with Ultrahigh-Molecular-Weight Capabilities. <i>Organometallics</i> , 2011, 30, 1695-1709.	1.1	51
5639	Coordination of Ethylene to a Zwitterionic Rh(III) Half-Sandwich Complex: Influence of Amphiphilic Ligands on Reactivity. <i>Organometallics</i> , 2011, 30, 511-519.	1.1	39
5640	Mechanisms for Selective Catalytic Oxidation of Ammonia over Vanadium Oxides. <i>Journal of Physical Chemistry C</i> , 2011, 115, 21218-21229.	1.5	48
5641	Detailed Investigation of the OH Radical Quenching by Natural Antioxidant Caffeic Acid Studied by Quantum Mechanical Models. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4218-4233.	2.3	100
5642	Excited-State Intramolecular Proton Transfer in Hydroxyoxime-Based Chemical Sensors. <i>Journal of Physical Chemistry A</i> , 2011, 115, 834-840.	1.1	40
5643	Quantifying Water-Mediated Protein-Ligand Interactions in a Glutamate Receptor: A DFT Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7085-7096.	1.2	16

#	CO-Induced Formation of an Interpenetrating Bicuboctahedral Au ₂ Pd ₁₈ Kernel in Nanosized Au ₂ Pd ₂₈ (CO) ₂₆ (PEt ₃) ₁₀ : Formal Replacement of an Interior (1/4-Pd) ₂ Fragment in the Corresponding Known Isostructural Homopalladium Pd ₃₀ (CO) ₂₆ (PEt ₃) ₁₀ with Nonisovalent (1/4-Au) ₂ and Resulting Experimental/Theoretical Implications	IF	CITATIONS
5644	Characterization of Tunable Radical Metal-Carbenes: Key Intermediates in Catalytic Cyclopropanation. <i>Organometallics</i> , 2011, 30, 2739-2746.	1.1	73
5646	Rearrangement of 3-Deoxy- <i>d</i> -erythro- <i>l</i> -hexos-2-ulose in Aqueous Solution: NMR Evidence of Intramolecular 1,2-Hydrogen Transfer. <i>Journal of Organic Chemistry</i> , 2011, 76, 8151-8158.	1.7	9
5647	How Is a Co-Methyl Intermediate Formed in the Reaction of Cobalamin-Dependent Methionine Synthase? Theoretical Evidence for a Two-Step Methyl Cation Transfer Mechanism. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4066-4077.	1.2	44
5648	pB ₂ Intermediate of the Photoactive Yellow Protein: Structure and Excitation Energies. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2097-2106.	1.2	8
5649	Atomic-Resolution Kinked Structure of an Alkylporphyrin on Highly Ordered Pyrolytic Graphite. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 62-66.	2.1	21
5650	Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1647-1666.	2.3	63
5651	Computational Study of the Mechanism of Cyclic Acetal Formation via the Iridium(I)-Catalyzed Double Hydroalkoxylation of 4-Pentyn-1-ol with Methanol. <i>Organometallics</i> , 2011, 30, 618-626.	1.1	17
5652	Coupled Cluster in Condensed Phase. Part I: Static Quantum Chemical Calculations of Hydrogen Fluoride Clusters. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 843-851.	2.3	39
5653	Changes in the Electronic Structures of a Single Sheet of Sashlike Polydiacetylene Atomic Sash upon Structural Transformations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9518-9525.	1.5	4
5654	Osazone Anion Radical Complex of Rhodium(III). <i>Inorganic Chemistry</i> , 2011, 50, 1331-1338.	1.9	14
5655	Theoretical Methodology for Prediction of Tropospheric Oxidation of Dimethyl Phosphonate and Dimethyl Methylphosphonate. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1946-1954.	1.1	5
5656	Theoretical Investigation of Raman Optical Activity Signatures of Tröger's Base. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13706-13713.	1.1	6
5657	Controlling the Selectivity for C-H and C-CN Bond Activation at Rhodium: A DFT Examination of Ligand Effects. <i>Organometallics</i> , 2011, 30, 3371-3377.	1.1	33
5658	DFT Calculations of the Isomerization of 2-Methyl-3-butenenitrile by [Ni(bisphosphine)] in Relation to the DuPont Adiponitrile Process. <i>Organometallics</i> , 2011, 30, 547-555.	1.1	28
5659	Asymmetric Imine <i>N</i> -Inversion in 3-Methyl-4-pyrimidinimine. Molecular Dipole Analysis of Solvation Effects. <i>Journal of Organic Chemistry</i> , 2011, 76, 3987-3996.	1.7	7
5660	About the Barriers to Reaction of CCl ₄ with HFeOH and FeCl ₂ . <i>Journal of Physical Chemistry A</i> , 2011, 115, 8713-8720.	1.1	4
5661	Revisiting the Aufbau Reaction with Acetylene: Further Insights from Experiment and Theory. <i>Organometallics</i> , 2011, 30, 1569-1576.	1.1	10

#	ARTICLE	IF	CITATIONS
5662	Regioselective Bis-functionalization of Endohedral Dimetallofullerene, La ₂ @C ₈₀ : Extremal La–La Distance. <i>Journal of the American Chemical Society</i> , 2011, 133, 7128-7134.	6.6	47
5663	Controlling the Photoreactivity of the Photoactive Yellow Protein Chromophore by Substituting at the <i>p</i> -Coumaric Acid Group. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7021-7028.	1.2	28
5664	Experimental Charge Density Analysis of a Gallium(I) N-Heterocyclic Carbene Analogue. <i>Inorganic Chemistry</i> , 2011, 50, 8418-8426.	1.9	33
5665	Ab Initio Analysis and Harmonic Force Fields of Gallium Nitride Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 6467-6477.	1.5	16
5666	C–H and C–CN Bond Activation of Acetonitrile and Succinonitrile by [Tp–Rh(PR ₃) ₃]. <i>Organometallics</i> , 2011, 30, 834-843.	1.1	44
5667	Ditopic Complexation of Selenite Anions or Calcium Cations by Pirenoxine: An Implication for Anti-Cataractogenesis. <i>Inorganic Chemistry</i> , 2011, 50, 365-377.	1.9	25
5668	Theoretical Study on the Formation of Silacyclopropene from Acylsilane and Acetylene via Silene-to-Silylene Rearrangement. <i>Organometallics</i> , 2011, 30, 3160-3167.	1.1	10
5669	Molybdenum-Catalyzed Transformation of Molecular Dinitrogen into Silylamine: Experimental and DFT Study on the Remarkable Role of Ferrocenyldiphosphine Ligands. <i>Journal of the American Chemical Society</i> , 2011, 133, 3498-3506.	6.6	148
5670	Electron Transport in Pure and Doped Hematite. <i>Nano Letters</i> , 2011, 11, 1775-1781.	4.5	267
5671	Complexation, Computational, Magnetic, and Structural Studies of the Maillard Reaction Product Isomaltol Including Investigation of an Uncommon π – π Interaction with Copper(II). <i>Inorganic Chemistry</i> , 2011, 50, 1498-1505.	1.9	18
5672	Optical Excitations in Hematite (Fe ₂ O ₃) via Embedded Cluster Models: A CASPT2 Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20795-20805.	1.5	57
5673	Internal Alkyne Isomerization to Vinylidene versus Stable π -Alkyne: Theoretical and Experimental Study on the Divergence of Analogous Cp*–Ru and Tp–Ru Systems. <i>Organometallics</i> , 2011, 30, 4014-4031.	1.1	36
5674	Reversible Capture of Small Molecules On Bimetalloborane Clusters: Synthesis, Structural Characterization, and Photophysical Aspects. <i>Inorganic Chemistry</i> , 2011, 50, 7511-7523.	1.9	19
5675	An ab initio study of cooperative effects in ternary complexes X:CNH:Z with X, Z=CNH, FH, ClH, FCl, and HLi: structures, binding energies, and spin–spin coupling constants across intermolecular bonds. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13951.	1.3	40
5676	Ligand Exchange Reaction Involving Ru(III) Compounds in Aqueous Solution: A Hybrid Quantum Mechanical/Effective Fragment Potential Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2030-2037.	1.2	7
5677	Theoretical investigation of growth, stability, and electronic properties of beaded ZnO nanoclusters. <i>Journal of Materials Chemistry</i> , 2011, 21, 16905.	6.7	34
5678	Field-Extremum Model for Short-Range Contributions to Hydration Free Energy. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3952-3960.	2.3	22
5679	1,3-Dipolar cycloaddition between a metal–azide (Ph ₃ PAuN ₃) and a metal–acetylide (Ph ₃ PAuC≡CPh): an inorganic version of a click reaction. <i>Dalton Transactions</i> , 2011, 40, 8140.	1.6	73

#	ARTICLE	IF	CITATIONS
5680	Nonradiative Decay Mechanism of Fluoren-9-ylidene Malononitrile Ambipolar Derivatives. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2184-2195.	1.1	13
5681	Intramolecular Nitrile C-H Bond Activation in Nickel NHC Complexes: A Route to New Nickelacycles. <i>Organometallics</i> , 2011, 30, 3400-3411.	1.1	52
5682	Inorganic-organic hybrid compounds based on face-sharing octahedral [PbI ₃] ²⁻ chains: self-assemblies, crystal structures, and ferroelectric, photoluminescence properties. <i>Dalton Transactions</i> , 2011, 40, 1672.	1.6	41
5683	First Experimental Characterization of a Non-nuclear Attractor in a Dimeric Magnesium(I) Compound. <i>Journal of Physical Chemistry A</i> , 2011, 115, 194-200.	1.1	106
5684	Theoretical Study on the Mechanism of the Oxygen Activation Process in Cysteine Dioxygenase Enzymes. <i>Journal of the American Chemical Society</i> , 2011, 133, 3869-3882.	6.6	197
5685	Bottom-up synthesis of finite models of helical (n,m)-single-wall carbon nanotubes. <i>Nature Communications</i> , 2011, 2, .	5.8	284
5686	Revisiting Fluorenone Photophysics via Dipolar Fluorenone Derivatives. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6366-6375.	1.1	46
5687	Geometry optimization using tuned and balanced redistributed charge schemes for combined quantum mechanical and molecular mechanical calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10556.	1.3	20
5688	Gd ₂ @C ₇₉ N: Isolation, Characterization, and Monoadduct Formation of a Very Stable Heterofullerene with a Magnetic Spin State of $\langle S \rangle = 15/2$. <i>Journal of the American Chemical Society</i> , 2011, 133, 9741-9750.	6.6	104
5689	DFT Study of the Homogeneous Hydroformylation of Propene Promoted by a Heterobimetallic Pt-Sn Catalyst. <i>Organometallics</i> , 2011, 30, 4257-4268.	1.1	21
5690	Prediction of the Reactivity Hazards for Organic Peroxides Using the QSPR Approach. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 1515-1522.	1.8	45
5691	Imino-Amido Hf and Zr Complexes: Synthesis, Isomerization, and Olefin Polymerization. <i>Organometallics</i> , 2011, 30, 251-262.	1.1	42
5692	From computational discovery to experimental characterization of a high hole mobility organic crystal. <i>Nature Communications</i> , 2011, 2, 437.	5.8	321
5693	Theoretical Analysis of Proton Relays in Electrochemical Proton-Coupled Electron Transfer. <i>Journal of the American Chemical Society</i> , 2011, 133, 8282-8292.	6.6	54
5694	Mechanistic Insights on N-Heterocyclic Carbene-Catalyzed Annulations: The Role of Base-Assisted Proton Transfers. <i>Journal of Organic Chemistry</i> , 2011, 76, 5606-5613.	1.7	86
5695	Theoretical Study on the Ring-Opening Polymerization of μ -Caprolactone by [YMeX(THF) ₅] ⁺ with X = BH ₄ ⁻ , NMe ₂ . <i>Organometallics</i> , 2011, 30, 1326-1333.	1.1	22
5696	Copper-Mediated C-H Activation/C-S Cross-Coupling of Heterocycles with Thiols. <i>Journal of Organic Chemistry</i> , 2011, 76, 8999-9007.	1.7	230
5697	Single Strand Break in DNA Coupled to the O-P Bond Cleavage. A Computational Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1911-1917.	1.2	23

#	ARTICLE	IF	CITATIONS
5698	Binding Ligands and Cofactor to α -Lactate Dehydrogenase from Human Skeletal and Heart Muscles. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6366-6376.	1.2	13
5699	Experimental and theoretical study on the absorption and fluorescence properties of substituted aryl hydrazones of 1,8-naphthalimide. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18530.	1.3	35
5700	Quantum Mechanical Investigation of the Effect of Catalyst Fluorination in the Intermolecular Asymmetric Stetter Reaction. <i>Journal of the American Chemical Society</i> , 2011, 133, 11249-11254.	6.6	89
5701	QM/MM calculation of protein magnetic shielding tensors with generalized hybrid-orbital method: A GIAO approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14490.	1.3	3
5702	Density Functional Theory Studies of Interactions of Ruthenium ^{II} Arene Complexes with Base Pair Steps. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11293-11302.	1.1	24
5703	Diarylethene-Containing Cyclometalated Platinum(II) Complexes: Tunable Photochromism via Metal Coordination and Rational Ligand Design. <i>Journal of the American Chemical Society</i> , 2011, 133, 12690-12705.	6.6	171
5704	DFT investigations on the ring-opening polymerization of cyclic carbonates catalyzed by zinc-dithiolate complexes. <i>Polymer Chemistry</i> , 2011, 2, 2564.	1.9	21
5705	Ruthenium Complexes Containing 2-(2-Nitrosoaryl)pyridine: Structural, Spectroscopic, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2011, 50, 11636-11643.	1.9	26
5706	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6145.	1.3	84
5707	Co-Crystals of Sulfamethazine with Some Carboxylic Acids and Amides: Co-Former Assisted Tautomerism in an Active Pharmaceutical Ingredient and Hydrogen Bond Competition Study. <i>Crystal Growth and Design</i> , 2011, 11, 3489-3503.	1.4	129
5708	Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5247-5255.	1.1	84
5709	What can molecular modelling bring to the design of artificial inorganic cofactors?. <i>Faraday Discussions</i> , 2011, 148, 137-159.	1.6	26
5710	Ammonia Activation by μ_3 -Alkylidyne Fragments Supported on a Titanium Molecular Oxide Model. <i>Inorganic Chemistry</i> , 2011, 50, 6269-6279.	1.9	39
5712	A Simple QM/MM Approach for Capturing Polarization Effects in Protein-Ligand Binding Free Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4911-4926.	1.2	97
5713	Cyano-bridged Homodinuclear Copper(II) Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 6890-6901.	1.9	28
5714	Basis Set Dependence of Vibrational Raman and Raman Optical Activity Intensities. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3323-3334.	2.3	128
5715	Ligand Self-Assembling through Complementary Hydrogen-Bonding in the Coordination Sphere of a Transition Metal Center: The 6-Diphenylphosphanylpyridin-2(1 <i>H</i>)-one System. <i>Journal of the American Chemical Society</i> , 2011, 133, 964-975.	6.6	44
5716	Four-Electron Oxygen Reduction by Tetrathiafulvalene. <i>Journal of the American Chemical Society</i> , 2011, 133, 12115-12123.	6.6	56

#	ARTICLE	IF	CITATIONS
5717	Experimental and Theoretical Charge Density Studies at Subatomic Resolution. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13061-13071.	1.1	95
5718	Facile, high-yielding synthesis of deepened cavitands: a synthetic and theoretical study. <i>Supramolecular Chemistry</i> , 2011, 23, 710-719.	1.5	15
5719	Unsymmetrical diimine complexes of iron(ii) and manganese(ii): synthesis, structure and photoluminescence of an isomer. <i>Dalton Transactions</i> , 2011, 40, 146-155.	1.6	10
5720	Adsorption of Glycine on Au(111) and Gold Thin Film Electrodes: An in Situ Spectroelectrochemical Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16439-16450.	1.5	31
5721	Computational investigation on the mechanism and stereochemistry of guanidine-catalyzed enantioselective isomerization of 3-alkynoates to allenates. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6034.	1.5	18
5722	Phosphine and solvent effects on oxidative addition of CH ₃ Br to Pd(PR ₃) and Pd(PR ₃) ₂ complexes. <i>Dalton Transactions</i> , 2011, 40, 11089.	1.6	50
5723	Solvation and Crystal Effects in Bilirubin Studied by NMR Spectroscopy and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11696-11714.	1.1	10
5724	Molecular Conductors with a 8-Hydroxy cobalt Bis(dicarbollide) Anion. <i>Inorganic Chemistry</i> , 2011, 50, 444-450.	1.9	29
5725	Water Oxidation by a Mononuclear Ruthenium Catalyst: Characterization of the Intermediates. <i>Journal of the American Chemical Society</i> , 2011, 133, 14649-14665.	6.6	180
5726	DFT Calculations of Isotropic Hyperfine Coupling Constants of Nitrogen Aromatic Radicals: The Challenge of Nitroxide Radicals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 169-179.	2.3	38
5727	Adsorption and Diffusion of Gallium Adatoms on the Si(100)-2 × 1 Reconstructed Surface: A Multiconfiguration Self-Consistent Field Study Utilizing Molecular Surface Clusters. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23488-23500.	1.5	4
5728	Investigation of the valence electronic states of Ti(IV) in Ti silicalite-1 coupling X-ray emission spectroscopy and density functional calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19409.	1.3	46
5729	A computational insight into a metal mediated pathway for the ring-opening polymerization (ROP) of lactides by an ionic {(NHC) ₂ Ag}+X ⁻ (X = halide) type N-heterocyclic carbene (NHC) complex. <i>Dalton Transactions</i> , 2011, 40, 10156.	1.6	22
5730	Enantioselective Synthesis of Endohedral Metallofullerenes. <i>Journal of the American Chemical Society</i> , 2011, 133, 17746-17752.	6.6	56
5731	Gas-Phase and Ar-Matrix SQM Scaling Factors for Various DFT Functionals with Basis Sets Including Polarization and Diffuse Functions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4640-4649.	1.1	47
5732	Semiclassical dynamics simulations of charge transport in stacked π-systems. <i>Journal of Chemical Physics</i> , 2011, 134, 034309.	1.2	27
5733	Novel C-H...C contacts involving 3,5-dimethylpyrazole ligands in a tetracoordinate Co(II) complex. <i>Dalton Transactions</i> , 2011, 40, 11605.	1.6	26
5734	Ab Initio and DFT Predictions of Infrared Intensities and Raman Activities. <i>Journal of Physical Chemistry A</i> , 2011, 115, 63-69.	1.1	132

#	ARTICLE	IF	CITATIONS
5735	Computational Studies of the Luciferase Light-Emitting Product: Oxyluciferin. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 809-817.	2.3	78
5736	Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3491-3496.	1.1	117
5737	Gold(III) N-Heterocyclic Carbene Complexes Mediated Synthesis of β^2 -Enaminones From 1,3-Dicarbonyl Compounds and Aliphatic Amines. <i>Inorganic Chemistry</i> , 2011, 50, 1840-1848.	1.9	54
5738	Nature of Intramolecular Transannular Interaction in Group 13 Atranes: A Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 1361-1367.	1.9	20
5739	A Theoretical Study of the Physicochemical Mechanisms Associated with DNA Recognition Modulation in Artificial Zinc-Finger Proteins. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4774-4780.	1.2	10
5740	DFT study of the interaction free energy of π - π complexes of fullerenes with buckybowls and viologen dimers. <i>New Journal of Chemistry</i> , 2011, 35, 1453.	1.4	32
5741	Bis(2-pyridylimino)isoindolato iron(ii) and cobalt(ii) complexes: Structural chemistry and paramagnetic NMR spectroscopy. <i>Dalton Transactions</i> , 2011, 40, 10406.	1.6	49
5742	Density Functional Calculation of the Structure and Electronic Properties of Cu_nO_n ($n = 1\text{--}8$) Clusters. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2087-2095.	1.1	39
5743	Estimation of Mayr Electrophilicity with a Quantitative Structure-Property Relationship Approach Using Empirical and DFT Descriptors. <i>Journal of Organic Chemistry</i> , 2011, 76, 9312-9319.	1.7	21
5744	Bridging Interactions and Selective Nanoparticle Aggregation Mediated by Monovalent Cations. <i>ACS Nano</i> , 2011, 5, 530-536.	7.3	71
5745	Ab Initio Studies of Aromatic Excimers Using Multiconfiguration Quasi-Degenerate Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7687-7699.	1.1	73
5746	Evaluation of Theoretical Approaches for Describing the Interaction of Water with Linear Acenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5955-5964.	1.1	24
5747	Probing the electronic and optical properties of silica-coated quantum dots with first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 14476.	1.3	4
5748	An approximate density-functional method using the Harris-Foulkes functional. <i>Journal of Chemical Physics</i> , 2011, 135, 084105.	1.2	8
5749	Adaptive-Partitioning Redistributed Charge and Dipole Schemes for QM/MM Dynamics Simulations: On-the-fly Relocation of Boundaries that Pass through Covalent Bonds. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3625-3634.	2.3	48
5750	Evaluation of the Nonlinear Optical Properties for Annulenes with Hückel and Möbius Topologies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3935-3943.	2.3	86
5751	Effects of Peripheral and Axial Substitutions on Electronic Transitions of Tin Naphthalocyanines. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9265-9272.	1.1	11
5752	Synthesis, Isolation, Characterization, and Theoretical Studies of $\text{Sc}_3\text{NC}@C_{78}\text{-}C_{72}$. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23755-23759.	1.5	54

#	ARTICLE	IF	CITATIONS
5753	Spectroscopic, structural, computational and (spectro)electrochemical studies of icosahedral carboranes bearing fluorinated aryl groups. <i>Dalton Transactions</i> , 2011, 40, 4200.	1.6	40
5754	Oxazoles revisited: On the nature of binding of benzoxazole and 2-methylbenzoxazole with the zinc and palladium halides. <i>Dalton Transactions</i> , 2011, 40, 1594.	1.6	11
5755	Rhodium-Catalyzed Oxidative 1:1, 1:2, and 1:4 Coupling Reactions of Phenylazoles with Internal Alkynes through the Regioselective Cleavages of Multiple C-H Bonds. <i>Journal of Organic Chemistry</i> , 2011, 76, 13-24.	1.7	207
5756	Shattering dissociation in high-energy molecular collisions between nitrate esters. <i>Journal of Chemical Physics</i> , 2011, 135, 114306.	1.2	0
5757	Controlled Radiation Damage and Edge Structures in Boron Nitride Membranes. <i>ACS Nano</i> , 2011, 5, 3977-3986.	7.3	33
5758	Predicting Selectivity in Oxidative Addition of C-S Bonds of Substituted Thiophenes to a Platinum(0) Fragment: An Experimental and Theoretical Study. <i>Organometallics</i> , 2011, 30, 4578-4588.	1.1	21
5759	Ground-State Electronic Structure in Charge-Transfer Complexes Based on Carbazole and Diarylamine Donors. <i>Journal of Physical Chemistry C</i> , 2011, 115, 10823-10835.	1.5	24
5760	Proton management as a design principle for hydrogenase-inspired catalysts. <i>Energy and Environmental Science</i> , 2011, 4, 3008.	15.6	50
5761	An Extension of the Hirshfeld Method to Open Shell Systems Using Fractional Occupations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1328-1335.	2.3	50
5762	Doubly charged protonated a ions derived from small peptides. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18307.	1.3	4
5763	Adsorption CO ₂ on the perfect and oxygen vacancy defect surfaces of anatase TiO ₂ and its photocatalytic mechanism of conversion to CO. <i>Applied Surface Science</i> , 2011, 257, 10322-10328.	3.1	106
5764	Differences and similarities in binding of pyruvate and l-lactate in the active site of M4 and H4 isoforms of human lactate dehydrogenase. <i>Archives of Biochemistry and Biophysics</i> , 2011, 505, 33-41.	1.4	16
5765	Complexation of alkali-metal cations by conformationally rigid, stereoisomeric calix[4]arene crown ethers: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 235-242.	1.1	8
5766	Quantum chemical studies on peroxodisulfuric acid-sulfuric acid-water clusters. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 219-225.	1.1	1
5767	Superhalogen plus anion : A recently discovered anion with the formula. <i>Computational and Theoretical Chemistry</i> , 2011, 973, 9-12.	1.1	11
5768	How does electron delocalization affect the electronic energy? A survey of neutral poly-nitrogen clusters. <i>Computational and Theoretical Chemistry</i> , 2011, 974, 86-91.	1.1	20
5769	Increasing complexity models for describing the generation of substrate radicals at the active site of ethanolamine ammonia-lyase/B12. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 52-60.	1.1	3
5770	A comparison of density functional theory (DFT) methods for estimating the singlet-triplet (S ₀ -T ₁) excitation energies of benzene and polyacenes. <i>Computational and Theoretical Chemistry</i> , 2011, 976, 105-112.	1.1	36

#	ARTICLE	IF	CITATIONS
5771	A theoretical study of boron tetrahalides: Structures and electron affinities. Computational and Theoretical Chemistry, 2011, 976, 201-208.	1.1	3
5772	Torsional potential and nonlinear optical properties of phenyldiazines and phenyltetrazines. Computational and Theoretical Chemistry, 2011, 977, 22-28.	1.1	11
5773	Singlet \leftrightarrow triplet ($S_0 \leftrightarrow T_1$) excitation energies of the $[4n-2]$ rectangular graphene nanoribbon series ($n=2-6$): A comparative theoretical study. Computational and Theoretical Chemistry, 2011, 977, 163-167.	1.1	13
5774	A computational study on the chemical fixation of carbon dioxide with 2-aminobenzonitrile catalyzed by 1-butyl-3-methyl imidazolium hydroxide ionic liquids. Computational and Theoretical Chemistry, 2011, 978, 47-56.	1.1	19
5775	Covalent hydration of nitrobenzofurazans compounds from the perspective of the HSAB principle and reactivity \leftrightarrow selectivity descriptor. Comptes Rendus Chimie, 2011, 14, 911-915.	0.2	0
5776	Calculation of equilibrium stable isotope partition function ratios for aqueous zinc complexes and metallic zinc. Geochimica Et Cosmochimica Acta, 2011, 75, 769-783.	1.6	83
5777	The Elward Reaction: A DFT Study. Inorganic Chemistry, 2011, 50, 5833-5840.	1.9	5
5778	Covalent Lanthanide Chemistry Near the Limit of Weak Bonding: Observation of $(\text{CpSiMe}_3)_3\text{Ce}^{\sim}\text{ECp}^*$ and a Comprehensive Density Functional Theory Analysis of $\text{Cp}_3\text{Ln}^{\sim}\text{ECp}$ ($E = \text{Al, Ga}$). Inorganic Chemistry, 2011, 50, 345-357.	1.9	58
5779	Accurate Molecular Crystal Lattice Energies from a Fragment QM/MM Approach with On-the-Fly Ab Initio Force Field Parametrization. Journal of Chemical Theory and Computation, 2011, 7, 3733-3742.	2.3	125
5780	Calculating the Response of NMR Shielding Tensor χ^{P} and χ^{C} Coupling Constants in Nucleic Acid Phosphate to Coordination of the Mg^{2+} Cation. Journal of Physical Chemistry A, 2011, 115, 2385-2395.	1.1	21
5781	Synthesis of Tetrahydronaphthalene Lignan Esters by Intramolecular Cyclization of Ethyl <i>p</i> -Azidophenyl-2-phenylalkanoates and Evaluation of the Growth Inhibition of Human Tumor Cell Lines. Journal of Medicinal Chemistry, 2011, 54, 3175-3187.	2.9	21
5782	Hydrogenation of Carbon Dioxide Catalyzed by PNP Pincer Iridium, Iron, and Cobalt Complexes: A Computational Design of Base Metal Catalysts. ACS Catalysis, 2011, 1, 849-854.	5.5	176
5783	Total Synthesis of Natural and Non-Natural $\hat{\text{I}}^{5,6}$ - $\hat{\text{I}}^{12,13}$ -Jatrophone Diterpenes and Their Evaluation as MDR Modulators. Journal of Organic Chemistry, 2011, 76, 512-522.	1.7	49
5784	A new approach to local hardness. Physical Chemistry Chemical Physics, 2011, 13, 15003.	1.3	36
5785	Theoretical study of metallasilatranes; Bonding nature and prediction of new metallasilatrane. Collection of Czechoslovak Chemical Communications, 2011, 76, 619-629.	1.0	8
5786	Role of Conformation in C^{\sim}C Interactions and Polymer/Fullerene Miscibility. Journal of Physical Chemistry B, 2011, 115, 8989-8995.	1.2	24
5787	Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062.	1.5	38
5788	Robust Scoring Functions for Protein \leftrightarrow Ligand Interactions with Quantum Chemical Charge Models. Journal of Chemical Information and Modeling, 2011, 51, 2528-2537.	2.5	47

#	ARTICLE	IF	CITATIONS
5789	A Theoretical Study of Abiotic Methylation Reactions of Gaseous Elemental Mercury by Halogen-Containing Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5602-5608.	1.1	13
5790	Discovering the chemical reactivity of the molecular oxonitride $[\{Ti(\eta^5-C_5Me_5)(\eta^4-O)\}_3(\eta^4-N)]$. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 4011-4017.	0.8	9
5791	Theoretical investigation of thermally and photochemically induced haptotropic rearrangements of chromium ligands on naphthalene systems. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 3861-3866.	0.8	8
5792	Spontaneous Proton Transfer to a Conserved Inein Residue Determines On-Pathway Protein Splicing. <i>Journal of Molecular Biology</i> , 2011, 406, 430-442.	2.0	24
5793	Theoretical study of the solvation of $HgCl_2$, $HgClOH$, $Hg(OH)_2$ and $HgCl_3^-$: a density functional theory cluster approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16772.	1.3	32
5794	Comparison of quantum Monte Carlo with time-dependent and static density-functional theory calculations of diamondoid excitation energies and Stokes shifts. <i>Physical Review B</i> , 2011, 84, .	1.1	24
5795	Tungsten(VI) N-Heterocyclic Carbene Complexes: Synthetic, Structural, and Computational Study. <i>Organometallics</i> , 2011, 30, 6262-6269.	1.1	17
5796	Stereoselective Synthesis of <i>cis</i> -3,4-Disubstituted Piperidines through Ring Transformation of 2-(2-Mesyloxyethyl)azetidines. <i>Journal of Organic Chemistry</i> , 2011, 76, 8364-8375.	1.7	33
5797	Can Human Prolidase Enzyme Use Different Metals for Full Catalytic Activity?. <i>Inorganic Chemistry</i> , 2011, 50, 3394-3403.	1.9	37
5798	Computational Investigation of Amine-Oxygen Exciplex Formation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10159-10165.	1.1	11
5799	Ab Initio Investigation of the Hydration of the Tetrahedral Perchlorate, Perbromate, Selenate, Arsenate, and Vanadate Anions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13007-13015.	1.1	13
5800	Substituents dependent capability of bis(ruthenium-dioxolene-terpyridine) complexes toward water oxidation. <i>Dalton Transactions</i> , 2011, 40, 2225-2233.	1.6	36
5801	Inductive Effect: A Quantum Theory of Atoms in Molecules Perspective. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12544-12554.	1.1	11
5802	DFT Studies on the Reaction of $CpCo(PPh_3)_2$ with Diphenylphosphinoalkynes: Formation of Cobaltacycles and Cyclobutadiene-Substituted $CpCoCb$ Diphosphines. <i>Organometallics</i> , 2011, 30, 3740-3748.	1.1	13
5803	Theoretical studies of the mechanism of catalytic hydrogen production by a cobaloxime. <i>Chemical Communications</i> , 2011, 47, 12456.	2.2	213
5804	Synthesis and Transformations of Novel Benzo[c]furans. <i>Heterocycles</i> , 2011, 83, 591.	0.4	1
5805	Bonding in negative ions: the role of d orbitals in the heavy analogues of pyridine and furanradical anions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1663-1668.	1.3	8
5806	Theoretical investigation of the conformational intricacies and thermodynamic functions of noradrenaline. <i>Canadian Journal of Chemistry</i> , 2011, 89, 1010-1020.	0.6	1

#	ARTICLE	IF	CITATIONS
5807	The Cause for Tremendous Acceleration of Chloride Substitution via Base Catalysis in the Chloro Pentaammine Cobalt(III) Ion. <i>Inorganic Chemistry</i> , 2011, 50, 8728-8740.	1.9	13
5808	Self-assembly of metal-organic frameworks: From packing helical channels to 2-fold interpenetration helical layers. <i>CrystEngComm</i> , 2011, 13, 6373.	1.3	4
5809	Theoretical Determination of One-Electron Redox Potentials for DNA Bases, Base Pairs, and Stacks. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4804-4810.	1.1	76
5810	Effects of geminal methyl groups on the tunnelling rates in the ring opening of cyclopropylcarbonyl radical at cryogenic temperature. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 3142.	1.5	12
5811	On the interaction of ascorbic acid and the tetrachlorocuprate ion $[CuCl_4]^{2-}$ in CuCl nanoplatelet formation from an ionic liquid precursor (ILP). <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13537.	1.3	31
5812	Thermodynamic and Kinetic Studies on Novel Dinuclear Platinum(II) Complexes Containing Bidentate N-donor ligands. <i>Inorganic Chemistry</i> , 2011, 50, 8984-8996.	1.9	41
5813	Aromatic versus Benzylic CH Bond Activation of Alkylaromatics by a Transient η^2 -Cyclopropene Complex. <i>Organometallics</i> , 2011, 30, 3999-4007.	1.1	17
5814	Theoretical Study for Pyridinium-Based Ionic Liquid 1-Ethylpyridinium Trifluoroacetate: Synthesis Mechanism, Electronic Structure, and Catalytic Reactivity. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8255-8263.	1.1	26
5815	Mean Excitation Energies for Biomolecules. <i>Advances in Quantum Chemistry</i> , 2011, 62, 215-242.	0.4	18
5816	Chemical Indices of the Biomimetic Models of Oxyhemocyanin and Oxytyrosinase. , 2011, , .		0
5817	Semiempirical, Hartree-Fock, density functional, and second order Moller-Plesset perturbation theory methods do not accurately predict ionization energies and electron affinities of short- through long-chain [n]acenes. <i>Nature Precedings</i> , 2011, , .	0.1	1
5818	Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4MP2/G4 theoretical study. <i>Nature Precedings</i> , 2011, , .	0.1	0
5819	DISCOVERY OF ENERGETIC MATERIALS BY A THEORETICAL METHOD (DEMTM). <i>International Journal of Energetic Materials and Chemical Propulsion</i> , 2011, 10, 33-44.	0.2	0
5821	Synthetic 3-Arylidene flavanones as Inhibitors of the Initial Stages of Biofilm Formation by <i>Staphylococcus aureus</i> and <i>Enterococcus faecalis</i> . <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2011, 66, 104-114.	0.6	16
5822	Carboxylated Lysine is Required for Higher Activities in Hydantoinases. <i>Protein and Peptide Letters</i> , 2011, 18, 663-669.	0.4	8
5823	A Nonadiabatic Ab Initio Dynamics Study on Rhodopsin and Its Analog Isorhodopsin: Chemical Dynamics Reasons behind Selection of Rhodopsin by Life. <i>Chemistry Letters</i> , 2011, 40, 1395-1397.	0.7	1
5824	Study on Reactions of Long-Lived Phenoxathiin Radical Cation with Aliphatic Alcohols, Phenol and Phenyl Halides in Ambient Condition by Fused-Droplet Electrospray Ionization Mass Spectrometry. <i>European Journal of Mass Spectrometry</i> , 2011, 17, 385-394.	0.5	5
5825	Comparison of Inhibitory Activities of Stereo-Isomers of Cyclic Phosphatidic Acid (cPA) on Autotaxin. <i>Cytologia</i> , 2011, 76, 73-80.	0.2	4

#	ARTICLE	IF	CITATIONS
5826	Theoretical study of adsorption of lithium atom on carbon nanotube. <i>AIP Advances</i> , 2011, 1, .	0.6	28
5827	A fluctuating quantum model of the CO vibration in carboxyhemoglobin. <i>Journal of Chemical Physics</i> , 2011, 134, 214106.	1.2	10
5828	Structural and photophysical characterization, topological and conformational analysis of 2-o-tolyl-4-(3-N,N-dimethylaminophenyl-methylene)-oxazol-5-one. <i>Journal of Structural Chemistry</i> , 2011, 52, 405-411.	0.3	3
5829	Role of the surface hydroxyl groups of modified titanium oxide in catalytic ethylene oxide hydration. <i>Kinetics and Catalysis</i> , 2011, 52, 659-671.	0.3	4
5830	Cyclization of C-phosphorylated (PIII) arylformamidines to 3H-1,3-benzazaphospholes. <i>Tetrahedron</i> , 2011, 67, 7748-7758.	1.0	44
5831	Mechanistic studies on the enantioselective BINOLAM/titanium(IV)-catalyzed cyanobenzoylation of aldehydes: Part 1. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 1282-1291.	1.8	8
5832	Synthesis and olefin polymerization activity of (quinolin-8-ylamino)phenolate and (quinolin-8-ylamido)phenolate Group 4 metal complexes. <i>Journal of Molecular Catalysis A</i> , 2011, 351, 112-119.	4.8	15
5833	Experimental and theoretical investigation on the vibrational spectroscopy of l-theanine. <i>Journal of Molecular Structure</i> , 2011, 1006, 559-565.	1.8	2
5834	Determination of the optimal position of adjacent proton-donor centers for the activation or inhibition of peptide bond formation â€“ A computational model study. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 30, 10-14.	1.3	1
5835	Synthesis, X-ray crystal structure and fluorescent spectra of novel pyrazolo[1,5-a]pyrazin-4(5H)-one derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 372-379.	2.0	5
5836	Synthesis, spectroscopic characterization, DFT studies and biological assays of a novel gold(I) complex with 2-mercaptothiazoline. <i>Polyhedron</i> , 2011, 30, 2354-2359.	1.0	18
5837	Vibrational spectra and structure of methyl-derivatives of imidazo[4,5-c]pyridine based on DFT quantum chemical calculations and XRD studies. <i>Vibrational Spectroscopy</i> , 2011, 57, 229-241.	1.2	9
5838	Multi-equilibrium system based on sertraline and Î²-cyclodextrin supramolecular complex in aqueous solution. <i>International Journal of Pharmaceutics</i> , 2011, 421, 24-33.	2.6	47
5839	Investigation into the shape selectivity of zeolite catalysts for biomass conversion. <i>Journal of Catalysis</i> , 2011, 279, 257-268.	3.1	963
5840	Methyltrioxorhenium-catalyzed oxidation of pseudocumene for vitamin E synthesis: A study of solvent and ligand effects. <i>Journal of Catalysis</i> , 2011, 283, 55-67.	3.1	32
5841	Transformation mechanism of a H ₂ molecule from physisorption to chemisorption in pristine and B-doped C ₂₀ fullerenes. <i>Chemical Physics Letters</i> , 2011, 511, 393-398.	1.2	22
5842	A density-functional theory investigation of the electronic structure of the active carbon graphite-like and amorphous domains. <i>Chemical Physics Letters</i> , 2011, 513, 261-266.	1.2	25
5843	Inclusion complexes of Î±-cyclodextrin and the cisplatin analogues oxaliplatin, carboplatin and nedaplatin: A theoretical approach. <i>Chemical Physics Letters</i> , 2011, 515, 127-131.	1.2	19

#	ARTICLE	IF	CITATIONS
5844	Examining the impact of steric and electronic variation in N2S scorpionate ligands on the properties of zinc(II) and cadmium(II) complexes. <i>Inorganica Chimica Acta</i> , 2011, 376, 562-573.	1.2	12
5845	Electron transfer pathways in cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2011, 1807, 1305-1313.	0.5	34
5846	Theoretical study of the excited states of the photosynthetic reaction center in photosystem II: Electronic structure, interactions, and their origin. <i>Biophysical Chemistry</i> , 2011, 159, 227-236.	1.5	9
5847	A theoretical investigation of gas phase NO ₃ initiated nitration of p-cresol. <i>Chemical Physics</i> , 2011, 389, 39-46.	0.9	11
5848	Indenyl effect in dissociative reactions. Nucleophilic substitution in iron carbonyl complexes: a case study. <i>Dalton Transactions</i> , 2011, 40, 11138.	1.6	18
5849	A combined effective fragment potentialâ€“fragment molecular orbital method. II. Analytic gradient and application to the geometry optimization of solvated tetraglycine and chignolin. <i>Journal of Chemical Physics</i> , 2011, 134, 034110.	1.2	44
5850	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6670.	1.3	1,627
5851	Regioselectivity in the Nitration of Dialkoxybenzenes. <i>Journal of Organic Chemistry</i> , 2011, 76, 1285-1294.	1.7	24
5852	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10930-10949.	1.1	110
5853	Synthesis, Characterization, and Cytotoxicity of Platinum(IV) Carbamate Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 3103-3115.	1.9	102
5854	Unexpected Direct Reduction Mechanism for Hydrogenation of Ketones Catalyzed by Iron PNP Pincer Complexes. <i>Inorganic Chemistry</i> , 2011, 50, 12836-12843.	1.9	71
5855	Covalent assistance in supramolecular synthesis: in situ modification and masking of the hydrogen bonding functionality of the supramolecular reagent isoniazid in co-crystals. <i>CrystEngComm</i> , 2011, 13, 5692.	1.3	24
5856	Interpretation of substituent effects on ¹³ C and ¹⁵ N NMR chemical shifts in 6-substituted purines. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15854.	1.3	31
5857	Do Two Different Reaction Mechanisms Contribute to the Hydroxylation of Primary Amines by Cytochrome P450?. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3399-3404.	2.3	28
5858	New Insights into Kegginâ€“Type 12â€“tungstophosphoric Acid from ³¹ P MAS NMR Analysis of Absorbed Trimethylphosphine Oxide and DFT Calculations. <i>Chemistry - an Asian Journal</i> , 2011, 6, 137-148.	1.7	42
5859	Arginineâ€“Facilitated Î±â€“and Î³â€“Radical Migrations in Glycylarginyltryptophan Radical Cations. <i>Chemistry - an Asian Journal</i> , 2011, 6, 888-898.	1.7	28
5860	Synthesis of a Novel Lithocene that has Aromaticâ€“Like Nature with Nonaromatic Rings. <i>Chemistry - an Asian Journal</i> , 2011, 6, 2907-2910.	1.7	12
5861	Unusual Metal Ion Selectivities of the Highly Preorganized Tetradentrate Ligand 1,10-Phenanthroline-2,9-dicarboxamide: A Thermodynamic and Fluorescence Study. <i>Inorganic Chemistry</i> , 2011, 50, 8348-8355.	1.9	46

#	ARTICLE	IF	CITATIONS
5862	Synthesis and Characterization of Silver(I), Gold(I), and Gold(III) Complexes Bearing Amino-Functionalized N-Heterocyclic Carbenes. <i>Organometallics</i> , 2011, 30, 2755-2764.	1.1	58
5863	Chemoselective Sulfide and Sulfoxide Oxidations by CpMo(CO) ₃ Cl/HOOR: a DFT Mechanistic Study. <i>Organometallics</i> , 2011, 30, 1454-1465.	1.1	26
5864	Indenyl ring slippage in crown thioether complexes [IndMo(CO) ₂ L] ⁺ and C≡S activation of trithiacyclononane: Experimental and theoretical studies. <i>Dalton Transactions</i> , 2011, 40, 10513.	1.6	19
5865	Theoretical Study on the Mechanism of Al(salalen)-Catalyzed Hydrophosphonylation of Aldehydes. <i>Organometallics</i> , 2011, 30, 2095-2104.	1.1	22
5866	Ruthenium complexes of chelating amido-functionalized N-heterocyclic carbene ligands: Synthesis, structure and DFT studies. <i>Journal of Chemical Sciences</i> , 2011, 123, 791-798.	0.7	7
5867	Calculations of complexes of 9-diphenylaminoacridine fluorescent indicator with analyte molecules using density functional theory with dispersion correction. <i>Nanotechnologies in Russia</i> , 2011, 6, 298-302.	0.7	0
5868	An analysis of SCF and geometry convergence for diatomic molecules. <i>Open Chemistry</i> , 2011, 9, 567-571.	1.0	1
5869	Theoretical study on energy transfer from the excited C60 to molecular oxygen. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2011, 111, 248-256.	0.2	6
5870	Theoretical investigation of the structure and properties of H ₂ B=NH ₂ ...M ⁿ⁺ , HB≡NH...M ⁿ⁺ , and Borazine...M ⁿ⁺ complexes (M = Alkaline and Earth Alkaline Metals). <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 2148-2155.	0.1	3
5871	Prediction of Charge Mobility in Amorphous Organic Materials through the Application of Hopping Theory. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2556-2567.	2.3	24
5872	Water-compatible one-pot organocatalytic asymmetric synthesis of cyclic nitrones. Application in intramolecular 1,3-dipolar cycloadditions. <i>Tetrahedron Letters</i> , 2011, 52, 5976-5979.	0.7	18
5873	Theoretical Study on the Reaction Mechanism of NH ₂ ≡N with O ₂ (a ¹ g). <i>Journal of Physical Chemistry A</i> , 2011, 115, 13581-13588.	1.1	1
5874	Glutathione radical cation in the gas phase; generation, structure and fragmentation. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7384.	1.5	14
5875	Theoretical Analysis of Mechanistic Pathways for Hydrogen Evolution Catalyzed by Cobaloximes. <i>Inorganic Chemistry</i> , 2011, 50, 11252-11262.	1.9	199
5876	Mechanisms of Oxygen Reduction Reaction on Nitrogen-Doped Graphene for Fuel Cells. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11170-11176.	1.5	1,235
5877	Porous metal organic framework nanoparticles to address the challenges related to busulfan encapsulation. <i>Nanomedicine</i> , 2011, 6, 1683-1695.	1.7	95
5878	New chemistry of 1,2-closo-P ₂ B ₁₀ H ₁₀ and 1,2-closo-As ₂ B ₁₀ H ₁₀ ; in silico and gas electron diffraction structures, and new metalladiphospha- and metalladiarsaboranes. <i>Dalton Transactions</i> , 2011, 40, 7181.	1.6	21
5879	Structures of the I-, II- and H-Methane Clathrates and the Ice [∞] Methane Clathrate Phase Transition from Quantum-Chemical Modeling with Force-Field Thermal Corrections. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6169-6176.	1.1	61

#	ARTICLE	IF	CITATIONS
5880	Synthesis, Structure, and Bonding Nature of Ethynediyl-Bridged Bis(silylene) Dinuclear Complexes of Tungsten and Molybdenum. <i>Organometallics</i> , 2011, 30, 4515-4531.	1.1	22
5881	Density Functional Theory Study of Photophysical Properties of Iridium(III) Complexes with Phenylisoquinoline and Phenylpyridine Ligands. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20724-20731.	1.5	74
5883	Characterization of <i>Rubus fruticosus</i> mitochondria and salicylic acid inhibition of reactive oxygen species generation at Complex III/Q cycle: potential implications for hypersensitive response in plants. <i>Journal of Bioenergetics and Biomembranes</i> , 2011, 43, 237-246.	1.0	18
5884	Influence of Prototropic Reactions on the Absorption and Fluorescence Spectra of Methyl p-dimethylaminobenzoate and Its Two Ortho Derivatives. <i>Journal of Fluorescence</i> , 2011, 21, 1749-1762.	1.3	12
5885	Parity-Violation Energy of Biomoleculesâ€”IV: Protein Secondary Structure. <i>Origins of Life and Evolution of Biospheres</i> , 2011, 41, 249-259.	0.8	4
5886	Modeling of NMR spectra and signal assignment using real-time DFT/GIAO calculations. <i>Russian Chemical Bulletin</i> , 2011, 60, 783-789.	0.4	16
5887	Unusual asymmetry in halobenzenes, a solid-state, gas-phase and theoretical investigation. <i>Structural Chemistry</i> , 2011, 22, 279-285.	1.0	3
5888	Conformational analysis of vitamin K1 model molecule: a theoretical study. <i>Structural Chemistry</i> , 2011, 22, 305-311.	1.0	6
5889	Computational studies on tetrazole derivatives as potential high energy materials. <i>Structural Chemistry</i> , 2011, 22, 775-782.	1.0	24
5890	Theoretical study of the neutral hydrolysis of methyl formate via a concerted and stepwise water-assisted mechanism using free-energy curves and molecular dynamics simulation. <i>Structural Chemistry</i> , 2011, 22, 909-915.	1.0	9
5891	Novel guanidinium zwitterion and derived ionic liquids: physicochemical properties and DFT theoretical studies. <i>Structural Chemistry</i> , 2011, 22, 1119-1130.	1.0	10
5892	Theoretical study on interactions of β -cyclodextrin with helicobacter pylori eradicating agent (TG44). <i>Journal of Molecular Modeling</i> , 2011, 17, 913-920.	0.8	2
5893	A new scheme to calculate isotope effects. <i>Journal of Molecular Modeling</i> , 2011, 17, 2175-2182.	0.8	3
5894	Theoretical study on the interactions between methanol and imidazolium-based ionic liquids. <i>Journal of Molecular Modeling</i> , 2011, 17, 1997-2004.	0.8	17
5895	New insight into the formation mechanism of imidazolium-based halide salts. <i>Journal of Molecular Modeling</i> , 2011, 17, 2099-2102.	0.8	7
5896	Light activation of the isomerization and deprotonation of the protonated Schiff base retinal. <i>Journal of Molecular Modeling</i> , 2011, 17, 2539-2547.	0.8	15
5897	Formation of the Vilsmeier-Haack complex: the performance of different levels of theory. <i>Journal of Molecular Modeling</i> , 2011, 17, 3209-3217.	0.8	3
5898	The importance of conformational search: a test case on the catalytic cycle of the Suzukiâ€”Miyaura cross-coupling. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 639-646.	0.5	67

#	ARTICLE	IF	CITATIONS
5899	Electronic spectra of the linear cationic chains $NC_2n N^+$ ($n=1-7$): an ab initio study. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 793-801.	0.5	6
5900	Theoretical study of the excited states and the redox potentials of unusually distorted β -trifluoromethylporphycene. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 175-185.	0.5	4
5901	Finite-field evaluation of static (hyper)polarizabilities based on the linear-scaling divide-and-conquer method. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 701-709.	0.5	14
5902	MPI/OpenMP hybrid parallel implementation of second-order Møller-Plesset perturbation theory using numerical quadratures. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 317-321.	0.5	13
5903	An application of double exponential formula to radial quadrature grid in density functional calculation. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 645-669.	0.5	11
5904	Linear-scaling divide-and-conquer second-order Møller-Plesset perturbation calculation for open-shell systems: implementation and application. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 411-417.	0.5	26
5905	Application of resolution of identity approximation of second-order Møller-Plesset perturbation theory to three-body fragment molecular orbital method. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 449-453.	0.5	15
5906	The concerted and stepwise chemisorption mechanisms of isothiazole and thiazole on $Si(100)2 \times 1$ surface. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 507-513.	0.5	1
5907	Electronic stress tensor analysis of hydrogenated palladium clusters. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 531-542.	0.5	10
5908	Sensitive and selective fluorescence detection of guanosine nucleotides by nanoparticles conjugated with a naphthyridine receptor. <i>Analytical and Bioanalytical Chemistry</i> , 2011, 399, 1215-1222.	1.9	16
5909	Energy expression of the chemical bond between atoms in metal oxides. <i>Journal of Physics and Chemistry of Solids</i> , 2011, 72, 853-861.	1.9	13
5910	A theoretical study of the vibrational spectrum of maleimide. <i>Journal of Molecular Structure</i> , 2011, 993, 431-434.	1.8	8
5911	Prediction of protein ^{13}C NMR chemical shifts using a combination scheme of statistical modeling and quantum-mechanical analysis. <i>Journal of Molecular Structure</i> , 2011, 995, 163-172.	1.8	10
5912	Theoretical study of the reactions $M^{++}H_2O$ ($M=Sr, Ba, La, Hf$). <i>Chemical Physics Letters</i> , 2011, 504, 113-117.	1.2	2
5913	Experimental and theoretical study of a Diels-Alder reaction between a sugar-derived nitroalkene and cyclopentadiene. <i>Carbohydrate Research</i> , 2011, 346, 460-464.	1.1	8
5914	Effect of regular hydration on gas phase structural stability of [zwitterionic alanine+ M^+] ($M=Li^+$). <i>Journal of Physical Chemistry B</i> , 2011, 115, 10784-10793.	0.9	3
5915	Vibrational spectroscopic studies of N,N -dimethylpropyleneurea-water system: Affected solvent spectra and factor analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 712-721.	2.0	6
5916	Characterization of pentacarbonyl(4-methylpyridine)chromium(0) complex using density functional theory (DFT) and Hartree-Fock (HF) computational methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 1715-1721.	2.0	9

#	ARTICLE	IF	CITATIONS
5917	Silver complexes of 1,2,4-triazole derived N-heterocyclic carbenes: Synthesis, structure and reactivity studies. <i>Journal of Chemical Sciences</i> , 2011, 123, 97-106.	0.7	21
5918	Loss of 45 ÅDa from a₂ Ions and Preferential Loss of 48 ÅDa from a₂ Ions Containing Methionine in Peptide Ion Tandem Mass Spectra. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 280-289.	1.2	13
5919	Kinetics, <i>in silico</i> docking, molecular dynamics, and MMâ€GSA binding studies on prototype indirubins, KT5720, and staurosporine as phosphorylase kinase ATPâ€binding site inhibitors: The role of water molecules examined. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 703-719.	1.5	82
5920	Organocatalytic depolymerization of poly(ethylene terephthalate). <i>Journal of Polymer Science Part A</i> , 2011, 49, 1273-1281.	2.5	172
5921	Theoretical study of spectroscopic properties of insulated molecular wires formed by substituted oligothiophenes and crossâ€linked 1â€cyclodextrin. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1101-1111.	2.4	9
5922	Donorâ€acceptor diethynylsilane oligomers: A secondâ€order nonlinear optical material. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2011, 49, 1410-1419.	2.4	13
5923	A DFT study of structures of dipicolyl urea isomers and their recognition with carboxylic acids and their carboxylate anions. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 92-100.	0.9	1
5924	Regiospecific naphthyl nitration of 5,10,15,20â€tetranaphthylporphyrin. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 1030-1038.	0.9	2
5925	EPR spectroscopic and computational characterization of the 2â€dehydroâ€i>â€xylene and 4â€dehydroâ€i>â€xylene triradicals. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 976-992.	0.9	7
5926	Density functional investigations of endohedral metallofullerenes TM@C₂₄ (TM = Mn, Fe,) Tj ETQq1 1,0,784314 rgBT /Ove	1.0	18
5927	A screened hybrid density functional study on energetic complexes: Metal carbohydrazide nitrates. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2311-2316.	1.0	2
5928	Quantitative evaluation of catalytic effect of metal chlorides on the decomposition reaction of NaAlH₄. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 950-960.	1.0	6
5929	DFT study of the structure and property of small organic holeâ€transporting molecules. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2039-2044.	1.0	1
5930	A mechanism of the 1,3â€dipolar cycloaddition between the hydrogen nitril HNO₂ and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2378-2389.	1.0	9
5931	Effect of amino acid polarization in force field biomolecular calculations. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2555-2559.	1.0	2
5932	Theoretical study on the smallest endohedral metallofullerenes: TM@C₂₀ (TM = Ce and) Tj ETQq1 1,0,784314 rgBT /Ove	1.0	16
5933	Structural analysis of sterically hindered 1,4â€diols from the naturally occurring lignan hydroxymatairesinol a quantum chemical study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4309-4317.	1.0	6
5934	Multireference theoretical studies on the solvent effect of firefly multicolor bioluminescence. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3371-3377.	1.0	14

#	ARTICLE	IF	CITATIONS
5935	Comparison of the deactivation mechanism of 5-fluorouracil with that of its parent system, uracil: The need of the use of the MS-CASPT2 method. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3405-3415.	1.0	6
5936	Unique QM/MM potential energy surface exploration using microiterations. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3339-3346.	1.0	55
5937	Understanding the Terahertz Spectra of Crystalline Pharmaceuticals: Terahertz Spectroscopy and Solid-State Density Functional Theory Study of (S)-(+)-ibuprofen and (RS)-ibuprofen. <i>Journal of Pharmaceutical Sciences</i> , 2011, 100, 1116-1129.	1.6	65
5938	New Alternating Copolymers of 3,6-Carbazoles and Dithienylbenzothiadiazoles: Synthesis, Characterization, and Application in Photovoltaics. <i>Macromolecular Chemistry and Physics</i> , 2011, 212, 2127-2141.	1.1	21
5939	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorine-Substituted Phenylpyridine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2517-2524.	1.0	82
5940	Synthesis of Cyclopalladated Derivatives of (<i>E</i>)-N-(benzylidene(2,6-dichlorophenyl)ethanamine and Their Reactivity towards Monodentate and Symmetric Bidentate Lewis Bases. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 3617-3631.	1.0	17
5941	Helical Complexes of Chiral Quaterpyridines – Mononuclear Cu ^{II} and Dinuclear Cu ^I Complexes. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 5112-5124.	1.0	10
5942	Photophysical and Electrochemical Properties of Phenanthroline-Based Bis-cyclometallated Iridium Complexes in Aqueous and Organic Media. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 4816-4825.	1.0	46
5943	1,2,4-Triazine vs. 1,3- and 1,4-Oxazinones in Normal- and Inverse-Electron-Demand Hetero-Diels-Alder Reactions: Establishing a Status Quo by Computational Analysis. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 983-992.	1.2	19
5944	The Mechanism of the Acid-Catalyzed Benzidine Rearrangement of Hydrazobenzene: A Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 2326-2333.	1.2	27
5945	A Convenient Road to 1-Chloropentacycloundecanes – A Joint Experimental and Computational Investigation. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 2554-2561.	1.2	12
5946	Planar Chirality of Imidazole-Containing Macrocycles – Understanding and Tuning Atropisomerism. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 6649-6655.	1.2	20
5947	Effects of heterole spacers on the structural, optical, and electrochemical properties of 2,5-bis(1,5-diphenylphosphol-2-yl)heteroles. <i>Heteroatom Chemistry</i> , 2011, 22, 457-470.	0.4	13
5948	Synthesis and structure of peri-substituted boron/pnictogen naphthalene derivatives. <i>Heteroatom Chemistry</i> , 2011, 22, 500-505.	0.4	17
5949	Camptothecin and Thiocamptothecin: the Role of Sulfur in Shifting the Hydrolysis Equilibrium towards the Closed Lactone Form. <i>ChemMedChem</i> , 2011, 6, 1706-1714.	1.6	6
5950	Aggregation of 2-Aminobenzimidazole – A Combined Experimental and Theoretical Investigation. <i>ChemPhysChem</i> , 2011, 12, 1747-1755.	1.0	5
5951	A Theoretical Study of the 3d ^M (smif) ₂ Complexes: Structure, Magnetism, and Oxidation States. <i>ChemPhysChem</i> , 2011, 12, 3236-3244.	1.0	7
5952	Spin-Orbit Coupling in Phosphorescent Iridium(III) Complexes. <i>ChemPhysChem</i> , 2011, 12, 2429-2438.	1.0	73

#	ARTICLE	IF	CITATIONS
5953	Differences in Two-Photon and One-Photon Absorption Profiles Induced by Vibronic Coupling: The Case of Dioxaborine Heterocyclic Dye. <i>ChemPhysChem</i> , 2011, 12, 3392-3403.	1.0	22
5954	Basis-Set Quality and Basis-Set Bias in Molecular Property Calculations. <i>ChemPhysChem</i> , 2011, 12, 3404-3413.	1.0	7
5955	Influence of Electron Doping on the Hydrogenation of Fullerene C ₆₀ : A Theoretical Investigation. <i>ChemPhysChem</i> , 2011, 12, 2581-2589.	1.0	4
5956	Transformation of Nickelalactones to Methyl Acrylate: On the Way to a Catalytic Conversion of Carbon Dioxide. <i>ChemSusChem</i> , 2011, 4, 1275-1279.	3.6	59
5957	A method to calculate the one-electron reduction potentials for nitroaromatic compounds based on gas-phase quantum mechanics. <i>Journal of Computational Chemistry</i> , 2011, 32, 226-239.	1.5	35
5958	Generation of Kekulé valence structures and the corresponding valence bond wave function. <i>Journal of Computational Chemistry</i> , 2011, 32, 696-708.	1.5	6
5959	Vibrational spectral signatures of peptide secondary structures: N-methylation and side chain hydrogen bond in cyclosporin A. <i>Journal of Computational Chemistry</i> , 2011, 32, 1500-1518.	1.5	2
5960	Assessment of TD-DFT and TD-CF based approaches for the prediction of exciton coupling parameters, potential energy curves, and electronic characters of electronically excited aggregates. <i>Journal of Computational Chemistry</i> , 2011, 32, 1971-1981.	1.5	70
5961	Alkaline hydrolysis of ethylene phosphate: An <i>ab initio</i> study by supermolecule model and polarizable continuum approach. <i>Journal of Computational Chemistry</i> , 2011, 32, 2545-2554.	1.5	11
5962	Two-level hierarchical parallelization of second-order Møller-Plesset perturbation calculations in divide-and-conquer method. <i>Journal of Computational Chemistry</i> , 2011, 32, 2756-2764.	1.5	21
5963	Toward a new approach for determination of solute's charge distribution to analyze interatomic electrostatic interactions in quantum mechanical/molecular mechanical simulations. <i>Journal of Computational Chemistry</i> , 2011, 32, 3092-3104.	1.5	6
5966	The Dinitrogen-Ligated Triaurum Cation, Aurodiazenylium, Auronitrenium, Auroammonia, and Auroammonium. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 2166-2170.	7.2	7
5967	Radical Derivatives of Insoluble La@C ₇₄ : X-ray Structures, Metal Positions, and Isomerization. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 6356-6359.	7.2	48
5968	Zirconium-Catalyzed Multistep Reaction of Hydrazines with Alkynes: A Non-Fischer-Type Pathway to Indoles. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 5757-5761.	7.2	56
5969	Aspergiolides C and D: Spirocyclic Aromatic Polyketides with Potent Protein Kinase <i>c-Met</i> Inhibitory Effects. <i>Chemistry - A European Journal</i> , 2011, 17, 1319-1326.	1.7	21
5970	Mechanism of the Dehydrogenative Silylation of Alcohols Catalyzed by Cationic Gold Complexes: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2011, 17, 2256-2265.	1.7	36
5971	[Ir(PCy ₃) ₂ (H) ₂ Bi ₂ NMe ₂] ⁺ as a Latent Source of Aminoborane: Probing the Role of Metal in the Dehydrocoupling of H ₃ B...NMe ₂ H and Retrodimerisation of [H ₂ BNMe ₂] ₂ . <i>Chemistry - A European Journal</i> , 2011, 17, 3011-3020.	1.7	116
5972	Chloropupukeanolides <i>C</i> : Cytotoxic Pupukeanane Chlorides with a Spiroketal Skeleton from <i>Pestalotiopsis fici</i> . <i>Chemistry - A European Journal</i> , 2011, 17, 2604-2613.	1.7	78

#	ARTICLE	IF	CITATIONS
5973	Effect of the Axial Ligand on Substrate Sulfoxidation Mediated by Iron(IV)â€œOxo Porphyrin Cation Radical Oxidants. <i>Chemistry - A European Journal</i> , 2011, 17, 6196-6205.	1.7	82
5974	Synthesis and Conformational Analysis of Î±,Î²â€œDifluoroâ€œÎ³â€œamino Acid Derivatives. <i>Chemistry - A European Journal</i> , 2011, 17, 2340-2343.	1.7	51
5975	Mechanistic Insights into Ringâ€œClosing Enyne Metathesis with the Secondâ€œGeneration Grubbsâ€œHoveyda Catalyst: A DFT Study. <i>Chemistry - A European Journal</i> , 2011, 17, 7506-7520.	1.7	56
5976	Molecular Structures of THFâ€œSolvated Alkaliâ€œMetal 2,2,6,6â€œTetramethylpiperidides Finally Revealed: Xâ€œray Crystallographic, DFT, and NMR (including DOSY) Spectroscopic Studies. <i>Chemistry - A European Journal</i> , 2011, 17, 6725-6730.	1.7	42
5977	A Tale of Two Polymorphic Pharmaceuticals: Pyrithyldione and Propyphenazone and their 1937 Coâ€œCrystal Patent. <i>Chemistry - A European Journal</i> , 2011, 17, 13445-13460.	1.7	21
5978	Expanding the Utility of BrÃ¼nsted Base Catalysis: Biomimetic Enantioselective Decarboxylative Reactions. <i>Chemistry - A European Journal</i> , 2011, 17, 8363-8370.	1.7	93
5979	Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. <i>Chemistry - A European Journal</i> , 2011, 17, 12027-12036.	1.7	23
5980	Developing a Heteroâ€œAlkaliâ€œMetal Chemistry of 2,2,6,6â€œTetramethylpiperidide (TMP): Stoichiometric and Structural Diversity within a Series of Lithium/Sodium, Lithium/Potassium and Sodium/Potassium TMP Compounds. <i>Chemistry - A European Journal</i> , 2011, 17, 8820-8831.	1.7	31
5981	Hexaazatriphenylene (HAT) versus triâ€œHAT: The Bigger the Better?. <i>Chemistry - A European Journal</i> , 2011, 17, 10312-10322.	1.7	40
5982	Enantioselective and Diastereoselective Tsujiâ€œTrost Allylic Alkylation of Lactones: An Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2011, 17, 11243-11249.	1.7	32
5983	Stitching Phospholanes Together Piece by Piece: New Modular Diâ€œand Tridentate Stereodirecting Ligands. <i>Chemistry - A European Journal</i> , 2011, 17, 14047-14062.	1.7	34
5984	Synthesis and properties of a meso-tetraphenylporphyrin and its Zn (II) complex with a dicyanoisophorone borne by double bond in the Î² pyrrolic position. <i>Inorganic Chemistry Communication</i> , 2011, 14, 1311-1313.	1.8	11
5985	Theoretical investigation of electronic structure and field emission properties of carbon nanotubeâ€œZnO nanocontacts. <i>Carbon</i> , 2011, 49, 3835-3841.	5.4	11
5986	The interaction between D3hâ€œC74 and fluorine. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 314-318.	1.1	0
5987	Theoretical studies on the structure and properties of BN clusters (BN) _n and endohedral metallo-BN clusters M@(BN) _n . <i>Computational and Theoretical Chemistry</i> , 2011, 964, 56-64.	1.1	18
5988	Proline- and thioproline-derived enamines: The theoretical study of torsional and ring-puckering conformations. <i>Computational and Theoretical Chemistry</i> , 2011, 964, 133-140.	1.1	3
5989	Density functional study for the Câ€œF bond activation of the reaction of [Pt(PCy3)2] with C6F6. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 92-100.	1.1	12
5990	Solvent effects on the antioxidant activity of 3,4-dihydroxyphenylpyruvic acid : DFT and TD-DFT studies. <i>Computational and Theoretical Chemistry</i> , 2011, 966, 232-243.	1.1	73

#	ARTICLE	IF	CITATIONS
5991	Density functional study on ionic liquid of 1-propyl-4,5-dibromo-3-methylimidazolium bromide. <i>Chemical Physics Letters</i> , 2011, 505, 87-91.	1.2	11
5992	Do nitrogen bases form chlorine-shared and ion-pair halogen bonds?. <i>Chemical Physics Letters</i> , 2011, 508, 6-9.	1.2	24
5993	Chemical-intuition based LMO transformation simplifies excited-state wave functions of peptides. <i>Chemical Physics Letters</i> , 2011, 508, 171-176.	1.2	12
5994	4f-in-core model core potentials for trivalent lanthanides. <i>Chemical Physics Letters</i> , 2011, 510, 261-266.	1.2	13
5995	Modeling short-range contributions to hydration energies with minimal parameterization. <i>Chemical Physics Letters</i> , 2011, 511, 161-165.	1.2	21
5996	The molecular basis of working mechanism of natural polyphenolic antioxidants. <i>Food Chemistry</i> , 2011, 125, 288-306.	4.2	917
5997	A combined theoretical and experimental study of mechanisms of fragmentation active for PHB oligomers in negative-ion mode multistage mass spectrometry. <i>International Journal of Mass Spectrometry</i> , 2011, 304, 15-24.	0.7	9
5998	Molecular modeling investigation of para-nitrobenzoic acid interaction in β -cyclodextrin. <i>Journal of Molecular Liquids</i> , 2011, 160, 1-7.	2.3	15
5999	Bichromophoric hemicyanine dyes as fluorescence probes applied for monitoring of the photochemically initiated polymerization. <i>Journal of Molecular Structure</i> , 2011, 985, 95-104.	1.8	11
6000	Synthesis, characterization, and computational study of N,N'-bis(2,4-dihydroxyphenyl)-1,4-quinonediimine, a hydroxyl-capped three-ring quinonediimine with sterically hindered substituent on outer rings. <i>Journal of Molecular Structure</i> , 2011, 985, 299-306.	1.8	7
6001	High-efficiency blue-green electrophosphorescent light-emitting devices using a bis-sulfone as host in the emitting layer. <i>Organic Electronics</i> , 2011, 12, 1314-1318.	1.4	28
6002	Luminescence and spectroscopic studies of organometallic rhodium and rhenium multichromophore systems carrying polypyridyl acceptor sites and phenylethynyl antenna subunits. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2252-2258.	0.8	17
6003	Synthesis of (E)-2-(1-ferrocenylmethylidene)malonic acid derivatives by a cobalt-catalyzed domino reaction of ethyl diazoacetate, carbon monoxide and ferrocenylimines. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 1394-1403.	0.8	14
6004	A DFT study of the mechanism of palladium-catalyzed alkoxy carbonylation and aminocarbonylation of alkynes: Hydride versus amine pathways. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2355-2363.	0.8	16
6005	New platinum(II) and palladium(II) quinoline-imine-pyridine, quinoline-imine-thiazole and quinoline-imine-imidazole complexes by metal-assisted condensation reactions. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2565-2575.	0.8	11
6006	Understanding the stability, electronic and molecular structure of some copper(III) complexes containing alkyl and non alkyl ligands: Insights from DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2627-2634.	0.8	12
6007	Trinuclear copper(I) acetylide complexes bearing carbonyl moiety: Synthesis, characterization, and photophysical properties. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 2654-2659.	0.8	13
6008	Rhenium(I) carbonyl complex of 4,7-diphenyl-1,10-phenanthroline—Spectroscopic properties, X-Ray structure, theoretical studies of ground and excited electronic states. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 3068-3075.	0.8	19

#	ARTICLE	IF	CITATIONS
6009	Theoretical study of inclusion complexation of 3-amino-5-nitrobenzothiazole with β -cyclodextrin. <i>Journal of Molecular Liquids</i> , 2011, 160, 8-13.	2.3	14
6010	Palladium(II) complex with S-allyl-L-cysteine: New solid-state NMR spectroscopic measurements, molecular modeling and antibacterial assays. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 313-318.	2.0	16
6011	Synthesis, X-ray studies, spectroscopic characterization and DFT calculations of p-tolylimido rhenium(V) complexes bearing an imidazole-based ligand. <i>Polyhedron</i> , 2011, 30, 142-153.	1.0	15
6012	Chemical, spectroscopic characterization, DFT studies and initial pharmacological assays of a silver(I) complex with N-acetyl-L-cysteine. <i>Polyhedron</i> , 2011, 30, 579-583.	1.0	24
6013	Synthesis, structure, UV-Vis-IR spectra, magnetism and theoretical studies on $\text{Cu}[\text{II}[(2\text{-aminomethyl})\text{pyridine}](\text{thiocyanate})_2]$ and comparisons with an analogous Cu complex. <i>Polyhedron</i> , 2011, 30, 754-763.	1.0	39
6014	Ground-state properties of ruthenium(II) and osmium(II) tin trihydride complexes: A DFT study. <i>Polyhedron</i> , 2011, 30, 1524-1529.	1.0	7
6015	Synthesis, spectroscopic and structural properties of $\text{CF}_3\text{SO}_2\text{OCCl}_3$. <i>Vibrational Spectroscopy</i> , 2011, 55, 153-159.	1.2	5
6016	Synthesis of 3-aryl-4-methyl-1,2-benzenedisulfonimides, new chiral Brønsted acids. A combined experimental and theoretical study. <i>Tetrahedron</i> , 2011, 67, 5789-5797.	1.0	14
6017	Adsorption mechanisms of isoxazole and oxazole on $\text{Si}(100)\text{-}2\times 1$ surface: Si-N dative bond addition vs. [4+2] cycloaddition. <i>Journal of Chemical Physics</i> , 2011, 135, 244707.	1.2	2
6018	Heterocyclization of Allenes Catalyzed by Late Transition Metals: Mechanisms and Regioselectivity. <i>Topics in Current Chemistry</i> , 2011, 302, 183-224.	4.0	19
6019	Effects of strong and weak hydrogen bond formation on VCD spectra: a case study of 2-chloropropionic acid. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13972.	1.3	40
6020	OHphenol-OH alcohol hydrogen-bonding as the preferred hydrogen-bonded interaction in the crystal structures of three isomers of methylolphenol: analysis of hydrogen-bonding interactions in phenol and alcohol containing molecules. <i>CrystEngComm</i> , 2011, 13, 5773.	1.3	11
6021	Thermal decomposition mechanisms of methylamine, ethylamine, and 1-propylamine on $\text{Si}(100)\text{-}2\times 1$ surface. <i>Journal of Chemical Physics</i> , 2011, 134, 194701.	1.2	11
6023	Absorption spectra of nucleic acid bases studied by the symmetry-adapted-cluster configuration-interaction (SAC-CI) method. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 537-552.	1.0	4
6024	Photodynamics of the adenine model 4-aminopyrimidine embedded within double strand of DNA. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 631-643.	1.0	10
6025	Explicitly time-dependent coupled cluster singles doubles calculations of laser-driven many-electron dynamics. <i>Journal of Chemical Physics</i> , 2011, 134, 054113.	1.2	78
6026	Valence anions of N-acetylproline in the gas phase: Computational and anion photoelectron spectroscopic studies. <i>Journal of Chemical Physics</i> , 2011, 135, 114301.	1.2	9
6027	QUANTUM CHEMICAL STUDY OF CISPLATIN-WATER COMPLEXES: AN INVESTIGATION OF ELECTRON CORRELATION EFFECTS. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 371-391.	1.8	12

#	ARTICLE	IF	CITATIONS
6028	Quasi-degenerate second-order perturbation theory for occupation restricted multiple active space self-consistent field reference functions. <i>Journal of Chemical Physics</i> , 2011, 135, 044101.	1.2	35
6029	Tris(dialkylamino)phosphine Chalcogenide Complexes of Tin(IV) Chloride: A Multinuclear (³¹ P, ⁷⁷ Se, and ¹¹⁹ Sn) NMR Characterization. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2011, 186, 1922-1931.	0.8	5
6030	Synthesis and Photophysical Properties of Blue Mono-Cyclometalated Ir(III) Complexes with Phenylpyridine Based Ligands and Phosphines. <i>Molecular Crystals and Liquid Crystals</i> , 2011, 539, 73/[413]-82/[422].	0.4	1
6031	Theoretical Indicators for Proposing Reductive Dechlorination Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans. , 2011, , .		0
6032	THE PERFORMANCE OF SELECTED <i>ab initio</i> METHODS IN ESTIMATING ELECTRON BINDING ENERGIES OF SUPERHALOGEN ANIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 93-109.	1.8	28
6033	Reconsidering an analytical gradient expression within a divide-and-conquer self-consistent field approach: Exact formula and its approximate treatment. <i>Journal of Chemical Physics</i> , 2011, 134, 034105.	1.2	45
6034	In vivomolecular labeling of halogenated volatile anesthetics via intrinsic molecular vibrations using nonlinear Raman spectroscopy. <i>Journal of Chemical Physics</i> , 2011, 134, 024525.	1.2	9
6035	Electronic coupling calculation and pathway analysis of electron transfer reaction using <i>ab initio</i> fragment-based method. I. FMO–LCMO approach. <i>Journal of Chemical Physics</i> , 2011, 134, 204109.	1.2	35
6036	Inner-shell single and double ionization potentials of aminophenol isomers. <i>Journal of Chemical Physics</i> , 2011, 135, 084302.	1.2	40
6037	On basis set superposition error corrected stabilization energies for large <i>n</i> -body clusters. <i>Journal of Chemical Physics</i> , 2011, 135, 134118.	1.2	9
6038	A tiered approach to Monte Carlo sampling with self-consistent field potentials. <i>Journal of Chemical Physics</i> , 2011, 135, 184107.	1.2	1
6039	Calculations of hyperfine coupling constant of the TMPD molecule. <i>Acta Chimica Slovaca</i> , 2012, 5, .	0.5	0
6040	Properties of Reaction Intermediates from Unzipping Nanotubes via the Diketone Formation: A Computational Study. <i>Journal of Nanomaterials</i> , 2012, 2012, 1-10.	1.5	2
6041	O ⁺ –C ₂ H ₄ potential energy surface: lowest-lying singlet at the multireference level. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	5
6042	Local Dielectric Property of Cubic, Tetragonal, and Monoclinic Hafnium Oxides. <i>Japanese Journal of Applied Physics</i> , 2012, 51, 031101.	0.8	9
6043	A First Principles Study on Zinc–Porphyrin Interaction with O ₂ in Zinc–Porphyrin(Oxygen) Complex. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 124301.	0.7	17
6044	Electronic excitation spectrum of the photosensitizer [Ir(ppy) ₂ (bpy)] ⁺ . <i>Journal of Chemical Physics</i> , 2012, 136, 214305.	1.2	37
6045	Universal state-selective corrections to multi-reference coupled-cluster theories with single and double excitations. <i>Journal of Chemical Physics</i> , 2012, 136, 124102.	1.2	21

#	ARTICLE	IF	CITATIONS
6046	Longitudinal static optical properties of hydrogen chains: Finite field extrapolations of matrix product state calculations. <i>Journal of Chemical Physics</i> , 2012, 136, 134110.	1.2	56
6047	Methodological aspects of the quantum-chemical description of interface dipoles at tetrathiafulvalene/tetracyanoquinodimethane interfaces. <i>Journal of Chemical Physics</i> , 2012, 137, 174708.	1.2	7
6048	On the fundamental processes in molecular electrical doping of organic semiconductors. <i>AIP Conference Proceedings</i> , 2012, , .	0.3	11
6049	Extension of local response dispersion method to excited-state calculation based on time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 124106.	1.2	21
6050	Calculation of electronic excitations using wave-function in wave-function frozen-density embedding. <i>Journal of Chemical Physics</i> , 2012, 137, 204120.	1.2	34
6051	Modeling the electron-impact dissociation of methane. <i>Journal of Chemical Physics</i> , 2012, 137, 22A510.	1.2	20
6052	Molecular dynamics simulations of surface-specific bonding of the hydrogen network of water: A solution to the low sum-frequency spectra. <i>Physical Review B</i> , 2012, 86, .	1.1	28
6053	Photoelectron spectroscopy and density functional theory studies on the uridine homodimer radical anions. <i>Journal of Chemical Physics</i> , 2012, 137, 205101.	1.2	4
6054	Optimizing large parameter sets in variational quantum Monte Carlo. <i>Physical Review B</i> , 2012, 85, .	1.1	91
6055	Spectral Assignment of Phenanthrene Derivatives Based on ⁶ H-Dibenzo[^{C,E}][1,2] Oxaphosphinine 6-Oxide by NMR and Quantum Chemical Calculations. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2012, 187, 781-798.	0.8	12
6056	Potential energy surface for dissociation including spin-orbit effects. <i>Molecular Physics</i> , 2012, 110, 2599-2609.	0.8	6
6057	Photoelectron spectroscopy and ab initio study of boron-carbon mixed clusters: CB ₉ ⁺ and C ₂ B ₈ ⁺ . <i>Journal of Chemical Physics</i> , 2012, 137, 234306.	1.2	19
6058	THEORETICAL INVESTIGATIONS ON THE MECHANISM OF ACTIVATION OF AMMONIA BY A p-DIMETHYLAMINOPYRIDINE COORDINATED ^{Si=O} DOUBLE BOND. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 437-481.	1.8	1
6059	A spin-adapted size-extensive state-specific multi-reference perturbation theory with various partitioning schemes. II. Molecular applications. <i>Journal of Chemical Physics</i> , 2012, 136, 024106.	1.2	31
6060	AN EVALUATION OF QUANTUM CHEMICAL CALCULATIONS OF REACTION ENERGIES FOR CATALYTIC ACTIVATION PROCESSES: THE ACTIVATION OF PROPANE BY A RHODIUM CATALYST REVISITED. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 297-312.	1.8	5
6061	Implementation of the multireference Brillouin-Wigner and Mukherjee's coupled cluster methods with non-iterative triple excitations utilizing reference-level parallelism. <i>Journal of Chemical Physics</i> , 2012, 137, 094112.	1.2	19
6062	Electronic excitations of C ₆₀ fullerene calculated using the ab initio cluster expansion method. <i>Journal of Chemical Physics</i> , 2012, 137, 134304.	1.2	13
6063	Will water act as a photocatalyst for cluster phase chemical reactions? Vibrational overtone-induced dehydration reaction of methanediol. <i>Journal of Chemical Physics</i> , 2012, 136, 164302.	1.2	30

#	ARTICLE	IF	CITATIONS
6064	Dielectronic recombination and resonant transfer excitation processes for helium-like krypton. Chinese Physics B, 2012, 21, 103401.	0.7	3
6065	On the Coulson-Fischer wave function and a local static correlation potential. Molecular Physics, 2012, 110, 149-161.	0.8	7
6066	INSIGHTS INTO THE SOLVATO-/THERMO-PROMOTED INTRAMOLECULAR ELECTRON TRANSFER IN A TTF- <i>f</i> -TCNQ DYAD WITH AN EXTREMELY LOW HOMO-LUMO GAP. Journal of Theoretical and Computational Chemistry, 2012, 11, 599-609.	1.8	5
6067	Mechanistic Consideration of Asymmetric C-N and C-C Bond Formations with Bifunctional Chiral Ir and Ru Catalysts. Bulletin of the Chemical Society of Japan, 2012, 85, 316-334.	2.0	13
6068	Amino-Acrylamido Carbenes: Modulating Carbene Reactivity via Decoration with an $\hat{1}\pm, \hat{1}^2$ -Unsaturated Carbonyl Moiety. Organometallics, 2012, 31, 4862-4870.	1.1	25
6069	Extreme oxatriquinanes and a record C-O bond length. Nature Chemistry, 2012, 4, 1018-1023.	6.6	48
6070	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. Journal of Organic Chemistry, 2012, 77, 10824-10834.	1.7	407
6071	A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. Journal of Chemical Physics, 2012, 136, 154101.	1.2	556
6072	The equation-of-motion coupled cluster method for triple electron attached states. Journal of Chemical Physics, 2012, 137, 174102.	1.2	26
6073	Refined Transition-State Models for Proline-Catalyzed Asymmetric Michael Reactions under Basic and Base-Free Conditions. Journal of Organic Chemistry, 2012, 77, 10516-10524.	1.7	21
6074	Polyoxopalladates Encapsulating 8-Coordinated Metal Ions, [MO ₈ Pd ₁₂ L ₈] ⁿ⁺ (M = Tl, ET, Q, O, O, rg, BT, /Overlock 10 Tf 50)	1.9	58
6075	13214-13228 Coordination and Metalation Bifunctionality of Cu with 5,10,15,20-Tetra(4-pyridyl)porphyrin: Toward a Mixed-Valence Two-Dimensional Coordination Network. Journal of the American Chemical Society, 2012, 134, 6401-6408.	6.6	199
6076	Mechanistic Features of Isomerizing Alkoxyacylation of Methyl Oleate. Journal of the American Chemical Society, 2012, 134, 17696-17703.	6.6	137
6077	TD-DFT Assessment of Functionals for Optical $\hat{0}$ Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372.	2.3	403
6078	Merging Active-Space and Renormalized Coupled-Cluster Methods via the CC(<i>P</i> ; <i>Q</i>) Formalism, with Benchmark Calculations for Singlet-Triplet Gaps in Biradical Systems. Journal of Chemical Theory and Computation, 2012, 8, 4968-4988.	2.3	53
6079	The $\hat{0}$ -conjugated P-flowers C ₁₆ (PH) ₈ and C ₁₆ (PF) ₈ are potential materials for organic n-type semiconductors. Physical Chemistry Chemical Physics, 2012, 14, 14832.	1.3	23
6080	Carbon-Oxygen Bond Activation in Esters by Platinum(0): Cleavage of the Less Reactive Bond. Organometallics, 2012, 31, 5018-5024.	1.1	20
6081	Theoretical Study on the Reaction Mechanisms of CH ₃ O $\hat{0}$ with O ₂ (X $\hat{1}$) and O ₂ (a $\hat{1}$). Journal of Physical Chemistry A, 2012, 116, 11656-11667.	1.1	1

#	ARTICLE	IF	CITATIONS
6082	Methyl [¹³ C]Glucopyranosiduronic Acids: Effect of COOH Ionization and Exocyclic Structure on NMR Spin-Couplings. <i>Journal of Organic Chemistry</i> , 2012, 77, 9521-9534.	1.7	9
6083	2-Acylamino-6-pyridones: Breaking of an Intramolecular Hydrogen Bond by Self-association and Complexation with Double and Triple Hydrogen Bonding Counterparts. Uncommon Steric Effect on Intermolecular Interactions. <i>Journal of Organic Chemistry</i> , 2012, 77, 1653-1662.	1.7	28
6084	Photochromism of a Diarylethene Having an Azulene Ring. <i>Journal of Organic Chemistry</i> , 2012, 77, 3270-3276.	1.7	39
6085	Investigating the Dearomative Rearrangement of Biaryl Phosphine-Ligated Pd(II) Complexes. <i>Journal of the American Chemical Society</i> , 2012, 134, 19922-19934.	6.6	80
6086	Theoretical study on the relationship between the molecular structure and corrosion inhibition efficiency of long alkyl side chain acetamide and isoxazolidine derivatives. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2012, 48, 710-721.	0.3	17
6087	Configurational Assignment of Cyclic Bisbibenzyls by HPLC-CD and Quantum-Chemical CD Calculations. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 6878-6887.	1.2	13
6088	Natural Chlorophyll-Related Porphyrins and Chlorins for Dye-Sensitized Solar Cells. <i>Molecules</i> , 2012, 17, 4484-4497.	1.7	48
6089	Atomic Hydrogen Activated TiO ₂ Nanocluster: DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18139-18145.	1.5	25
6090	Preparation and characterization of zinc-exchanged montmorillonite and its effectiveness as aflatoxin B1 adsorbent. <i>Materials Chemistry and Physics</i> , 2012, 137, 213-220.	2.0	20
6091	A remarkable anion effect on palladium nanoparticle formation and stabilization in hydroxyl-functionalized ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6026.	1.3	59
6092	¹⁵ N NMR Studies of tautomerism. <i>International Reviews in Physical Chemistry</i> , 2012, 31, 567-629.	0.9	25
6093	Mechanistic Studies on the pH-Controllable Hydrogenation of NAD ⁺ by H ₂ and Generation of H ₂ from NADH by a Water-Soluble Biomimetic Iridium Complex. <i>Organometallics</i> , 2012, 31, 8525-8536.	1.1	3
6094	Monomer- and polymer radicals of vinyl compounds: EPR and DFT studies of geometric and electronic structures in the adsorbed state. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 98, 367-377.	2.0	3
6095	Using Efficient Predictor-Corrector Reaction Path Integrators for Studies Involving Projected Frequencies. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5013-5019.	2.3	6
6096	A Phosphorescent C [∞] C* Cyclometalated Platinum(II) Dibenzothiophene NHC Complex. <i>Organometallics</i> , 2012, 31, 7447-7452.	1.1	58
6097	Synthesis and Characterization of Novel Iron(II) Complexes with Tetradentate Bis(N-heterocyclic) Tj ETQq1 1 0.784314 rgBT /Overlock 1 1.1 64	1.1	64
6098	Catalytic olefin epoxidation with a fluorinated organomolybdenum complex. <i>Journal of Molecular Catalysis A</i> , 2012, 363-364, 237-244.	4.8	21
6099	Origins of enantioselectivity in the chiral diphosphine-ligated CuH-catalyzed asymmetric hydrosilylation of ketones. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 597-604.	1.5	17

#	ARTICLE	IF	CITATIONS
6100	A Configuration Interaction Picture for a Molecular Environment Using Localized Molecular Orbitals: The Excited States of Retinal Proteins. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4452-4461.	2.3	9
6101	Revisiting sesquiterpene biosynthetic pathways leading to santalene and its analogues: a comprehensive mechanistic study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7996.	1.5	14
6102	Photoelectron Spectroscopy and Computational Modeling of Thymidine Homodimer Anions. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13975-13981.	1.2	3
6103	Low-lying electronic states and their nonradiative deactivation of thieno[3,4-b]pyrazine: An <i>ab initio</i> study. <i>Journal of Chemical Physics</i> , 2012, 137, 224313.	1.2	11
6104	A Free Energy Approach to the Prediction of Olefin and Epoxide Mutagenicity and Carcinogenicity. <i>Chemical Research in Toxicology</i> , 2012, 25, 2780-2787.	1.7	18
6105	Natural Atomic Orbital Representation for Optical Spectra Calculations in the Exciton Scattering Approach. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3734-3739.	2.1	5
6106	<i>o</i> -Benzenedisulfonimide and its chiral derivative as Brønsted acids catalysts for one-pot three-component Strecker reaction. Synthetic and mechanistic aspects. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4058.	1.5	26
6107	Free Base and Metal Complexes of 5,15-Diaza-10,20-dimesitylporphyrins: Synthesis, Structures, Optical and Electrochemical Properties, and Aromaticities. <i>Inorganic Chemistry</i> , 2012, 51, 12879-12890.	1.9	63
6108	On the electronic structure of second generation Hoveyda–Grubbs alkene metathesis precursors. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 57-67.	1.1	21
6109	Iron-Catalyzed Direct Suzuki–Miyaura Reaction: Theoretical and Experimental Studies on the Mechanism and the Regioselectivity. <i>ACS Catalysis</i> , 2012, 2, 1829-1837.	5.5	28
6110	Structural and Electronic Comparison of 1st Row Transition Metal Complexes of a Tripodal Iminopyridine Ligand. <i>Inorganic Chemistry</i> , 2012, 51, 12493-12502.	1.9	22
6111	In situ selective N-alkylation of pendant pyridyl functionality in mixed-valence copper complexes with methanol and copper(II) bromide. <i>Dalton Transactions</i> , 2012, 41, 4255.	1.6	10
6112	Formation of nano-plate silver particles in the presence of polyampholyte copolymer. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2012, 414, 17-25.	2.3	19
6114	Versatile Bottom-up Approach to Stapled π -Conjugated Helical Scaffolds: Synthesis and Chiroptical Properties of Cyclic <i>o</i> -Phenylene Ethynylene Oligomers. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 13036-13040.	7.2	31
6115	Synthesis of Amino, Azido, Nitro, and Nitrogen-Rich Azole-Substituted Derivatives of 1 <i>H</i> -Benzotriazole for High-Energy Materials Applications. <i>Chemistry - A European Journal</i> , 2012, 18, 15031-15037.	1.7	44
6116	Enantiomerization Mechanism of Thalidomide and the Role of Water and Hydroxide Ions. <i>Chemistry - A European Journal</i> , 2012, 18, 14305-14313.	1.7	30
6117	Mixed (P $\frac{1}{2}$ S/P $\frac{1}{2}$ O)-Stabilized Geminal Dianion: Facile Diastereoselective Intramolecular C–H Activations by a Related Ruthenium–Carbene Complex. <i>Chemistry - A European Journal</i> , 2012, 18, 16136-16144.	1.7	36
6118	Photochemistry of <i>fac</i> -[Re(bpy)(CO) ₃ Cl]. <i>Chemistry - A European Journal</i> , 2012, 18, 15722-15734.	1.7	74

#	ARTICLE	IF	CITATIONS
6119	Investigation of the Substrate Range of CYP199A4: Modification of the Partition between Hydroxylation and Desaturation Activities by Substrate and Protein Engineering. <i>Chemistry - A European Journal</i> , 2012, 18, 16677-16688.	1.7	53
6120	Novel Organic Dyes Based on Bulky Tri(triphenylamine)-Substituted Styrene for Dye-Sensitized Solar Cells. <i>Chinese Journal of Chemistry</i> , 2012, 30, 2779-2785.	2.6	5
6121	Facile Oxidative Rearrangements Using Hypervalent Iodine Reagents. <i>ChemistryOpen</i> , 2012, 1, 245-250.	0.9	66
6122	Density functional study on the derivatives of purine. <i>Journal of Molecular Modeling</i> , 2012, 18, 3501-3506.	0.8	8
6123	Molecular structure and vibrational spectra analysis of diethylsilanediol by IR and Raman spectroscopies and DFT calculations. <i>Journal of Sol-Gel Science and Technology</i> , 2012, 64, 54-66.	1.1	4
6124	Studies of the tautomeric equilibrium of 1,3-thiazolidine-2-thione: Theoretical and experimental approaches. <i>Chemical Physics</i> , 2012, 408, 62-68.	0.9	20
6125	QM/MM studies of cisplatin complexes with DNA dimer and octamer. <i>Computational and Theoretical Chemistry</i> , 2012, 993, 60-65.	1.1	20
6126	Structures of the α_2 ions of Ala-Ala-Ala and Phe-Phe-Phe. <i>International Journal of Mass Spectrometry</i> , 2012, 330-332, 254-261.	0.7	11
6127	Mechanistic insights into the hydrosilylation of allyl compounds – Evidence for different coexisting reaction pathways. <i>Journal of Catalysis</i> , 2012, 295, 1-14.	3.1	30
6128	Comparative DFT study of $[\text{Mg}(\text{CHZ})_3](\text{ClO}_4)_2$ and $[\text{Mg}(\text{CHZ})_3](\text{NO}_3)_2$ ($\text{CHZ}=\text{Carbohydrazide}$). <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2012, 27, 679-683.	0.4	2
6129	Ionization of chlorophyll-c2 in liquid methanol. <i>Chemical Physics Letters</i> , 2012, 546, 67-73.	1.2	7
6130	Synthesis and Characterization of a Rhodium(I) η^3 -Alkane Complex in the Solid State. <i>Science</i> , 2012, 337, 1648-1651.	6.0	131
6131	Differences in the Activation Processes of Phosphine-Containing and Grubbs-Hoveyda-Type Alkene Metathesis Catalysts. <i>Organometallics</i> , 2012, 31, 4203-4215.	1.1	85
6132	Synthesis and structural characterization of novel cyclam-based zirconium complexes and their use in the controlled ROP of rac-lactide: access to cyclam-functionalized polylactide materials. <i>Dalton Transactions</i> , 2012, 41, 14288.	1.6	26
6133	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4159-4169.	1.1	107
6134	A new 2,2',2''-terpyridine-based ligand and its complexes: structures, photophysical properties and DFT calculations to evaluate the halogen effect on the TPA. <i>CrystEngComm</i> , 2012, 14, 5613.	1.3	20
6135	Investigation of LiAlH_4 -THF formation by direct hydrogenation of catalyzed Al and LiH. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6569.	1.3	12
6136	Crystal structure, electronic properties and cytotoxic activity of palladium chloride complexes with monosubstituted pyridines. <i>Dalton Transactions</i> , 2012, 41, 658-666.	1.6	30

#	ARTICLE	IF	CITATIONS
6137	Computational studies on the mechanism of the gold(i)-catalysed rearrangement of cyclopropenes. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4433.	1.5	29
6138	Probing differences in binding of methylbenzylamine enantiomers to chiral cobalt(ii) salen complexes. <i>Dalton Transactions</i> , 2012, 41, 6861.	1.6	3
6139	An Oligosilsesquioxane Cage Functionalized with Molybdenum(II) Organometallic Fragments. <i>Organometallics</i> , 2012, 31, 4495-4503.	1.1	28
6140	Dimethylalkoxygallanes: Monomeric versus Dimeric Gas-Phase Structures. <i>Inorganic Chemistry</i> , 2012, 51, 3324-3331.	1.9	18
6141	Platinum(ii) and palladium(ii) complexes derived from 1-ferrocenylmethyl-3,5-diphenylpyrazole. Coordination, cyclometallation or transannulation?. <i>RSC Advances</i> , 2012, 2, 1986.	1.7	11
6142	How does it become possible to treat delocalized and/or open-shell systems in fragmentation-based linear-scaling electronic structure calculations? The case of the divide-and-conquer method. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7629.	1.3	68
6143	A binuclear silver complex with l-buthionine sulfoximine: synthesis, spectroscopic characterization, DFT studies and antibacterial assays. <i>RSC Advances</i> , 2012, 2, 10372.	1.7	13
6144	Photochromism of 1,2-Bis(2-thienyl)perfluorocyclopentene Derivatives: Substituent Effect on the Reactive Carbon Atoms. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10973-10979.	1.1	22
6145	Synthesis of Oxorhenium Acetyl and Benzoyl Complexes Incorporating Diamidopyridine Ligands: Implications for the Mechanism of CO Insertion. <i>Organometallics</i> , 2012, 31, 4295-4301.	1.1	20
6146	Theoretical Study of Negatively Charged Fe ⁻ (H ₂ O) _n Clusters. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5529-5540.	1.1	7
6147	Critical appraisal of excited state nonadiabatic dynamics simulations of 9 <i>H</i> -adenine. <i>Journal of Chemical Physics</i> , 2012, 137, 22A503.	1.2	102
6148	Sustainable and efficient methodology for CLA synthesis and identification. <i>Green Chemistry</i> , 2012, 14, 2584.	4.6	18
6149	Molecular tuning in highly fluorescent dithieno[3,2- <i>b</i> :2',3'- <i>d</i>]pyrrole-based oligomers: effects of N-functionalization and terminal aryl unit. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6101.	1.3	36
6150	Theoretical study on the difference of OH vibrational spectra between OH ⁺ (H ₂ O) ₃ and OH ⁺ (H ₂ O) ₄ . <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2797.	1.3	29
6151	Theoretical investigation on copper hydrides catalyzed hydrosilylation reaction of 3-methylcyclohex-2-enone: mechanism and ligands' effect. <i>Catalysis Science and Technology</i> , 2012, 2, 564-569.	2.1	8
6152	Intramolecular hydrogen atom migration along the backbone of cationic and neutral radical tripeptides and subsequent radical-induced dissociations. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8723.	1.3	31
6153	A density functional study of the relative stability of intermediates in a McMurry coupling reaction. <i>Journal of Coordination Chemistry</i> , 2012, 65, 1484-1492.	0.8	2
6154	Theoretical Study on CuCl-Catalyzed Coupling of Thiol Esters with Organostannane. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11736-11744.	1.1	3

#	ARTICLE	IF	CITATIONS
6155	Cis-Trans Ring Substituent Isomerism in Cyano-Substituted Metallathietane-3,3-dioxide Complexes of Platinum(II) and Palladium(II). <i>Organometallics</i> , 2012, 31, 4662-4669.	1.1	4
6156	Bis-Silylation of Lu ₃ N@C ₈₀ : Considerable Variation in the Electronic Structures. <i>Organic Letters</i> , 2012, 14, 5908-5911.	2.4	21
6157	¹⁷ O NMR Gives Unprecedented Insights into the Structure of Supported Catalysts and Their Interaction with the Silica Carrier. <i>Journal of the American Chemical Society</i> , 2012, 134, 9263-9275.	6.6	93
6158	Electron-Induced Elimination of the Bromide Anion from Brominated Nucleobases. A Computational Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 5612-5619.	1.2	52
6159	Mechanisms Behind the Generation of Protonated Ions for Polyaromatic Hydrocarbons by Atmospheric Pressure Photoionization. <i>Analytical Chemistry</i> , 2012, 84, 1146-1151.	3.2	30
6160	Construction of the two-electron contribution to the Fock matrix by numerical integration. <i>Molecular Physics</i> , 2012, 110, 2569-2578.	0.8	5
6161	Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7261-7271.	1.1	36
6162	Atmospheric Fate of Methacrolein. 2. Formation of Lactone and Implications for Organic Aerosol Production. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5763-5768.	1.1	58
6163	Synthesis, Characterization, and Thermal Rearrangement of Zirconium Tetraazadienyl and Pentaazadienyl Complexes. <i>Organometallics</i> , 2012, 31, 4504-4515.	1.1	28
6164	Buckyplates and Buckybowls: Examining the Effects of Curvature on π-π Interactions. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11920-11926.	1.1	58
6165	Coupling of Aromatic Aldehydes with CO ₂ -Me-Substituted Tp ^{Me2} Ir(III) Metallacyclopentadienes. <i>Organometallics</i> , 2012, 31, 3185-3198.	1.1	19
6166	Synthesis and characterization of benzodithiophene-isoindigo polymers for solar cells. <i>Journal of Materials Chemistry</i> , 2012, 22, 2306-2314.	6.7	156
6167	An Endohedral Metallofullerene as a Pure Electron Donor: Intramolecular Electron Transfer in Donor-Acceptor Conjugates of La ₂ @C ₈₀ and 11,11,12,12-Tetracyano-9,10-anthra-quinodimethane (TCAQ). <i>Journal of the American Chemical Society</i> , 2012, 134, 19401-19408.	6.6	35
6168	Iodine Bonding Stabilizes Iodomethane in MIDAS Pesticide. Theoretical Study of Intermolecular Interactions between Iodomethane and Chloropicrin. <i>Journal of Agricultural and Food Chemistry</i> , 2012, 60, 1776-1787.	2.4	4
6169	Influence of the Alkyl Substituents Spacing on the Solar Cell Performance of Benzodithiophene Semiconducting Polymers. <i>Macromolecules</i> , 2012, 45, 772-780.	2.2	26
6170	Theoretical Study on the Intermolecular Interactions of Black Dye Dimers and Black Dye-Deoxycholic Acid Complexes in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23906-23914.	1.5	24
6171	The Central Role of Gln63 for the Hydrogen Bonding Network and UV-Visible Spectrum of the AppA BLUF Domain. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8064-8073.	1.2	27
6172	Scope of Stereoselective Mn-Mediated Radical Addition to Chiral Hydrazones and Application in a Formal Synthesis of Quinine. <i>Journal of Organic Chemistry</i> , 2012, 77, 3159-3180.	1.7	35

#	ARTICLE	IF	CITATIONS
6173	Modeling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding for Geometry Optimizations and Molecular Property Calculations in the Solid. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 498-508.	2.3	39
6174	Modification of Lipid Bilayer Structure by Diacylglycerol: A Comparative Study of Diacylglycerol and Cholesterol. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 749-758.	2.3	41
6175	Charge-Transport Parameters of Acenedithiophene Crystals: Realization of One-, Two-, or Three-Dimensional Transport Channels through Alkyl and Phenyl Derivatizations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 5215-5224.	1.5	25
6176	CF ₃ â€“Ph Reductive Elimination from [(Xantphos)Pd(CF ₃)(Ph)]. <i>Organometallics</i> , 2012, 31, 1315-1328.	1.1	89
6177	Cleavage of Carbon Monoxide Promoted by a Dinuclear Tantalum Tetrahydride Complex. <i>Organometallics</i> , 2012, 31, 8516-8524.	1.1	24
6178	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. <i>Journal of the American Chemical Society</i> , 2012, 134, 13662-13669.	6.6	31
6179	Evaluation of the nonlinear optical properties for an expanded porphyrin H ₂ ckel-M ₂ bius aromaticity switch. <i>Journal of Chemical Physics</i> , 2012, 137, 184306.	1.2	35
6180	Benchmark Calculations of the Energies for Binding Excess Electrons to Water Clusters. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 893-900.	2.3	39
6181	Î±-Cleavage of Phenyl Groups from GePh ₃ Ligands in Iridium Carbonyl Cluster Complexes. A Mechanism and Its Role in the Synthesis of Bridging Germylene Ligands. <i>Organometallics</i> , 2012, 31, 2621-2630.	1.1	14
6182	Cp* Iridium Precatalysts for Selective C-H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. <i>ACS Catalysis</i> , 2012, 2, 208-218.	5.5	82
6183	Tunneling and Conformational Flexibility Play Critical Roles in the Isomerization Mechanism of Vitamin D. <i>Journal of the American Chemical Society</i> , 2012, 134, 346-354.	6.6	32
6184	Kinetically Blocked Stable Heptazethrene and Octazethrene: Closed-Shell or Open-Shell in the Ground State?. <i>Journal of the American Chemical Society</i> , 2012, 134, 14913-14922.	6.6	256
6185	Photoionization-Induced Water Migration in the Hydratedtrans-Formanilide Cluster Cation Revealed by Gas-Phase Spectroscopy and Ab Initio Molecular Dynamics Simulation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3816-3823.	1.1	31
6186	Intersubunit Electron Transfer (IET) in Quantum Dots/Graphene Complex: What Features Does IET Endow the Complex with?. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15833-15838.	1.5	28
6187	Electronic Excitations in Epicocconone Analogues: TDDFT Methodological Assessment Guided by Experiment. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8634-8643.	1.1	19
6188	A Pragmatic Approach Using First-Principle Methods to Address Site of Metabolism with Implications for Reactive Metabolite Formation. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 686-695.	2.5	7
6189	Dipole and Coulomb Forces in Electron Capture Dissociation and Electron Transfer Dissociation Mass Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1828-1837.	1.1	18
6190	Theoretical Study of the Switching between H ₂ ckel and M ₂ bius Topologies for Expanded Porphyrins. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24358-24366.	1.5	28

#	ARTICLE	IF	CITATIONS
6191	Folding-Reaction Coupling in a Self-Cleaving Protein. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3871-3879.	2.3	12
6192	Atmospheric Fate of Methacrolein. 1. Peroxy Radical Isomerization Following Addition of OH and O ₂ . <i>Journal of Physical Chemistry A</i> , 2012, 116, 5756-5762.	1.1	166
6193	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. <i>Organometallics</i> , 2012, 31, 1664-1672.	1.1	104
6194	Parallel Implementation of Multireference Coupled-Cluster Theories Based on the Reference-Level Parallelism. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 487-497.	2.3	25
6195	Imino Hydrogen Positions in Nucleic Acids from Density Functional Theory Validated by NMR Residual Dipolar Couplings. <i>Journal of the American Chemical Society</i> , 2012, 134, 6956-6959.	6.6	2
6196	Delocalization-to-Localization Charge Transition in Diferrocenyl-Oligothiophene-Vinylene Molecular Wires as a Function of the Size by Raman Spectroscopy. <i>Journal of the American Chemical Society</i> , 2012, 134, 5675-5681.	6.6	33
6197	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. <i>Organometallics</i> , 2012, 31, 4055-4062.	1.1	19
6198	Computer Simulation of the Nonlinear Optical Properties of Langmuir-Blodgett Films of a Squaraine Derivative. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15449-15457.	1.5	5
6199	Insights into the ultraviolet spectrum of liquid water from model calculations: The different roles of donor and acceptor hydrogen bonds in water pentamers. <i>Journal of Chemical Physics</i> , 2012, 137, 184301.	1.2	20
6200	QM/MM Trajectory Surface Hopping Approach to Photoisomerization of Rhodopsin and Isorhodopsin: The Origin of Faster and More Efficient Isomerization for Rhodopsin. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8009-8023.	1.2	43
6201	Influence of the Molecular Environment on Phosphorylated Amino Acid Models: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2751-2757.	1.2	12
6202	Theoretical Characterization of Absorption and Emission Spectra of an Asymmetric Porphycene. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3366-3376.	1.1	9
6203	Hole Transport in Nonstoichiometric and Doped W _{1/4} stite. <i>Journal of Physical Chemistry C</i> , 2012, 116, 17403-17413.	1.5	22
6204	Computational Insights into Uranium Complexes Supported by Redox-Active $\hat{\pm}$ -Diimine Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 2058-2064.	1.9	25
6205	Molecular-Level Insight into the Spectral Tuning Mechanism of the DsRed Chromophore. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3513-3521.	2.1	54
6206	Inner-Sphere Activation, Outer-Sphere Catalysis: Theoretical Study on the Mechanism of Transfer Hydrogenation of Ketones Using Iron(II) PNNP Eneamido Complexes. <i>Organometallics</i> , 2012, 31, 7375-7385.	1.1	79
6207	Highly Fluorinated Aryl-Substituted Tris(indazolyl)borate Thallium Complexes: Diverse Regiochemistry at the B-N Bond. <i>Inorganic Chemistry</i> , 2012, 51, 2893-2901.	1.9	22
6208	Experimental and Computational Evidence for the Participation of Nonclassical Dihydrogen Species in Proton Transfer Processes on Ru-Arene Complexes with Uncoordinated N Centers. Efficient Catalytic Deuterium Labeling of H ₂ with CD ₃ OD. <i>Organometallics</i> , 2012, 31, 3087-3100.	1.1	12

#	ARTICLE	IF	CITATIONS
6209	SERS on (111) Surface Nanofacets at Pt Nanoparticles: The Case of Acetaldehyde Oxime Reduction. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10781-10789.	1.5	11
6210	DFT Study of Internal Alkyne-to-Disubstituted Vinylidene Isomerization in [CpRu(PhC≡CAr)(dppe)] ⁺ . <i>Journal of the American Chemical Society</i> , 2012, 134, 17746-17756.	6.6	55
6211	Obtaining Enhanced Circular Dichroism in [4]Heterohelicenium Analogues. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8744-8752.	1.1	14
6212	Resonance and Aromaticity: An Ab Initio Valence Bond Approach. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4778-4788.	1.1	19
6213	Sequentially Coupled Hole- ⁺ Electron Transfer Pathways for Bridge-Mediated Triplet Excitation Energy Transfer. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23252-23256.	1.5	0
6214	Methane Adsorption on Graphitic Nanostructures: Every Molecule Counts. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2598-2603.	2.1	24
6215	Large-Scale MP2 Calculations on the Blue Gene Architecture Using the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 75-79.	2.3	45
6216	Spirobifluorene Bridged Ir(III) and Os(II) Polypyridyl Arrays: Synthesis, Photophysical Characterization, and Energy Transfer Dynamics. <i>Inorganic Chemistry</i> , 2012, 51, 2832-2840.	1.9	18
6217	1 <i>H</i> -Pyrrolo[3,2- <i>h</i>]quinoline: A Benchmark Molecule for Reliable Calculations of Vibrational Frequencies, IR Intensities, and Raman Activities. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11973-11986.	1.1	13
6218	Charged, but Found "Not Guilty": Innocence of the Suspect Bridging Ligands [RO(O)CNC(O)OR] ²⁺ = L ²⁺ in [(acac) ₂ Ru($\frac{1}{4}$ -L)Ru(acac) ₂] ⁺ , <i>i>n</i> = +, 0, "2". <i>Inorganic Chemistry</i> , 2012, 51, 9273-9281.	1.9	34
6219	Structure and Dynamics of the 1-Hydroxyethyl-4-amino-1,2,4-triazolium Nitrate High-Energy Ionic Liquid System. <i>Journal of Physical Chemistry B</i> , 2012, 116, 503-512.	1.2	38
6220	Investigating Hydrogen-Bonded Phosphonic Acids with Proton Ultrafast MAS NMR and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 18824-18830.	1.5	16
6221	Fascinating effect of dehydrogenation on the transport properties of N-heteropentacenes: transformation from p- to n-type semiconductor. <i>Journal of Materials Chemistry</i> , 2012, 22, 18181.	6.7	44
6222	A Density Functional Theory and Experimental Study of CO ₂ Interaction with Brookite TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 19755-19764.	1.5	84
6223	Intrinsic Energy Landscapes of Amino Acid Side-Chains. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1559-1572.	2.5	19
6224	Turning on Red and Near-Infrared Phosphorescence in Octahedral Complexes with Metalated Quinones. <i>Inorganic Chemistry</i> , 2012, 51, 1739-1750.	1.9	31
6225	Arginine-Facilitated Isomerization: Radical-Induced Dissociation of Aliphatic Radical Cationic Glycylarginyl(iso)leucine Tripeptides. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7627-7634.	1.2	15
6226	Dual-Copper Catalytic Site Formed in CuMFI Zeolite Makes Effective Activation of Ethane Possible Even at Room Temperature. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10680-10691.	1.5	14

#	ARTICLE	IF	CITATIONS
6227	Computational Elucidation of the Internal Oxidant-Controlled Reaction Pathways in Rh(III)-Catalyzed Aromatic C-H Functionalization. <i>Journal of Organic Chemistry</i> , 2012, 77, 3017-3024.	1.7	206
6228	Synthesis, X-ray studies, spectroscopic characterization and DFT calculations of [ReO(hmbzim) ₂ (py)]Cl·H ₂ O and [ReO(hpbzim) ₂ (Hhpbzim)]Cl. <i>Polyhedron</i> , 2012, 44, 156-164.	1.0	4
6229	Synthesis of ferrocene-labeled steroids via copper-catalyzed azide-alkyne cycloaddition. Reactivity difference between 2 ¹² -, 6 ¹² - and 16 ¹² -azido-androstanes. <i>Steroids</i> , 2012, 77, 738-744.	0.8	15
6230	DFT studies of unique stereoelectronic effects of substituents on divergent reaction pathways of methylenecyclobutanone radical cations. <i>Tetrahedron</i> , 2012, 68, 5564-5571.	1.0	3
6231	Controlling 6-endo-selectivity in oxidation/bromocyclization cascades for synthesis of aplysiapyranoids and other 2,2,6,6-substituted tetrahydropyrans. <i>Tetrahedron</i> , 2012, 68, 6968-6980.	1.0	13
6232	Direct dynamics simulation of dioxetane formation and decomposition via the singlet \hat{A} -O \hat{O} -CH ₂ -CH ₂ -biradical: Non-RRKM dynamics. <i>Journal of Chemical Physics</i> , 2012, 137, 044305.	1.2	22
6233	Mechanism of the MeReO ₃ -Catalyzed Deoxygenation of Epoxides. <i>Organometallics</i> , 2012, 31, 6139-6147.	1.1	39
6234	Gaussian Expansions of Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4891-4898.	2.3	20
6235	Carbon Monoxide Induced Double Cyclometalation at the Iridium Center. <i>Organometallics</i> , 2012, 31, 5533-5540.	1.1	12
6236	Catalytic Arene H/D Exchange with Novel Rhodium and Iridium Complexes. <i>Organometallics</i> , 2012, 31, 1943-1952.	1.1	66
6237	Acetate-Bridged Platinum(III) Complexes Derived from Cisplatin. <i>Inorganic Chemistry</i> , 2012, 51, 9852-9864.	1.9	37
6238	Dimerization Mechanism of Bis(triphenylphosphine)copper(I) Tetrahydroborate: Proton Transfer via a Dihydrogen Bond. <i>Inorganic Chemistry</i> , 2012, 51, 6486-6497.	1.9	34
6239	Synthesis of Silylene-Bridged Endohedral Metallofullerene Lu ₃ N@I _h -C ₈₀ . <i>Journal of the American Chemical Society</i> , 2012, 134, 16033-16039.	6.6	35
6240	Post-assembly Functionalization of Organoplatinum(II) Metallacycles via Copper-free Click Chemistry. <i>Journal of the American Chemical Society</i> , 2012, 134, 14738-14741.	6.6	94
6241	Electronic excitation spectra of the [Ir(ppy) ₂ (bpy)] ⁺ photosensitizer bound to small silver clusters Ag _n (n = 1-6). <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4977.	1.3	6
6242	Oxidative Aliphatic C-H Fluorination with Fluoride Ion Catalyzed by a Manganese Porphyrin. <i>Science</i> , 2012, 337, 1322-1325.	6.0	478
6243	Accurate prediction of rate constants of Diels-Alder reactions and application to design of Diels-Alder ligation. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2673.	1.5	45
6244	The fragment molecular orbital and systematic molecular fragmentation methods applied to water clusters. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7752.	1.3	61

#	ARTICLE	IF	CITATIONS
6245	Coordination of a Di- <i>tert</i> -butylphosphidoboratabenzene Ligand to Electronically Unsaturated Group 10 Transition Metals. <i>Organometallics</i> , 2012, 31, 6428-6437.	1.1	24
6246	Experimental and theoretical studies on pyrene-grafted polyoxometalate hybrid. <i>Dalton Transactions</i> , 2012, 41, 12185.	1.6	32
6247	Thermodynamic and Kinetic Hydricity of Ruthenium(II) Hydride Complexes. <i>Journal of the American Chemical Society</i> , 2012, 134, 15743-15757.	6.6	117
6248	Stable Tetrabenzo-Chichibabin π Hydrocarbons: Tunable Ground State and Unusual Transition between Their Closed-Shell and Open-Shell Resonance Forms. <i>Journal of the American Chemical Society</i> , 2012, 134, 14513-14525.	6.6	218
6249	Thermal Decomposition Mechanism of 1-Ethyl-3-methylimidazolium Bromide Ionic Liquid. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5867-5876.	1.1	57
6250	Metal Hydride and Ligand Proton Transfer Mechanism for the Hydrogenation of Dimethyl Carbonate to Methanol Catalyzed by a Pincer Ruthenium Complex. <i>ACS Catalysis</i> , 2012, 2, 964-970.	5.5	58
6251	Mechanism of the N-protecting group dependent annulations of 3-aryloxy alkynyl indoles under gold catalysis: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4417.	1.5	23
6252	Quantification of Sophisticated Equilibria in the Reaction Pool and Amplifying Catalytic Cycle of the Soai Reaction. <i>ACS Catalysis</i> , 2012, 2, 2137-2149.	5.5	67
6253	Mechanism and Stereoselectivity of a Dual Amino-Catalyzed Robinson Annulation: Rare Duumvirate Stereocontrol. <i>Journal of the American Chemical Society</i> , 2012, 134, 13624-13631.	6.6	37
6254	Theoretical illumination of water-inserted structures of the CaMn ₄ O ₅ cluster in the S ₂ and S ₃ states of oxygen-evolving complex of photosystem II: full geometry optimizations by B3LYP hybrid density functional. <i>Dalton Transactions</i> , 2012, 41, 13727.	1.6	176
6255	Mechanistic Study of the Synthesis of CdSe Nanocrystals: Release of Selenium. <i>Journal of the American Chemical Society</i> , 2012, 134, 1400-1403.	6.6	53
6256	Mechanistic investigations on the adsorption of thiophene over Zn ₃ NiO ₄ bimetallic oxide cluster. <i>Applied Surface Science</i> , 2012, 258, 10148-10153.	3.1	20
6257	Noncovalent interactions between classical supramolecular synthons in solution: Hydrogen bonding in hindered 2-acylaminopyridine/2-pyridone associates. <i>Journal of Molecular Structure</i> , 2012, 1018, 84-87.	1.8	6
6258	Reactivity of [Ba(H ₂ O) _n] ²⁺ with neutral molecules in the gas-phase: An experimental and DFT study. <i>Journal of Molecular Structure</i> , 2012, 1021, 138-146.	1.8	0
6259	Bifunctional nickel precatalysts of amido-functionalized N-heterocyclic carbenes for base-free Michael reaction under ambient conditions. <i>Journal of Organometallic Chemistry</i> , 2012, 696, 4159-4165.	0.8	34
6260	Study of the different behaviour of thiazolin and thiazin indazole derivatives with palladium(II) acetate. <i>Journal of Organometallic Chemistry</i> , 2012, 701, 36-42.	0.8	2
6261	Preparation of half-sandwich ethylene complexes of Osmium(II). <i>Journal of Organometallic Chemistry</i> , 2012, 702, 45-51.	0.8	10
6262	1,1 π -Bis(diphenylphosphino)ferrocene bridging two mono(cyclopentadienyl) cobalt moieties: Synthesis, structure, electrochemistry and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2012, 712, 52-56.	0.8	4

#	ARTICLE	IF	CITATIONS
6263	Exploring the conformational space of amorphous cellulose using NMR chemical shifts. <i>Carbohydrate Polymers</i> , 2012, 90, 1197-1203.	5.1	61
6264	A dash of protons: A theoretical study on the hydrolysis mechanism of 1-substituted silatranes and their protonated analogs. <i>Computational and Theoretical Chemistry</i> , 2012, 987, 2-15.	1.1	25
6265	Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. <i>Computational and Theoretical Chemistry</i> , 2012, 979, 1-9.	1.1	8
6266	A QM/MM study on the spinach plastocyanin: Redox properties and absorption spectra. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 119-125.	1.1	55
6267	Revealing substituent effects on the electronic structure and planarity of Ni-porphyrins. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 73-85.	1.1	42
6268	The degree of proton transfer for $XH\cdots NH_3$ ($X=F, Br, HS, \text{ and } HCOO$) heterodimers upon attachment of an excess electron. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 95-100.	1.1	1
6269	Differences in hydration between cis- and trans-platin: Quantum insights by ab initio fragment molecular orbital-based molecular dynamics (FMO-MD). <i>Computational and Theoretical Chemistry</i> , 2012, 986, 30-34.	1.1	21
6270	Theoretical study on the mechanism and stereochemistry of salicylaldehyde-Al(III)-catalyzed hydrophosphonylation of benzaldehyde. <i>Computational and Theoretical Chemistry</i> , 2012, 989, 44-50.	1.1	7
6271	Metal salts reduction during parylenes polymerization. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 56-65.	1.1	2
6272	Mechanism of SO ₂ elimination from the aromatic sulfonamide anions: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 74-81.	1.1	12
6273	DFT study on the intramolecular nitrene-alkene cycloaddition reaction of the N-3-alkenylnitrene. <i>Computational and Theoretical Chemistry</i> , 2012, 992, 128-133.	1.1	2
6274	Towards large-scale calculations with State-Specific Multireference Coupled Cluster methods: Studies on dodecane, naphthynes, and polycarbenes. <i>Chemical Physics Letters</i> , 2012, 542, 128-133.	1.2	13
6275	Experimental and theoretical NMR determination of isoniazid and sodium p-sulfonatocalix[n]arenes inclusion complexes. <i>European Journal of Pharmaceutical Sciences</i> , 2012, 47, 539-548.	1.9	44
6276	Effect of Microstructure of Nitrogen-Doped Graphene on Oxygen Reduction Activity in Fuel Cells. <i>Langmuir</i> , 2012, 28, 7542-7550.	1.6	279
6277	Substitution Reactions in Dinuclear Ru-Hbpp Complexes: an Evaluation of Through-Space Interactions. <i>Inorganic Chemistry</i> , 2012, 51, 1889-1901.	1.9	21
6278	Ab Initio Molecular Orbital Study on the Excited States of [2.2]-, [3.3]-, and Siloxane-Bridged Paracyclophanes. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10194-10202.	1.1	15
6279	Single-Crystal X-ray Diffraction Study of Three Yb@C ₈₂ Isomers Cocrystallized with Ni ^{II} (octaethylporphyrin). <i>Journal of the American Chemical Society</i> , 2012, 134, 18772-18778.	6.6	71
6280	Solvent-Catalyzed Ring-Chain-Ring Tautomerization in Axially Chiral Compounds. <i>Chemistry - A European Journal</i> , 2012, 18, 12725-12732.	1.7	14

#	ARTICLE	IF	CITATIONS
6281	Disclosing the Structure/Activity Correlation in Trivalent Boron-Containing Compounds: A Tendency Map. <i>Chemistry - A European Journal</i> , 2012, 18, 12794-12802.	1.7	69
6282	Predicting the Enantioselectivity of the Copper-Catalysed Cyclopropanation of Alkenes by Using Quantitative Quadrant-Diagram Representations of the Catalysts. <i>Chemistry - A European Journal</i> , 2012, 18, 14026-14036.	1.7	39
6283	Iridium-Catalyzed Allylic Substitutions with Cyclometalated Phosphoramidite Complexes Bearing a Dibenzocyclooctatetraene Ligand: Preparation of (η^5 -Allyl)Ir Complexes and Computational and NMR Spectroscopic Studies. <i>Chemistry - A European Journal</i> , 2012, 18, 14314-14328.	1.7	34
6284	Reversible Double C-H Bond Activation of Linear and Cyclic Ethers To Form Iridium Carbenes. <i>Chemistry - A European Journal</i> , 2012, 18, 13149-13159.	1.7	30
6285	A π -Stacked Porphyrin-Fullerene Electron Donor-Acceptor Conjugate That Features a Surprising Frozen Geometry. <i>Chemistry - A European Journal</i> , 2012, 18, 14008-14016.	1.7	23
6286	Andraxylocarpins...A: Structurally Intriguing Limonoids from the True Mangroves <i>Xylocarpus granatum</i> and <i>Xylocarpus moluccensis</i> . <i>Chemistry - A European Journal</i> , 2012, 18, 14342-14351.	1.7	36
6287	Analysis of the Electronic Circular Dichroism Spectrum of (η^5)[9](2,5)Pyridinophane. <i>Chirality</i> , 2012, 24, 994-1004.	1.3	6
6288	Conformational Control of the Electronic Properties of an $\hat{\pi}$ -Terthiophene: Lessons from a Precursor Towards Dendritic Hyperbranched Oligo- and Poly-Thiophenes. <i>ChemPhysChem</i> , 2012, 13, 3893-3900.	1.0	11
6289	Redox Activity in a Vanadium(V)-Dioxolene Complex Is Modulated by Protonation State As Indicated by ^{51}V Solid-State NMR Spectroscopy and Density Functional Theory. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4644-4651.	1.0	9
6290	Structural Insight into the Prolyl Hydroxylase PHD2: A Molecular Dynamics and DFT Study. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4973-4985.	1.0	5
6291	Configurational Stable Tris(tetrathioaryl)methyl Molecular Propellers. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 6517-6525.	1.2	6
6292	Bond energies (Pt-NH ₃ , Pt-Cl) and proton affinity of cisplatin: A density functional theory approach. <i>Journal of Structural Chemistry</i> , 2012, 53, 436-442.	0.3	5
6293	Theoretical study of Rh(I) and Rh(III) bis(isonitrile) complexes as promising reagents for synthesis of N-heterocyclic carbenes. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 1576-1583.	0.3	2
6294	Facile Decarboxylation of Propiolic Acid on a Ruthenium Center and Related Chemistry. <i>Organometallics</i> , 2012, 31, 5262-5273.	1.1	13
6295	Photoinduced electron transfer and solvation dynamics in aqueous clusters: comparison of the photoexcited iodide-water pentamer and the water pentamer anion. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6257.	1.3	9
6296	<i>In Silico</i> Modeling of the Molecular Structure and Binding of Leukotriene A ₄ into Leukotriene A ₄ Hydrolase. <i>Chemical Biology and Drug Design</i> , 2012, 80, 902-908.	1.5	3
6297	Prediction of organic molecular crystal geometries from MP2-level fragment quantum mechanical/molecular mechanical calculations. <i>Journal of Chemical Physics</i> , 2012, 137, 174106.	1.2	60
6298	Theoretical Study on the Ground State Structure of Uranofullerene U@C ₈₂ . <i>Journal of Physical Chemistry A</i> , 2012, 116, 11651-11655.	1.1	34

#	ARTICLE	IF	CITATIONS
6299	Platinum Clusters on Vacancy-Type Defects of Nanometer-Sized Graphene Patches. <i>Molecules</i> , 2012, 17, 7941-7960.	1.7	15
6300	Rapid Access to Substituted Piperazines via Ti(NMe ₂) ₄ -Mediated C-C Bond-Making Reactions. <i>Organometallics</i> , 2012, 31, 6005-6013.	1.1	22
6301	On two alizarin polymorphs. <i>CrystEngComm</i> , 2012, 14, 3667.	1.3	21
6302	Computations of 36 Tautomer/Isomer Equilibria of Different Lactams. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6885-6893.	1.1	11
6303	Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2835-2843.	2.3	98
6304	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2868-2877.	2.3	54
6305	Insights on the binding ability of a new adenine analog: 7-amine-1,2,4-triazolo[1,5-a]pyrimidine. Synthesis and magnetic study of the first copper(II) complexes. <i>Dalton Transactions</i> , 2012, 41, 1755-1764.	1.6	17
6306	Density Functional Theory Study of N≡C-N and O≡C-N Bond Cleavage by an Iron Silyl Complex. <i>Organometallics</i> , 2012, 31, 3995-4005.	1.1	19
6307	Carbon Nanotube Container: Complexes of C ₅₀ H ₁₀ with Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4546-4555.	2.3	16
6308	Axial Ligand Effect On The Rate Constant of Aromatic Hydroxylation By Iron(IV)=Oxo Complexes Mimicking Cytochrome P450 Enzymes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 718-730.	1.2	64
6309	Decarbonylation of Aliphatic Aldehydes by a Tp ^{Me2} Ir(III) Metallacyclopentadiene. <i>Organometallics</i> , 2012, 31, 716-721.	1.1	31
6310	Convergence of Electronic Structure with the Size of the QM Region: Example of QM/MM NMR Shieldings. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2260-2271.	2.3	111
6311	A Theoretical Study of an Unusual Y-Shaped Three-Coordinate Pt Complex: Pt(0) η^2 -Disilane Complex or Pt(II) Disilyl Complex?. <i>Journal of the American Chemical Society</i> , 2012, 134, 11749-11759.	6.6	36
6312	Modified reactive empirical bond-order potential for heterogeneous bonding environments. <i>Journal of Chemical Physics</i> , 2012, 137, 054102.	1.2	8
6313	Decaborane Thiols as Building Blocks for Self-Assembled Monolayers on Metal Surfaces. <i>Inorganic Chemistry</i> , 2012, 51, 1685-1694.	1.9	23
6314	Dimeric Gold Bis(carbene) Complexes by Transmetalation in Water. <i>Organometallics</i> , 2012, 31, 619-626.	1.1	65
6315	Exploring Structural and Optical Properties of Fluorescent Proteins by Squeezing: Modeling High-Pressure Effects on the mStrawberry and mCherry Red Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12426-12440.	1.2	32
6316	Excited states and electronic spectra of annulated dinuclear free-base phthalocyanines: A theoretical study on near-infrared-absorbing dyes. <i>Journal of Chemical Physics</i> , 2012, 136, 114304.	1.2	9

#	ARTICLE	IF	CITATIONS
6317	Catalyst Chelation Effects in Organocatalyzed Ring-Opening Polymerization of Lactide. ACS Macro Letters, 2012, 1, 19-22.	2.3	64
6318	An Atomistic View on Human Hemoglobin Carbon Monoxide Migration Processes. Biophysical Journal, 2012, 102, 887-896.	0.2	43
6319	Theoretical studies on intramolecular methyl transfer in the S-2-alkenyl-dimethylsulfonium ion. Computational and Theoretical Chemistry, 2012, 997, 25-33.	1.1	2
6320	New five-coordinated mercury (II) dyes based on a novel 2,2',6',2'''-terpyridine ligand: Structures, photophysical properties and DFT calculations to evaluate the halogen effect on the two-photon absorption. Dyes and Pigments, 2012, 95, 723-731.	2.0	10
6321	Design, structural and spectroscopic elucidation, and the in vitro biological activities of new diorganotin dithiocarbamates. European Journal of Medicinal Chemistry, 2012, 58, 493-503.	2.6	42
6322	Synthesis and electrochemical properties of tetrathienyl-linked branched polymers with various aromatic cores. Electrochimica Acta, 2012, 79, 154-161.	2.6	16
6323	Theoretical studies on the spectroscopic properties of a series of halide Zinc (II) complexes with pyridinylimine and pyridinylmethylamine derivatives. Synthetic Metals, 2012, 162, 2138-2148.	2.1	7
6324	Crystal structure and theoretical studies of the keto-enol isomerism of N,N'-bis(salicylidene)-o-phenylenediamine (salophen). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 110-115.	2.0	44
6325	Interaction of alkali, alkaline earth and transition metal ions with a ketocyanine dye: A comparative electronic spectroscopic study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 37-45.	2.0	8
6326	Quantitative analysis of molecular surface based on improved Marching Tetrahedra algorithm. Journal of Molecular Graphics and Modelling, 2012, 38, 314-323.	1.3	1,449
6327	Mass spectrometric and theoretical studies on dissociation of the CS bond in the benzenesulfonic acid and benzenesulfonic acid anion series: Homolytic cleavage vs heterolytic cleavage. Journal of Molecular Structure, 2012, 1028, 1-6.	1.8	7
6328	Conformational Changes of <i>trans</i> -1,2-Dichlorocyclohexane Adsorbed in Zeolites Studied by FT-Raman Spectroscopy and Molecular QM/MM Simulations. Journal of Physical Chemistry C, 2012, 116, 8608-8618.	1.5	7
6329	Reactivity for boryl(phosphino)carbenyl carbene analogues with group 14 elements (C, Si, Ge, Sb, and) Tj ETQq0 0 Q rgBT /Overlock 10 T	1.6	9
6330	Effects of Ethynyl Substitution on Cyclobutadiene. Journal of Physical Chemistry A, 2012, 116, 483-490.	1.1	10
6331	Mechanisms of Organocatalytic Amidation and Trans-Esterification of Aromatic Esters As a Model for the Depolymerization of Poly(ethylene) Terephthalate. Journal of Physical Chemistry A, 2012, 116, 12389-12398.	1.1	73
6332	Ring-Opening Polymerization of Epoxides Catalyzed by Uranyl Complexes: An Experimental and Theoretical Study of the Reaction Mechanism. Inorganic Chemistry, 2012, 51, 9132-9140.	1.9	23
6333	Iridium-Catalyzed Allylic Alkylation Reaction with N-Aryl Phosphoramidite Ligands: Scope and Mechanistic Studies. Journal of the American Chemical Society, 2012, 134, 4812-4821.	6.6	182
6334	Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. Journal of Chemical Theory and Computation, 2012, 8, 5107-5123.	2.3	72

#	ARTICLE	IF	CITATIONS
6335	Spectral Properties and Orientation of Voltage-Sensitive Dyes in Lipid Membranes. <i>Langmuir</i> , 2012, 28, 10808-10817.	1.6	18
6336	Dâ€“Dâ€“i€“A-Type Organic Dyes for Dye-Sensitized Solar Cells with a Potential for Direct Electron Injection and a High Extinction Coefficient: Synthesis, Characterization, and Theoretical Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25653-25663.	1.5	153
6337	The para-substituent effect and pH-dependence of the organometallic Baeyerâ€“Villiger oxidation of rheniumâ€“carbon bonds. <i>Dalton Transactions</i> , 2012, 41, 3758.	1.6	9
6338	Diruthenium(III,III) Ethynyl-phenyleneimine Molecular Wires: Preparation via On-Complex Schiff Base Condensation. <i>Inorganic Chemistry</i> , 2012, 51, 7561-7568.	1.9	14
6339	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12992.	1.3	32
6340	Hole transport in pure and doped hematite. <i>Journal of Applied Physics</i> , 2012, 112, .	1.1	84
6341	Selectivity of bis-triazinyl bipyridine ligands for americium(iii) in Am/Eu separation by solvent extraction. Part 1. Quantum mechanical study on the structures of BTBP complexes and on the energy of the separation. <i>Dalton Transactions</i> , 2012, 41, 14416.	1.6	64
6342	Computational Insight into a Gold(I) N-Heterocyclic Carbene Mediated Alkyne Hydroamination Reaction. <i>Inorganic Chemistry</i> , 2012, 51, 5593-5604.	1.9	51
6343	Oxo vs Imido Alkylidene d⁰-Metal Species: How and Why Do They Differ in Structure, Activity, and Efficiency in Alkene Metathesis?. <i>Organometallics</i> , 2012, 31, 6812-6822.	1.1	81
6344	Charge Transfer in Model Peptides: Obtaining Marcus Parameters from Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2284-2293.	1.2	39
6345	Origin of Vibrational Spectroscopic Response at Ice Surface. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3001-3006.	2.1	52
6346	Improving Platinum Catalyst Durability with a Doped Graphene Support. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10548-10556.	1.5	113
6347	Epitaxial Growth of i€-Stacked Perfluoropentacene on Graphene-Coated Quartz. <i>ACS Nano</i> , 2012, 6, 10874-10883.	7.3	108
6348	The Cobaltâ€“Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1870-1894.	2.3	97
6349	Natural Bond Orbital Analysis of the Electronic Structure of [L_nM(CH₃)] and [L_nM(CF₃)] Complexes. <i>Organometallics</i> , 2012, 31, 1467-1476.	1.1	50
6350	Near-infrared laser induced conformational change and UV laser photolysis of glycine in low-temperature matrices: Observation of a short-lived conformer. <i>Journal of Molecular Structure</i> , 2012, 1025, 33-42.	1.8	50
6351	Tunneling Lifetime of the ttc/tp Conformer of Glycine in Low-Temperature Matrices. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10539-10547.	1.1	81
6352	Understanding of nonlinear optical properties of CS2 from a microscopic viewpoint. <i>Journal of Chemical Physics</i> , 2012, 137, 084315.	1.2	4

#	ARTICLE	IF	CITATIONS
6353	Luminescent Cyclometalated Alkynylgold(III) Complexes with 6-Phenyl-2,2'-Bipyridine Derivatives: Synthesis, Characterization, Electrochemistry, Photophysics, and Computational Studies. <i>Inorganic Chemistry</i> , 2012, 51, 7537-7545.	1.9	70
6354	Effects of Polarizability on the Adsorption of Noble Gases at Low Pressures in Monohalogenated Isorecticular Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19765-19772.	1.5	99
6355	Fragmentation Pathways in the Uracil Radical Cation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9217-9227.	1.1	32
6356	On the Interaction of Phosphines with High Surface Area Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25919-25927.	1.5	15
6357	Heteropolytopic Arsanylarylthiolato Ligands: Cis-Trans Isomerism of Nickel(II), Palladium(II), and Platinum(II) Complexes of 1-AsPh ₂ -2-SHC ₆ H ₄ . <i>Inorganic Chemistry</i> , 2012, 51, 7125-7133.	1.9	15
6358	Terahertz Spectroscopy of the Explosive Taggant 2,3-Dimethyl-2,3-Dinitrobutane. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6879-6884.	1.1	15
6359	On Two Recent Developments in the Description of Molecular Properties in Solution by Using the Polarizable Continuum Model (PCM): The Coupled-Cluster Theory and the Molecules at Extreme Pressures. , 2012, , 1-17.		0
6360	First-principles study of magnetic interactions in cupric oxide. <i>Physical Review B</i> , 2012, 85, .	1.1	26
6361	Mechanism of Metal-Free Hydrogen Transfer between Amine-Boranes and Aminoboranes. <i>Journal of the American Chemical Society</i> , 2012, 134, 16805-16816.	6.6	88
6362	Quantum Systems in Chemistry and Physics. <i>Progress in Theoretical Chemistry and Physics</i> , 2012, , .	0.2	6
6363	Untethered 4,1,2-MC2B10 supraicosahedral metallocarboranes, their C ₂ -dimethyl 4,1,6-, 4,1,8- and 4,1,12-MC2B10 analogues, and DFT study of the (4,1,2- to (4,1,6-isomerisations of C2B11 carboranes and MC2B10 metallocarboranes. <i>Dalton Transactions</i> , 2012, 41, 10957.	1.6	12
6364	Vibrational Analysis of Side Chain Model Compounds of Perfluorinated Alkyl Sulfonic Acid Ionomers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 10850-10863.	1.1	14
6365	Size Consistency Error in the Antisymmetric Geminal Power Wave Function can be Completely Removed. <i>Physical Review Letters</i> , 2012, 109, 203001.	2.9	83
6366	Calculations of nonlinear response properties using the intermediate state representation and the algebraic-diagrammatic construction polarization propagator approach: Two-photon absorption spectra. <i>Journal of Chemical Physics</i> , 2012, 136, 064107.	1.2	68
6367	Comparative parametric method 6 (PM6) and Recife model 1 (RM1) study of <i>trans</i> -stilbene. <i>Molecular Simulation</i> , 2012, 38, 1-7.	0.9	7
6368	New Linear π -Conjugated Diruthenium Compounds Containing Axial Tetrathiafulvalene-acetylide Ligands. <i>Organometallics</i> , 2012, 31, 8591-8597.	1.1	22
6369	Elucidating the Microscopic Origin of the Unique Optical Properties of Polypyrene. <i>Journal of Physical Chemistry C</i> , 2012, 116, 20191-20198.	1.5	5
6370	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2688-2697.	2.3	78

#	ARTICLE	IF	CITATIONS
6371	Distance-dependent Schwarz-based integral estimates for two-electron integrals: Reliable tightness vs. rigorous upper bounds. <i>Journal of Chemical Physics</i> , 2012, 136, 144107.	1.2	68
6372	Synthesis and Nâ€“H Reductive Elimination Study of Dinuclear Ruthenium Imido Dihydride Complexes. <i>Journal of the American Chemical Society</i> , 2012, 134, 17027-17035.	6.6	15
6373	Two-Photon Absorption-Molecular Structure Investigation Using a Porphycene Chromophore with Potential in Photodynamic Therapy. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11818-11828.	1.2	17
6374	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	22
6375	Can ORMAS be used for nonadiabatic coupling calculations? SiCH4 and butadiene contours. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	3
6376	Mechanism of ketone hydrosilylation using NHCâ€“Cu(I) catalysts: a computational study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	17
6377	Mechanistic Insight into the Chemiluminescent Decomposition of Firefly Dioxetanone. <i>Journal of the American Chemical Society</i> , 2012, 134, 11632-11639.	6.6	96
6378	A Computational Exploration of the CO Adsorption in Cation-Exchanged Faujasites. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24512-24521.	1.5	11
6379	DFT and QTAIM Study of Intramolecular and Intermolecular Feâ€“HÎˆ~ÂˆÂˆ-HÎˆ+â€“O Dihydrogen Bonds. <i>Journal of Cluster Science</i> , 2012, 23, 703-711.	1.7	2
6380	Crystal Structure of Two Anti-Porphyrin Antibodies with Peroxidase Activity. <i>PLoS ONE</i> , 2012, 7, e51128.	1.1	11
6381	Synthesis and evaluation of new guanidine-thiourea organocatalyst for the nitro-Michael reaction: Theoretical studies on mechanism and enantioselectivity. <i>Beilstein Journal of Organic Chemistry</i> , 2012, 8, 1485-1498.	1.3	36
6382	Synthesis and Properties of 2-Alkylidene-1,3-dithiolo[4,5-d]-4,5-ethylenediselenotetrathiafulvalene Derivatives and Crystal Structures of Their Cation Radical Salts. <i>Crystals</i> , 2012, 2, 393-412.	1.0	4
6383	Synthesis, Structures and Properties of Molecular Conductors Based on Bis-Fused Donors Composed of (Thio)Pyran-4-ylidene-1,3-dithiolo and Tetraselenafulvalene. <i>Crystals</i> , 2012, 2, 1092-1107.	1.0	4
6384	Conformationally Controlled Mechanistic Aspects of BACE 1 Inhibitors. <i>Central Nervous System Agents in Medicinal Chemistry</i> , 2012, 12, 28-37.	0.5	0
6385	Coupled-cluster, MÅ¶ller Plesset (MP2), density fitted local MP2, and density functional theory examination of the energetic and structural features of hydrophobic solvation: Water and pentane. <i>Journal of Chemical Physics</i> , 2012, 136, 054305.	1.2	8
6386	Theoretical study on photophysical properties of novel bis(BF₂)²â€“bidipyrrins dyes: Effect of variation in monomer structure. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 440-452.	1.0	9
6387	Structure and reactivity of baicalein radical cation. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2009-2017.	1.0	7
6388	Analysis of cipadesin limonoids from <i>Cipadessa cinerascens</i> using electrospray ionization quadrupole timeâ€“ofâ€“flight tandem mass spectrometry and quantum chemical calculations. <i>Rapid Communications in Mass Spectrometry</i> , 2012, 26, 563-571.	0.7	11

#	ARTICLE	IF	CITATIONS
6389	Kinetic investigation on carbamate formation from the reaction of carbon dioxide with amino acids in homogeneous aqueous solution. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 239-247.	0.9	20
6390	hCINAP is an atypical mammalian nuclear adenylate kinase with an ATPase motif: Structural and functional studies. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 206-220.	1.5	27
6391	Circular dichroism: electronic. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 150-166.	6.2	106
6392	EPR Spectroscopy of 4, 4'-bis(tert-butyl)-2, 2'-bipyridine-1, 2'-edithiolatocuprates(II) in Host Lattices with Different Coordination Geometries. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, 965-975.	0.6	4
6393	Reactions of substituted aspirins with amino acids. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 939-945.	0.9	2
6394	A proline mimetic for enantioselective aldol reaction: a quantum chemical study of a catalytic reaction with a sterically hindered α -prolinamide derivative. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 971-978.	0.9	3
6395	Aminonitrocyclopropanes as Possible High-Energy Materials. <i>Quantum Chemical Calculations. Propellants, Explosives, Pyrotechnics</i> , 2012, 37, 498-501.	1.0	3
6396	Basis set dependence of phosphate frequencies in density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2435-2439.	1.0	6
6397	Spin-orbit absorption spectroscopy of transition metal hydrides: A TD-DFT and MS-CASPT2 study of $\text{HM}(\text{CO})_5$ (M = Mn, Re). <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2085-2097.	1.0	22
6398	Prediction of conformational population of large cycloalkanes using <i>ab initio</i> correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3188-3197.	1.0	9
6399	ONIOM study of dissociated hydrogen and water on ZnO surface. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3223-3227.	1.0	10
6400	Theoretical study of inclusion of a dinuclear platinum(II) complex in $\hat{1}$, $\hat{2}$, and $\hat{3}$ -cyclodextrins. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3403-3408.	1.0	6
6401	A TD-DFT basis set and density functional assessment for the calculation of electronic excitation energies of fluorene. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3434-3438.	1.0	44
6402	Effect of the Substitution on the Protonation of Allyl Cyclopentadienyl Molybdenum(II) Compounds. <i>Organometallics</i> , 2012, 31, 2193-2202.	1.1	19
6403	Near-Infrared Radiation Induced Conformational Change and Hydrogen Atom Tunneling of 2-Chloropropionic Acid in Low-Temperature Ar Matrix. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4823-4832.	1.1	32
6404	Theoretical Analysis of the Sequential Proton-Coupled Electron Transfer Mechanisms for H_2 Oxidation and Production Pathways Catalyzed by Nickel Molecular Electrocatalysts. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3171-3180.	1.5	54
6405	Heteropolytopic phosphanylthiolato ligands: formation of cis isomers of nickel(ii), palladium(ii) and platinum(ii) complexes with 1-P(Biph)-2-SHC6H4 (Biph = 1,1'-biphenyl-2,2'-diyl). <i>Dalton Transactions</i> , 2012, 41, 7729.	1.6	9
6406	C-H Activation of Terminal Alkynes by Tris-(3,5-dimethylpyrazolyl)boraterhodiumneopentylisocyanide: New Metal-Carbon Bond Strengths. <i>Journal of the American Chemical Society</i> , 2012, 134, 9276-9284.	6.6	25

#	ARTICLE	IF	CITATIONS
6407	Gaseous Vanadium Molybdate and Tungstates: Thermodynamic Properties and Structures. <i>Inorganic Chemistry</i> , 2012, 51, 4918-4924.	1.9	15
6408	X-ray Spectroscopy of Heterocyclic Biochemicals: Xanthine, Hypoxanthine, and Caffeine. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5653-5664.	1.1	29
6409	Photochemistry of Cp ² Mn(CO) ₂ (NHC) (Cp ² = $\text{C}_5\text{H}_4\text{Me}$) Species: Synthesis, Time-Resolved IR Spectroscopy, and DFT Calculations. <i>Organometallics</i> , 2012, 31, 4971-4979.	1.1	21
6410	Observation of an Organic Acid Mediated Spin State Transition in a Co(II) Schiff Base Complex: An EPR, HYSCORE, and DFT Study. <i>Inorganic Chemistry</i> , 2012, 51, 8014-8024.	1.9	18
6411	Singlet Excitation Energy Transfer Mediated by Local Exciton Bridges. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13865-13876.	1.5	2
6412	Direct Asymmetric Allylic Alkenylation of <i>N</i> -Itaconimides with Morita-Baylis-Hillman Carbonates. <i>Journal of Organic Chemistry</i> , 2012, 77, 6600-6607.	1.7	26
6413	Preparation of novel polymorphic pigment 3,3'-((4,4'-biphenyldiylbisthio)bis-2-methyl-1,4-naphthoquinone and its polymorphic properties. <i>CrystEngComm</i> , 2012, 14, 1016-1020.	1.3	7
6414	Partial Atomic Charges and Screened Charge Models of the Electrostatic Potential. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1989-1998.	2.3	37
6415	Challenges for the Accurate Simulation of Anisotropic Charge Mobilities through Organic Molecular Crystals: The Γ^2 Phase of <i>mer</i> -Tris(8-hydroxyquinolino)aluminum(III) (Alq3) Crystal. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14826-14836.	1.5	66
6416	Nonagostic M ²⁺ -H ⁺ -C Interactions. Synthesis, Characterization, and DFT Study of the Titanium Amide Ti ₂ Cl ₆ [N(<i>t</i> -Bu) ₂] ₂ . <i>Organometallics</i> , 2012, 31, 4894-4903.	1.1	17
6417	Dimerization-Initiated Preferential Formation of Coronene-Based Graphene Nanoribbons in Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15141-15145.	1.5	87
6418	Rationalization of the behavior of M ₂ (CH ₃ CS ₂) ₄ (M) Tj ETQq1 1 0.784314 rgBT calculations. <i>Journal of Computational Chemistry</i> , 2012, 33, 1748-1761.	1.5	6
6419	On the importance of excited state dynamic response electron correlation in polarizable embedding methods. <i>Journal of Computational Chemistry</i> , 2012, 33, 2012-2022.	1.5	38
6420	¹ H NMR analysis of <i>O</i> -methylinositol isomers: a joint experimental and theoretical study. <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 608-614.	1.1	31
6421	Synthesis and Stereoselective Interconversion of Chiral 1,3,6-diphosphacycloheptanes. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 1857-1866.	1.0	21
6422	Metal Complexation of a ^D -Ribose-Based Ligand Decoded by Experimental and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3308-3319.	1.0	4
6423	Amide-Functionalized Bis(NHC) Systems: Anion Effect on Gold-Gold Interactions. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 3892-3898.	1.0	23
6424	[4+2] Cycloadditions of 3-tetrazolyl-1,2-diazabutadienes: Synthesis of 3-tetrazolyl-1,4,5,6-tetrahydropyridazines. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 2152-2160.	1.2	39

#	ARTICLE	IF	CITATIONS
6425	Assessment of <i>ab initio</i> MP2 and density functionals for characterizing the potential energy profiles of the S_N2 reactions at N center. <i>Journal of Computational Chemistry</i> , 2012, 33, 1347-1352.	1.5	13
6426	Shifts in Excitation Energies Induced by Hydrogen Bonding: A Comparison of the Embedding and Supermolecular Time-Dependent Density Functional Theory Calculations with the Equation-of-Motion Coupled-Cluster Results. <i>Progress in Theoretical Chemistry and Physics</i> , 2012, , 219-248.	0.2	7
6427	Cationic Ir(III) Alkylidenes Are Key Intermediates in C-H Bond Activation and C-C Bond-Forming Reactions. <i>Journal of the American Chemical Society</i> , 2012, 134, 7165-7175.	6.6	44
6428	Effects of Fluorination on Iridium(III) Complex Phosphorescence: Magnetic Circular Dichroism and Relativistic Time-Dependent Density Functional Theory. <i>Inorganic Chemistry</i> , 2012, 51, 2821-2831.	1.9	48
6429	Electronic Structures of Ruthenium and Osmium Complexes of 9,10-Phenanthrenequinone. <i>Inorganic Chemistry</i> , 2012, 51, 6687-6699.	1.9	29
6430	Quantum Mechanical Calculation of ^{13}C NMR Chemical Shifts in a Series of Isomeric Fucobiosides with the Account for Conformational Equilibrium. <i>Journal of Carbohydrate Chemistry</i> , 2012, 31, 93-104.	0.4	0
6431	Band Gap Engineering of MnO via ZnO Alloying: A Potential New Visible-Light Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9876-9887.	1.5	118
6432	Molecular Control of the Nanoscale: Effect of Phosphine-Chalcogenide Reactivity on CdS-CdSe Nanocrystal Composition and Morphology. <i>ACS Nano</i> , 2012, 6, 5348-5359.	7.3	101
6433	Photophysical and Computational Investigations of Bis(phosphine) Organoplatinum(II) Metallacycles. <i>Journal of the American Chemical Society</i> , 2012, 134, 10607-10620.	6.6	70
6434	Tuning redox potentials of bis(imino)pyridine cobalt complexes: an experimental and theoretical study involving solvent and ligand effects. <i>Dalton Transactions</i> , 2012, 41, 3562.	1.6	41
6435	Quantum kernel applications in medicinal chemistry. <i>Future Medicinal Chemistry</i> , 2012, 4, 1479-1494.	1.1	12
6436	Ultrafast exciton dynamics after Soret- or Q-band excitation of a directly \hat{I}^2, \hat{I}^2 -linked bisporphyrin. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8038.	1.3	37
6437	Conformational Solvation Studies of LIGNOLs with Molecular Dynamics and Conductor-Like Screening Model. <i>International Journal of Molecular Sciences</i> , 2012, 13, 9845-9863.	1.8	6
6438	Theoretical Study of the Cytochrome P450 Mediated Metabolism of Phosphorodithioate Pesticides. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2706-2712.	2.3	10
6439	Organic Dye Design Tools for Efficient Photocurrent Generation in Dye-Sensitized Solar Cells: Exciton Binding Energy and Electron Acceptors. <i>Advanced Functional Materials</i> , 2012, 22, 1606-1612.	7.8	143
6441	Superelectrophilic Amidine Dications: Dealkylation by Triflate Anion. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 8516-8519.	7.2	7
6442	Synthesis, characterization, biological studies and <i>in vitro</i> cytotoxicity on human cancer cell lines of titanium(IV) and tin(IV) derivatives with the \hat{I}, \hat{I} -dimercapto-o-xylene ligand. <i>Applied Organometallic Chemistry</i> , 2012, 26, 383-389.	1.7	7
6443	Molecular Structure and Electronic State of the Dibenzo[<i>a,e</i>]pentalene Anion Radical. <i>Chemistry - an Asian Journal</i> , 2012, 7, 480-483.	1.7	21

#	ARTICLE	IF	CITATIONS
6444	Catalytic Diastereoselective Tandem Conjugate Addition–Elimination Reaction of Morita–Baylis–Hillman Adducts by C–C Bond Cleavage. <i>Chemistry - an Asian Journal</i> , 2012, 7, 771-777.	1.7	6
6445	Naphthalene and Anthracene Complexes Sandwiched by Two $\{(Cp^*)Fe\}$ Fragments: Strong Electronic Coupling between the Fe Centers. <i>Chemistry - an Asian Journal</i> , 2012, 7, 1231-1242.	1.7	24
6446	Organocatalytic 1,4-Addition Reaction of α,β -Unsaturated Aldehydes versus 1,6-Addition Reaction. <i>ChemCatChem</i> , 2012, 4, 959-962.	1.8	52
6447	Mechanism of the Transition-Metal-Catalyzed Hydroarylation of Bromoalkynes Revisited: Hydrogen versus Bromine Migration. <i>Chemistry - A European Journal</i> , 2012, 18, 5401-5415.	1.7	52
6448	Tetrachlorinated Tetraazaperopyrenes (TAPPs): Highly Fluorescent Dyes and Semiconductors for Air-Stable Organic Channel Transistors and Complementary Circuits. <i>Chemistry - A European Journal</i> , 2012, 18, 3498-3509.	1.7	65
6449	Insights into the Mechanism of Reaction of $[(C_5Me_5)_2Sm(thf)_2]$ with CO_2 and COS by DFT Studies. <i>Chemistry - A European Journal</i> , 2012, 18, 7886-7895.	1.7	51
6450	Alternative Reaction Pathways in Domino Reactions of Hydrazinediidozirconium Complexes with Alkynes. <i>Chemistry - A European Journal</i> , 2012, 18, 3925-3941.	1.7	34
6451	DFT Studies on Cobalt-Catalyzed Cyclotrimerization Reactions: The Mechanism and Origin of Reaction Improvement under Microwave Irradiation. <i>Chemistry - A European Journal</i> , 2012, 18, 6217-6224.	1.7	36
6452	Bifunctional Rhenium Complexes for the Catalytic Transfer-Hydrogenation Reactions of Ketones and Imines. <i>Chemistry - A European Journal</i> , 2012, 18, 5701-5714.	1.7	40
6453	Insight into the Reaction Mechanisms of $(MeC_5H_4)_3U$ with Isoelectronic Heteroallenes CS_2 , COS, PhN_3 , and $PhNCO$ by DFT Studies: A Unique Pathway that Involves Bimetallic Complexes. <i>Chemistry - A European Journal</i> , 2012, 18, 6610-6615.	1.7	20
6454	En Route to Dinitroacetylene: Nitro(trimethylsilyl)acetylene and Nitroacetylene Harnessed by Dicobalt Hexacarbonyl. <i>Chemistry - A European Journal</i> , 2012, 18, 6588-6603.	1.7	10
6455	Chirality Effects on the IRMPD Spectra of Basket Resorcinarene/Nucleoside Complexes. <i>Chemistry - A European Journal</i> , 2012, 18, 8320-8328.	1.7	29
6456	Origin of Selectivity of Tsuji–Trost Allylic Alkylation of Lactones: Highly Ordered Transition States with Lithium-Containing Enolates. <i>Chemistry - A European Journal</i> , 2012, 18, 10408-10418.	1.7	16
6457	Conformational Flexibility and Absolute Stereochemistry of $(3R)$ - β -hydroxy- γ -lactams Investigated by Chiroptical Properties and TD-DFT Calculations. <i>Chirality</i> , 2012, 24, 741-750.	1.3	6
6458	Identification of the Most Stable Sc_2C_{80} Isomers: Structure, Electronic Property, and Molecular Spectra Investigations. <i>Chinese Journal of Chemistry</i> , 2012, 30, 765-770.	2.6	5
6459	Mechanism of Silver(I)-Catalyzed Enantioselective Synthesis of Axially Chiral Allenes Based on Propargylamines. <i>Chinese Journal of Chemistry</i> , 2012, 30, 951-958.	2.6	18
6460	Theoretical Study of Energetic Complexes (III): $Bis(5-nitro-2H-tetrazolato-N)^2$ tetraammine Cobalt(III) Perchlorate (BNCP) and Its Transition Metal (Ni/Fe/Cu/Zn) Perchlorate Analogues. <i>Chinese Journal of Chemistry</i> , 2012, 30, 1624-1630.	2.6	2
6461	Predicting Drug Metabolism by Cytochrome P450 2C9: Comparison with the 2D6 and 3A4 Isoforms. <i>ChemMedChem</i> , 2012, 7, 1202-1209.	1.6	46

#	ARTICLE	IF	CITATIONS
6462	Singleâ€Crystal Xâ€Ray Diffraction, Isolatedâ€Molecule and Cluster Electronic Structure Calculations, and Scanning Electron Microscopy in an Organic solid: Models for Intramolecular Motion in 4,4â€-Dimethoxybiphenyl. ChemPhysChem, 2012, 13, 2082-2089.	1.0	12
6463	Rationalization of Solvation and Stabilization of Palladium Nanoparticles in Imidazoliumâ€Based Ionic Liquids by DFT and Vibrational Spectroscopy. ChemPhysChem, 2012, 13, 1781-1790.	1.0	27
6464	Directionality of Dihydrogen Bonds: The Role of Transition Metal Atoms. ChemPhysChem, 2012, 13, 2677-2687.	1.0	22
6465	Aggregation and Solvation of Chiral N,â€Amide Ligands in Coordinating Solvents: A Computational and NMR Spectroscopic Study. ChemPlusChem, 2012, 77, 799-806.	1.3	11
6466	Synthesis of Fiveâ€Membered Cyclic Ethers by Reaction of 1,4â€Diols with Dimethyl Carbonate. ChemSusChem, 2012, 5, 1578-1586.	3.6	57
6467	Catalytic Adaptive Recognition of Thiol (SH) and Selenol (SeH) Groups Toward Synthesis of Functionalized Vinyl Monomers. Journal of the American Chemical Society, 2012, 134, 6637-6649.	6.6	97
6468	Steric effect for proton, hydrogen-atom, and hydride transfer reactions with geometric isomers of NADHâ€model ruthenium complexes. Faraday Discussions, 2012, 155, 129-144.	1.6	12
6469	Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening. Organic and Biomolecular Chemistry, 2012, 10, 6682.	1.5	57
6470	Intermolecular Interactions in Complex Liquids: Effective Fragment Potential Investigation of Waterâ€tert-Butanol Mixtures. Journal of Physical Chemistry B, 2012, 116, 2775-2786.	1.2	42
6471	Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484.	1.3	22
6472	Computational Study of the Mechanism of the Photochemical and Thermal Ring-Opening/Closure Reactions and Solvent Dependence in Spirooxazines. Journal of Physical Chemistry A, 2012, 116, 8148-8158.	1.1	17
6473	Substituent Effects in Thermal Reactions of a Silene with Silyl-Substituted Alkynes: A Theoretical Study. Organometallics, 2012, 31, 4737-4747.	1.1	7
6474	Supramolecular interactions between hexabromoethane and cyclopentadienyl ruthenium bromides: Halogen bonding or electrostatic organisation?. CrystEngComm, 2012, 14, 804-811.	1.3	19
6475	Performance assessment of density functional theory-based models using orbital momentum distributions. Molecular Simulation, 2012, 38, 468-480.	0.9	4
6476	Hydride Abstraction from [MCpBz(CO)3H] (M = Mo, W; CpBz= C5(CH2Ph)5): New Cationic Complexes Stabilized by Î-5:Î-2-C5H4:C6H5 Bonding of the Pentabenzylcyclopentadienyl Ligand. Organometallics, 2012, 31, 4387-4396.	1.1	3
6477	Symmetry Breaking: Polymorphic Form Selection by Enantiomers of the Melatonin Agonist and Its Missing Polymorph. Crystal Growth and Design, 2012, 12, 3964-3976.	1.4	16
6478	On the Origin of ^{35/37} Cl Isotope Effects on ¹⁹⁵ Pt NMR Chemical Shifts. A Density Functional Study. Journal of Chemical Theory and Computation, 2012, 8, 1344-1350.	2.3	19
6479	Axial Imidazole Binding Strengths in Porphyrinoid Cobalt(III) Complexes as Studied by Tandem Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2012, 23, 1135-1146.	1.2	9

#	ARTICLE	IF	CITATIONS
6480	An Assessment of Computational Methods for Obtaining Structural Information of Moderately Flexible Biomolecules from Ion Mobility Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 792-805.	1.2	29
6482	Density Functional Theory Study on the Identification of Pd(Me-Xanthate) ₂ . <i>Arabian Journal for Science and Engineering</i> , 2012, 37, 1283-1291.	1.1	7
6483	Energetics of dioxygen binding into graphene patches with various sizes and shapes. <i>Science China Chemistry</i> , 2012, 55, 787-795.	4.2	2
6484	Is the dynamical polarization a significant part of the contribution of the triples to the correlation energy?. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	0
6485	Numerical integration of atomic electron density with double exponential formula for density functional calculation. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	3
6486	Variationally determined electronic states for the theoretical analysis of intramolecular interaction: I. Resonance energy and rotational barrier of the C–N bond in formamide and its analogs. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	6
6487	Theoretical study on the structures and electronic properties of oligo(p-phenylenevinylene) carboxylic acid and its derivatives: effects of spacer and anchor groups. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	14
6488	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	14
6489	Electron momentum spectroscopy of metal carbonyls: a reinvestigation of the role of nuclear dynamics. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	19
6490	Proton transfer reaction and intermolecular interactions in associates of 2,5-dihydroxy-1,8-naphthyridine. <i>Journal of Molecular Modeling</i> , 2012, 18, 1633-1644.	0.8	9
6491	First-principles study of energetic complexes (II): (5-cyanotetrazolato-N ₂) pentaammine cobalt (III) perchlorate (CP) and Ni, Fe and Zn analogues. <i>Journal of Molecular Modeling</i> , 2012, 18, 2855-2860.	0.8	1
6492	Study of the picture change error at the 2nd order Douglas Kroll Hess level of theory. Electron and spin density and structure factors of the Bis[bis(methoxycarbimido) aminato] copper (II) complex. <i>Chemical Physics</i> , 2012, 395, 44-53.	0.9	14
6493	Non-Born–Oppenheimer self-consistent field calculations with cubic scaling. <i>Chemical Physics</i> , 2012, 400, 103-107.	0.9	9
6494	Modulation of ligand fluorescence by the Pt(II)/Pt(IV) redox couple. <i>Inorganica Chimica Acta</i> , 2012, 389, 77-84.	1.2	31
6495	The importance of London dispersion forces in crystalline magnesium nitrate hexahydrate. <i>Inorganica Chimica Acta</i> , 2012, 389, 176-182.	1.2	11
6496	Constrained self-consistent field method revisited toward theoretical designs of functional materials under external field. <i>Chemical Physics Letters</i> , 2012, 530, 132-136.	1.2	3
6497	Phosphorescence parameters for platinum (II) organometallic chromophores: A study at the non-collinear four-component Kohn–Sham level of theory. <i>Chemical Physics Letters</i> , 2012, 531, 229-235.	1.2	10
6498	Coordination effects on the electronic structure of the CuA site of cytochrome c oxidase. <i>Chemical Physics Letters</i> , 2012, 531, 197-201.	1.2	3

#	ARTICLE	IF	CITATIONS
6499	Theoretical study of 3,3- ² substitution of 9,9,9- ² ,9- ² -tetramethyl-fluorene-dimers. <i>Chemical Physics Letters</i> , 2012, 538, 67-71.	1.2	1
6500	Elimination of water from the backbone of protonated tetraglycine. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 268-272.	0.7	11
6501	Fragmentations of protonated cyclic-glycylglycine and cyclic-alanylalanine. <i>International Journal of Mass Spectrometry</i> , 2012, 316-318, 199-205.	0.7	14
6502	Influence of susceptibility to hydrolysis and hydrophobicity of arylsemicarbazones on their anti-nociceptive and anti-inflammatory activities. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 140-148.	2.6	7
6503	2-Acetylpyridine- and 2-benzoylpyridine-derived hydrazones and their gallium(III) complexes are highly cytotoxic to glioma cells. <i>European Journal of Medicinal Chemistry</i> , 2012, 50, 163-172.	2.6	58
6504	Density functional calculations on the effect of sulfur substitution for 2- ² -hydroxypropyl-p-nitrophenyl phosphate: C O vs. P O bond cleavage. <i>Bioorganic Chemistry</i> , 2012, 40, 99-107.	2.0	2
6505	Investigation of substituted 6-aminohexanoates as skin penetration enhancers. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 86-95.	1.4	6
6506	N-(4-Substituted-benzoyl)-N- ² -(¹ -d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 1801-1816.	1.4	13
6507	N4-Phenyl-substituted 2-acetylpyridine thiosemicarbazones: Cytotoxicity against human tumor cells, structure-activity relationship studies and investigation on the mechanism of action. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 3396-3409.	1.4	66
6508	Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 222-230.	2.0	7
6509	Chemical, spectroscopic characterization, DFT studies and antibacterial activities in vitro of a new gold(I) complex with rimantadine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 114-118.	2.0	10
6510	A theoretical study on cellular antioxidant activity of selected flavonoids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 235-239.	2.0	18
6511	Bis (trifluoromethyl) sulfone, CF ₃ SO ₂ CF ₃ : Synthesis, vibrational and conformational properties. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 332-339.	2.0	6
6512	W-band PELDOR with 1 kW microwave power: Molecular geometry, flexibility and exchange coupling. <i>Journal of Magnetic Resonance</i> , 2012, 216, 175-182.	1.2	54
6513	A first principles study of water adsorption on ¹ ±-Pu (020) surface. <i>Journal of Nuclear Materials</i> , 2012, 424, 138-145.	1.3	3
6514	Photoisomerization of fluorinated 1,3-dimethyl-5-propenyl uracils. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012, 231, 60-63.	2.0	0
6515	Structural characterization of a new dioxamic acid derivative by experimental (FT-IR, NMR, and X-ray) analyses and theoretical (HF and DFT) investigations. <i>Journal of Molecular Structure</i> , 2012, 1016, 13-21.	1.8	11
6516	Experimental and DFT study of cyclodehydration and acetylation of ferrocenyl diols. <i>Journal of Molecular Structure</i> , 2012, 1019, 7-15.	1.8	3

#	ARTICLE	IF	CITATIONS
6517	Synthesis, spectroscopic characterization and molecular modeling of a tetranuclear platinum(II) complex with thiazolidine-4-carboxylic acid. <i>Journal of Molecular Structure</i> , 2012, 1019, 21-26.	1.8	1
6518	Charged dioxomolybdenum(VI) complexes with pyridoxal thiosemicarbazone ligands as molybdenum(V) precursors in oxygen atom transfer process and epoxidation (pre)catalysts. <i>Polyhedron</i> , 2012, 33, 441-449.	1.0	67
6519	Silver(I) and gold(I) complexes with penicillamine: Synthesis, spectroscopic characterization and biological studies. <i>Polyhedron</i> , 2012, 34, 210-214.	1.0	29
6520	Synthesis, spectroscopic characterization, DFT studies and antibacterial assays of a novel silver(I) complex with the anti-inflammatory nimesulide. <i>Polyhedron</i> , 2012, 36, 112-119.	1.0	40
6521	Synthesis and characterization of novel pyridine- <i>iso</i> urea complexes of Pd(II). <i>Polyhedron</i> , 2012, 37, 66-76.	1.0	4
6522	A broad study of two new promising antimycobacterial drugs: Ag(I) and Au(I) complexes with 2-(2-thienyl)benzothiazole. <i>Polyhedron</i> , 2012, 38, 291-296.	1.0	41
6523	Catalytic effects of Lewis acids on 1,3-DC reaction: A luminescent study. <i>Journal of Luminescence</i> , 2012, 132, 1456-1461.	1.5	3
6524	Dimethylsilanediol: Structure and vibrational spectra by IR and Raman spectroscopies and quantum chemical calculations. <i>Vibrational Spectroscopy</i> , 2012, 58, 79-86.	1.2	8
6525	Synthesis and vibrational properties of trifluoromethyl trifluoromethanesulfonate and comparison with covalent sulfonates. <i>Vibrational Spectroscopy</i> , 2012, 59, 40-46.	1.2	7
6526	Initiation of the 3 \hat{e} :5 \hat{e} -AMP-induced protein kinase A \hat{I} regulatory subunit conformational transition. Part II. Inhibition by Rp-3 \hat{e} :5 \hat{e} -AMPS. <i>Biochemistry (Moscow)</i> , 2012, 77, 465-468.	0.7	1
6527	A theoretical study of kinetics and mechanism of the oxa 6 \hat{I} electrocyclization of naphthoquinones as antimalarial drugs. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1220-1225.	0.1	0
6528	Reactions of the biologically active palladium complexes (H ₂ A) ₂ [PdCl ₄] with glutamic acid as a model of their transformations in blood plasma. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2012, 38, 233-239.	0.3	5
6529	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. <i>ChemBioChem</i> , 2012, 13, 240-251.	1.3	72
6530	Theoretical Studies of Asymmetric Hydroformylation Using the Rh(\hat{I})-BINAPHOS Catalyst \hat{e} Origin of Coordination Preferences and Stereoinduction. <i>Chemistry - A European Journal</i> , 2012, 18, 995-1005.	1.7	45
6531	Template Effects in S _N 2 Displacements for the Preparation of Pseudopeptidic Macrocycles. <i>Chemistry - A European Journal</i> , 2012, 18, 2409-2422.	1.7	26
6532	Amination with Pd(\hat{I})-NHC Complexes: Rate and Computational Studies Involving Substituted Aniline Substrates. <i>Chemistry - A European Journal</i> , 2012, 18, 145-151.	1.7	96
6533	Catalytic Non \hat{e} Conventional <i>trans</i> - \hat{e} Hydroboration: A Theoretical and Experimental Perspective. <i>Chemistry - A European Journal</i> , 2012, 18, 1512-1521.	1.7	54
6534	Multifn: A multifunctional wavefunction analyzer. <i>Journal of Computational Chemistry</i> , 2012, 33, 580-592.	1.5	21,818

#	ARTICLE	IF	CITATIONS
6535	A [Fe(CB ₆)] platform for binding of small molecules: Insights from DFT calculations. <i>Journal of Computational Chemistry</i> , 2012, 33, 1047-1054.	1.5	4
6536	The Effects of Biological Environments on the Electron-Relay Functionality of Tryptophan Residues in Proteins. <i>ChemPhysChem</i> , 2012, 13, 183-192.	1.0	4
6537	Di-, Tetra-, Penta- and Polynuclear Zinc Complexes Supported by a Flexible Tetradentate Schiff Base Ligand. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 1130-1138.	1.0	15
6538	Gas-phase oxidation of cresol isomers initiated by OH or NO ₃ radicals in the presence of NO ₂ . <i>International Journal of Chemical Kinetics</i> , 2012, 44, 165-178.	1.0	9
6539	Surface Modification of Indium-Tin Oxide Via Self-Assembly of a Donor-Acceptor Complex: A Density Functional Theory Study. <i>Advanced Materials</i> , 2012, 24, 687-693.	11.1	10
6540	Novel C ⁺ Bond Cleavages of Tryptophan-Containing Peptide Radical Cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 264-273.	1.2	23
6541	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
6542	Examining the impact of ancillary ligand basicity on copper(I)-ethylene binding interactions: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
6543	Synthesis and structural study of ethylmethylsilanediol by quantum chemical calculations and IR and Raman spectroscopies. <i>Journal of Sol-Gel Science and Technology</i> , 2012, 61, 258-267.	1.1	3
6544	Theoretical study of the hydroboration reaction of cyclopropane with borane. <i>Journal of Molecular Modeling</i> , 2012, 18, 751-754.	0.8	3
6545	Influence of stereochemistry on proton transfer in protonated tripeptide models. <i>Journal of Molecular Modeling</i> , 2012, 18, 871-879.	0.8	0
6546	Solvent-Free Epoxidation of Olefins Catalyzed by [MoO ₂ (SAP)]-t-BuOOH: A New Mode of <i>tert</i> -Butylhydroperoxide Activation. <i>ChemCatChem</i> , 2013, 5, 601-611.	1.8	72
6547	Excitation energy transfer in GFP-X-CFP model peptides (X = amino acids): Direct versus through-bridge energy transfers. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 563-568.	1.0	4
6548	Divide-and-conquer-based symmetry adapted cluster method: Synergistic effect of subsystem fragmentation and configuration selection. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 218-223.	1.0	21
6549	Absorption and emission properties of various substituted cinnamic acids and cinnamates, based on TDDFT investigation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 542-554.	1.0	21
6550	Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6664-6670.	1.1	33
6551	Study of the Gas-Phase Intramolecular Aryltrifluoromethylation of Phenyl(Trifluoromethyl)Iodonium by ESI-MS/MS. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 761-767.	1.2	8
6552	Fragmentation Chemistry of [Met-Gly] ⁺ , [Gly-Met] ⁺ , and [Met-Met] ⁺ Radical Cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 543-553.	1.2	4

#	ARTICLE	IF	CITATIONS
6553	Which Hydrogen Atom of Toluene Protonates PAH molecules in (+)-Mode APPI MS Analysis?. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 316-319.	1.2	12
6554	Computational study on the structure and properties of ternary complexes of Ln ³⁺ (Ln = La, Ce, Nd) Tj ETQq1 1 0.784314 rgBT /Over 54, 283-291.	0.3	0
6555	Insight into Group 4 Metallocenium-Mediated Olefin Polymerization Reaction Coordinates Using a Metadynamics Approach. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3491-3497.	2.3	4
6556	Quantum chemical study of the mechanism of the catalytic oxyethylation of ethylene glycol on phosphorus-doped titanium dioxide: The role of the surface phosphoryl and hydroxyl groups of the catalyst. <i>Kinetics and Catalysis</i> , 2013, 54, 157-167.	0.3	3
6557	Analysis of energy-optimized Gaussian basis sets for condensed phase density functional calculations. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	9
6558	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	1
6559	A B3LYP study on the C-H activation in propane by neutral and +1 charged low-energy platinum clusters with 2-6 atoms. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2013, 109, 315-333.	0.8	9
6560	Synthesis, spectroscopic characterization, DFT studies, and antibacterial and antitumor activities of a novel water soluble Pd(II) complex with l-alliin. <i>Journal of Molecular Structure</i> , 2013, 1035, 421-426.	1.8	14
6561	Electrolyte effect on the aggregation behavior of 1-butyl-3-methylimidazolium dodecylsulfate in aqueous solution. <i>Journal of Colloid and Interface Science</i> , 2013, 402, 139-145.	5.0	49
6562	Optical Excitations in MnO and MnO:ZnO via Embedded CASPT2 Theory and Their Implications for Solar Energy Conversion. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13816-13826.	1.5	7
6563	An experimental and computational study of 1,1'-ferrocene diamines. <i>Polyhedron</i> , 2013, 52, 377-388.	1.0	19
6564	Zinc(ii), iron(ii/iii) and ruthenium(ii) complexes of o-phenylenediamine derivatives: oxidative dehydrogenation and photoluminescence. <i>Dalton Transactions</i> , 2013, 42, 15028.	1.6	8
6565	Density functional theory study of fullerene-carbene Lewis acid-base adducts: critical role of dispersion interactions. <i>RSC Advances</i> , 2013, 3, 10177.	1.7	7
6566	Photophysical Properties of Endohedral Amine-Functionalized Bis(phosphine) Pt(II) Complexes as Models for Emissive Metallacycles. <i>Inorganic Chemistry</i> , 2013, 52, 9254-9265.	1.9	16
6567	Molecular Structure and Chemical Property of a Divalent Metallofullerene Yb@C ₂ (13)-C ₈₄ . <i>Journal of the American Chemical Society</i> , 2013, 135, 12730-12735.	6.6	29
6568	Chemoselective Oxidation of Polyols with Chiral Palladium Catalysts. <i>Organometallics</i> , 2013, 32, 2257-2266.	1.1	30
6569	Probing Charge Transfer in Benzodifuran-C ₆₀ Dumbbell-Type Electron Donor-Acceptor Conjugates: Ground- and Excited-State Assays. <i>ChemPhysChem</i> , 2013, 14, 2910-2919.	1.0	9
6570	New dicoumarol sodium compound: crystal structure, theoretical study and tumoricidal activity against osteoblast cancer cells. <i>Chemistry Central Journal</i> , 2013, 7, 110.	2.6	9

#	ARTICLE	IF	CITATIONS
6571	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	12
6572	Failures of TDDFT in describing the lowest intramolecular charge-transfer excitation in <i>para</i> -nitroaniline. <i>Molecular Physics</i> , 2013, 111, 1235-1248.	0.8	79
6573	Impact of Organoaluminum Compounds on Phenoxyimine Ligands in Coordinative Olefin Polymerization. A Theoretical Study. <i>Organometallics</i> , 2013, 32, 3870-3876.	1.1	10
6574	Temperature influence on supramolecular structure formation. Synthesis, structure, spectral and DFT studies of Cu(II)-azide systems with symmetric diamines. <i>Polyhedron</i> , 2013, 61, 80-86.	1.0	16
6575	Effects of London dispersion correction in density functional theory on the structures of organic molecules in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16031.	1.3	238
6576	Pyrazolato-Bridged Dinuclear Complexes of Ruthenium(II) and Rhodium(III) with N-Heterocyclic Carbene Ligands: Synthesis, Characterization, and Electrochemical Properties. <i>Organometallics</i> , 2013, 32, 4082-4091.	1.1	22
6577	Nucleophilic Halogenations of Diazo Compounds, a Complementary Principle for the Synthesis of Halodiazo Compounds: Experimental and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2013, 78, 7488-7497.	1.7	42
6578	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. <i>Journal of Computational Chemistry</i> , 2013, 34, 2079-2090.	1.5	38
6579	Zirconium Hydrazides as Metallanitrene Synthons: Release of Molecular N ₂ from a Hydrazinediido Complex Induced by Oxidative N-N Bond Cleavage. <i>Organometallics</i> , 2013, 32, 3877-3889.	1.1	9
6580	How to Find Out Whether a 5-Substituted Uracil Could Be a Potential DNA Radiosensitizer. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2853-2857.	2.1	59
6581	Catalytic cross-coupling of diazo compounds with coinage metal-based catalysts: an experimental and theoretical study. <i>Dalton Transactions</i> , 2013, 42, 4132.	1.6	57
6582	Bisacenaphthopyrazinoquinoxaline derivatives: synthesis, physical properties and applications as semiconductors for n-channel field effect transistors. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 5683.	1.5	4
6583	The Mechanism of Borane-Amine Dehydrocoupling with Bifunctional Ruthenium Catalysts. <i>Journal of the American Chemical Society</i> , 2013, 135, 13342-13355.	6.6	141
6584	A new fluorescent probe for distinguishing Zn ²⁺ and Cd ²⁺ with high sensitivity and selectivity. <i>Dalton Transactions</i> , 2013, 42, 11465.	1.6	58
6585	Polymerization of Methyl Methacrylate with Lithium Triflate. A Kinetic and Structural Study. <i>Macromolecules</i> , 2013, 46, 5445-5454.	2.2	14
6586	Geometric and Electronic Structures of Manganese-Substituted Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2013, 52, 3356-3367.	1.9	19
6587	Effects of Odd-Even Side Chain Length of Alkyl-Substituted Diphenylbithiophenes on First Monolayer Thin Film Packing Structure. <i>Journal of the American Chemical Society</i> , 2013, 135, 11006-11014.	6.6	81
6588	TDDFT studies of electronic spectra and excited states of the triphenylamine-based organic sensitizers and organic sensitizer-titanium dioxide cluster complexes. <i>RSC Advances</i> , 2013, 3, 12133.	1.7	11

#	ARTICLE	IF	CITATIONS
6589	New Mechanism for the Ring-Opening Polymerization of Lactones? Uranyl Aryloxide-Induced Intermolecular Catalysis. <i>Inorganic Chemistry</i> , 2013, 52, 9077-9086.	1.9	45
6590	Assignment of Configuration in a Series of Dioxolanone-Type Secondary Metabolites from <i>Guignardia bidwellii</i> – A Comparison of VCD and ECD Spectroscopy. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 5946-5951.	1.2	17
6591	Structural and vibrational study of 8-hydroxyquinoline-2-carboxaldehyde isonicotinoyl hydrazone – A potential metal-protein attenuating compound (MPAC) for the treatment of Alzheimer's disease. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 41-48.	2.0	43
6592	Biomimetic Approaches to Reversible CO ₂ Capture from Air. N-Methylcarbaminoic Acid Formation in Rubisco-Inspired Models. , 2013, , 501-534.		5
6593	Hydrogenation and Redox Isomerization of Allylic Alcohols Catalyzed by a New Water-Soluble Pd-tetrahydrosalen Complex. <i>Organometallics</i> , 2013, 32, 4391-4401.	1.1	40
6594	Polymorphic Co-crystals from Polymorphic Co-crystal Formers: Competition between Carboxylic Acid-Pyridine and Phenol-Pyridine Hydrogen Bonds. <i>Crystal Growth and Design</i> , 2013, 13, 3935-3952.	1.4	80
6595	QM/MM description of platinum-DNA interactions: comparison of binding and DNA distortion of five drugs. <i>RSC Advances</i> , 2013, 3, 4066.	1.7	30
6596	Conformational Preferences of Modified Nucleoside N(4)-Acetylcytidine, ac4C Occur at the Wobble-34th Position in the Anticodon Loop of tRNA. <i>Cell Biochemistry and Biophysics</i> , 2013, 66, 797-816.	0.9	53
6597	Synthesis of 3,3-Disubstituted Oxindoles by Palladium-Catalyzed Asymmetric Intramolecular Arylation of Amides: Reaction Development and Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 11916-11927.	1.7	88
6598	Nonfitting protein-ligand interaction scoring function based on first-principles theoretical chemistry methods: Development and application on kinase inhibitors. <i>Journal of Computational Chemistry</i> , 2013, 34, 1636-1646.	1.5	37
6599	Modeling electron density distributions from X-ray diffraction to derive optical properties: Constrained wavefunction versus multipole refinement. <i>Journal of Chemical Physics</i> , 2013, 139, 064108.	1.2	30
6600	Geometrical Correction for the Inter- and Intramolecular Basis Set Superposition Error in Periodic Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 9282-9292.	1.1	123
6601	Theoretical studies of structure, energetics and properties of Ca ²⁺ complexes with alizarin glucoside. <i>Journal of Molecular Modeling</i> , 2013, 19, 4209-4214.	0.8	5
6602	Memory Effects in Carbocation Rearrangements: Structural and Dynamic Study of the Norborn-2-en-7-ylmethyl-X Solvolysis Case. <i>Journal of Organic Chemistry</i> , 2013, 78, 9041-9050.	1.7	13
6603	Heteroleptic Tin(II) Initiators for the Ring-Opening (Co)Polymerization of Lactide and Trimethylene Carbonate: Mechanistic Insights from Experiments and Computations. <i>Chemistry - A European Journal</i> , 2013, 19, 13463-13478.	1.7	56
6604	Theoretical study of the reactivity of Rh(I) and Rh(III) Bis(isonitrile) complexes in cycloaddition reactions with nitrones. <i>Russian Journal of Inorganic Chemistry</i> , 2013, 58, 320-330.	0.3	2
6605	Distance-Independent Charge Recombination Kinetics in Cytochrome c-Cytochrome c Peroxidase Complexes: Compensating Changes in the Electronic Coupling and Reorganization Energies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9129-9141.	1.2	23
6606	Bisanthracene Bis(dicarboxylic imide)s as Potential Photosensitizers in Photodynamic Therapy: A Theoretical Investigation. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2334-2340.	2.5	33

#	ARTICLE	IF	CITATIONS
6607	Spectroscopic and electric properties of C.I. Mordant Blue 29: a theoretical and experimental study. <i>New Journal of Chemistry</i> , 2013, 37, 2810.	1.4	2
6608	Mixed-ligand lanthanide complexes with acylpyrazolones and phosphorus-containing ligands. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2013, 39, 278-282.	0.3	4
6609	Theoretic study of DNA base guanine and adenine and protein residues TM binding mode of the trans geometries of new antitumor non-classical platinum complexes containing pyridine and picoline ligand. <i>Structural Chemistry</i> , 2013, 24, 2137-2148.	1.0	1
6610	Gas-phase molecular structure of 1,1,1,2-tetrabromo-2,2-dimethyldisilane: theoretical and experimental investigation of a super-halogenated disilane and computational investigation of the F, Cl and I analogues. <i>Structural Chemistry</i> , 2013, 24, 1201-1206.	1.0	12
6611	The structure of $\frac{1}{4}$ -oxo dimer of aluminium(III) porphyrin: a theoretical study. <i>Structural Chemistry</i> , 2013, 24, 877-881.	1.0	2
6612	Reversible crystal-to-crystal phase transition of a 4,4'-bipyridine-linked dinuclear copper(II) complex. <i>Structural Chemistry</i> , 2013, 24, 181-189.	1.0	2
6613	Syntheses, Structures, and Comparison of the Photophysical Properties of Cyclometalated Iridium Complexes Containing the Isomeric 1- and 2-(2-pyridyl)pyrene Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 9842-9860.	1.9	37
6614	Porphyrins bearing long alkoxy chains and carbazole for dye-sensitized solar cells: tuning cell performance through an ethynylene bridge. <i>RSC Advances</i> , 2013, 3, 14780.	1.7	56
6615	O-atom transport catalysis by neutral manganese oxide clusters in the gas phase: Reactions with CO, C ₂ H ₄ , NO ₂ , and O ₂ . <i>Journal of Chemical Physics</i> , 2013, 139, 084307.	1.2	26
6616	Conductometric and computational study of cationic polymer membranes in H ⁺ and Na ⁺ -forms at various hydration levels. <i>Journal of Membrane Science</i> , 2013, 444, 127-138.	4.1	24
6617	Photoabsorption of Acridine Yellow and Proflavin Bound to Human Serum Albumin Studied by Means of Quantum Mechanics/Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2069-2080.	1.2	18
6618	Electron Density Analysis. , 2013, , 187-226.		21
6619	Singlet [←] Triplet and Triplet [←] Triplet Transitions of Asphaltene PAHs by Molecular Orbital Calculations. <i>Energy & Fuels</i> , 2013, 27, 5017-5028.	2.5	24
6620	Mechanistic Studies on the Pd-Catalyzed Vinylation of Aryl Halides with Vinylalkoxysilanes in Water: The Effect of the Solvent and NaOH Promoter. <i>Journal of the American Chemical Society</i> , 2013, 135, 13749-13763.	6.6	46
6621	Foldamers of β -peptides: conformational preference of peptides formed by rigid building blocks. The first MI-IR spectra of a triamide nanosystem. <i>Amino Acids</i> , 2013, 45, 957-973.	1.2	9
6622	DFT studies of conversion of methyl chloride and three substituted chloromethyl tetrahydrofuran derivatives during reaction with trimethylamine. <i>Journal of Molecular Modeling</i> , 2013, 19, 4403-4417.	0.8	6
6623	Electronic structure theory based study of proline interacting with gold nano clusters. <i>Journal of Molecular Modeling</i> , 2013, 19, 4099-4109.	0.8	13
6624	DFT studies of the conversion of four mesylate esters during reaction with ammonia. <i>Journal of Molecular Modeling</i> , 2013, 19, 3015-3026.	0.8	6

#	ARTICLE	IF	CITATIONS
6625	Electron-induced reductive debromination of 2,3,4-tribromodiphenyl ether: a computational study. <i>Journal of Molecular Modeling</i> , 2013, 19, 3333-3338.	0.8	15
6626	Probing the Electronic Properties of a Trinuclear Molecular Wire Involving Isocyanoferrrocene and Iron(II) Phthalocyanine Motifs. <i>Inorganic Chemistry</i> , 2013, 52, 11004-11012.	1.9	54
6627	Theoretical Study on Ruthenium-Catalyzed Hydrocarboxylative Dimerization of Phenylacetylene with Acetic Acid Leading to (1 <i>E</i> ,3 <i>E</i>)-1,4-Diphenyl-1,3-butadienyl Acetate. <i>Organometallics</i> , 2013, 32, 5201-5211.	1.1	8
6628	Deep Red to Near-Infrared Emitting Rhenium(I) Complexes: Synthesis, Characterization, Electrochemistry, Photophysics, and Electroluminescence Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 13418-13427.	1.7	74
6629	Comparing the impact of different supporting ligands on copper(I)–ethylene interactions. <i>Polyhedron</i> , 2013, 52, 207-215.	1.0	12
6630	Pathways between superoxide and peroxide species on small La-O clusters. <i>Chinese Journal of Catalysis</i> , 2013, 34, 2130-2137.	6.9	3
6631	Analysis of matrine-type alkaloids using ESI-QTOF. <i>International Journal of Mass Spectrometry</i> , 2013, 341-342, 28-33.	0.7	13
6632	Simple and cheap steric and electronic characterization of the reactivity of Ru(II) complexes containing oxazoline ligands as epoxidation catalysts. <i>Chemical Physics Letters</i> , 2013, 577, 142-146.	1.2	6
6633	A nonlinear optical switch induced by conformation conversion of alkali metal doped nano-carbon bowls. <i>Chemical Physics Letters</i> , 2013, 588, 131-135.	1.2	15
6634	Direct Observation of a Bent Carbonyl Ligand in a 19-Electron Transition Metal Complex. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2317-2324.	1.1	8
6635	Kinetic and DFT Studies on the Mechanism of C–S Bond Formation by Alkyne Addition to the [Mo ₃ S ₄ (H ₂ O) ₉] ⁴⁺ Cluster. <i>Inorganic Chemistry</i> , 2013, 52, 14334-14342.	1.9	10
6637	Crystal band structure from the embedded cluster. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1877-1883.	1.0	4
6638	DFT studies on the reaction pathway of the catalytic olefin epoxidation with CpMoCF ₃ dioxo and oxo–peroxo complexes. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 36-45.	0.8	25
6639	<i>tert</i> -Butyl Hydroperoxide Oxygenation of Organic Sulfides Catalyzed by Diruthenium(II,III) Tetracarboxylates. <i>Inorganic Chemistry</i> , 2013, 52, 12545-12552.	1.9	24
6640	C [†] C*-cyclometalated platinum(II) complexes with trifluoromethyl-acetylacetonate ligands – Synthesis and electronic effects. <i>Journal of Organometallic Chemistry</i> , 2013, 730, 37-43.	0.8	16
6641	Dinuclear gold(I) and gold(III) complexes involving di(N-heterocyclic carbene) ligands – Synthesis, characterization and DFT studies. <i>Journal of Organometallic Chemistry</i> , 2013, 745-746, 242-250.	0.8	20
6642	The subtle effect of vdW interactions upon the C ₆₀ fullerene structure. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 12-16.	1.1	5
6643	Electronic states of porphycene-O ₂ complex and photoinduced singlet O ₂ production. <i>Journal of Chemical Physics</i> , 2013, 139, 074307.	1.2	7

#	ARTICLE	IF	CITATIONS
6644	Role of Silanol Group in Sn-Beta Zeolite for Glucose Isomerization and Epimerization Reactions. <i>ACS Catalysis</i> , 2013, 3, 2294-2298.	5.5	128
6645	Theoretical study on the mechanism and stereochemistry of the cinchona-thiourea organocatalytic hydrophosphonylation of an α -ketoester. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 7497.	1.5	13
6646	Computational Insight into 10^3 Rh Chemical Shift-Structure Correlations in Rhodium Bis(phosphine) Complexes. <i>Organometallics</i> , 2013, 32, 6437-6444.	1.1	8
6647	Quantum chemical analysis of salen-aluminum complexes for organic light emitting diodes. <i>Chemical Physics Letters</i> , 2013, 585, 143-148.	1.2	6
6648	Locally Refined Multigrid Solution of the All-Electron Kohn-Sham Equation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4744-4760.	2.3	14
6649	Luminescent Cyclometalated Alkynylplatinum(II) Complexes with a Tridentate Pyridine-Based N-Heterocyclic Carbene Ligand: Synthesis, Characterization, Electrochemistry, Photophysics, and Computational Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 10360-10369.	1.7	35
6650	RAFT-based Polystyrene and Polyacrylate Melts under Thermal and Mechanical Stress. <i>Macromolecules</i> , 2013, 46, 8079-8091.	2.2	29
6651	A first-principles study on the adsorption behavior of amphetamine on pristine, P- and Al-doped B ₁₂ N ₁₂ nano-cages. <i>Superlattices and Microstructures</i> , 2013, 64, 265-273.	1.4	56
6652	A hetero-alkali-metal version of the utility amide LDA: lithium-potassium diisopropylamide. <i>Dalton Transactions</i> , 2013, 42, 3704.	1.6	13
6653	Influence of Incorporating Different Electron-Rich Thiophene-Based Units on the Photovoltaic Properties of Isoindigo-Based Conjugated Polymers: An Experimental and DFT Study. <i>Macromolecules</i> , 2013, 46, 8488-8499.	2.2	58
6654	Role of the transition metal in Grignard metathesis polymerization (GRIM) of 3-hexylthiophene. <i>Journal of Materials Chemistry A</i> , 2013, 1, 12841.	5.2	27
6655	Cp*IrIII-Catalyzed Oxidative Coupling of Benzoic Acids with Alkynes. <i>ACS Catalysis</i> , 2013, 3, 2421-2429.	5.5	125
6656	Organic Acid-Catalyzed Polyurethane Formation via a Dual-Activated Mechanism: Unexpected Preference of N-Activation over O-Activation of Isocyanates. <i>Journal of the American Chemical Society</i> , 2013, 135, 16235-16241.	6.6	76
6657	Design of Nanosensors for Fissile Materials in Nuclear Waste Water. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24033-24041.	1.5	22
6658	Controlling the Structure of Reactive Intermediates via Incipient Covalent Bonding with the Counterions: Coexistence of Two Distinct Forms of the C ₆ F ₆ Cation Radical in a Single Crystal. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23568-23574.	1.5	2
6659	Atomistic multiscale simulation of the structure and properties of an amorphous OXD-7 layer. <i>Chemical Physics Letters</i> , 2013, 590, 101-105.	1.2	4
6660	Molecular engineering on a chlorophyll derivative, chlorin e6, for significantly improved power conversion efficiency in dye-sensitized solar cells. <i>Journal of Power Sources</i> , 2013, 242, 860-864.	4.0	35
6661	Facile Tuning of Luminescent Platinum(II) Schiff Base Complexes from Yellow to Near-Infrared: Photophysics, Electrochemistry, Electrochemiluminescence and Theoretical Calculations. <i>Chemistry - A European Journal</i> , 2013, 19, 15907-15917.	1.7	30

#	ARTICLE	IF	CITATIONS
6662	Cycloaddition of Benzyne to Armchair Single-Walled Carbon Nanotubes: [2 + 2] or [4 + 2]?. <i>Organic Letters</i> , 2013, 15, 5960-5963.	2.4	16
6663	Electron dynamics across molecular wires: A time-dependent configuration interaction study. <i>Chemical Physics</i> , 2013, 420, 44-49.	0.9	12
6664	Hydroxo- σ -Rhodium-N-Heterocyclic Carbene Complexes as Efficient Catalyst Precursors for Alkyne Hydrothiolation. <i>ACS Catalysis</i> , 2013, 3, 2910-2919.	5.5	53
6665	Presolvated Low Energy Electron Attachment to Peptide Methyl Esters in Aqueous Solution: C=O Bond Cleavage at 77 K. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2872-2877.	1.2	9
6666	Aerobic Oxidation of Methanol to Formic Acid on Au ₈ : Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10416-10427.	1.1	18
6667	Does Hydrogen Bonding Donation to Manganese(IV)-Oxo and Iron(IV)-Oxo Oxidants Affect the Oxygen-Atom Transfer Ability? A Computational Study. <i>Chemistry - A European Journal</i> , 2013, 19, 4058-4068.	1.7	76
6668	Coordination complexes of NbX ₅ (X = F, Cl) with (N,O)- and (O,O)-donor ligands and the first X-ray characterization of a neutral NbF ₅ adduct. <i>Dalton Transactions</i> , 2013, 42, 13054.	1.6	19
6669	Bimetallic Complexes for Enhancing Catalyst Efficiency: Probing the Relationship between Activity and Intermetallic Distance. <i>Organometallics</i> , 2013, 32, 5071-5081.	1.1	31
6670	Interaction analysis of HIV-1 antibody 2G12 and Man ₉ GlcNAc ₂ ligand: Theoretical calculations by fragment molecular orbital and MD methods. <i>Chemical Physics Letters</i> , 2013, 578, 144-149.	1.2	6
6671	A Self-Promotion Mechanism for Efficient Dehydrogenation of Ethanol Catalyzed by Pincer Ruthenium and Iron Complexes: Aliphatic versus Aromatic Ligands. <i>ACS Catalysis</i> , 2013, 3, 2684-2688.	5.5	68
6672	APPLICATIONS OF ENERGETIC MATERIALS BY A THEORETICAL METHOD (DISCOVER ENERGETIC MATERIALS BY) <i>Tj ETQq0 0 0 rgBT /Over</i> 12, 197-262.	0.2	10
6673	Theoretical Study of Nascent Solvation in Ni ⁺ (Benzene) _m , <i>m</i> = 3 and 4, Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12546-12559.	1.1	10
6674	Calculations on Tunneling in the Reactions of Noradamantyl Carbenes. <i>Journal of the American Chemical Society</i> , 2013, 135, 17274-17277.	6.6	42
6675	DFT model cluster studies of O ₂ adsorption on hydrogenated titania sub-nanoparticles. <i>Journal of Molecular Modeling</i> , 2013, 19, 5063-5073.	0.8	14
6676	DFT Investigation on Mechanisms and Stereoselectivities of [2 + 2 + 2] Multimolecular Cycloaddition of Ketenes and Carbon Disulfide Catalyzed by N-Heterocyclic Carbenes. <i>Journal of Organic Chemistry</i> , 2013, 78, 11849-11859.	1.7	38
6677	Theoretical insight into electronic spectra of carbon chain carbenes H ₂ C _n (<i>n</i> = 3~10). <i>Journal of Chemical Physics</i> , 2013, 138, 204303.	1.2	8
6678	Supramolecular Nano-Aggregates Based on Bis(Pyrene) Derivatives for Lysosome-Targeted Cell Imaging. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26811-26820.	1.5	79
6679	Ab initio study of electron and hole transport in pure and doped MnO and MnO:ZnO alloy. <i>Journal of Materials Chemistry A</i> , 2013, 1, 9246.	5.2	24

#	ARTICLE	IF	CITATIONS
6680	Theoretical study of structure and physical properties of $(Al_2O_3)_n$ clusters. <i>Physica Scripta</i> , 2013, 88, 058307.	1.2	20
6681	Immobilization and Characterization of $RuCl_2(PPh_3)_3$ Mesoporous Silica SBA-3. <i>Zeitschrift Fur Physikalische Chemie</i> , 2013, 227, 901-915.	1.4	7
6682	Thermal and Photoreductive Elimination from the Tellurium Center of π -Conjugated Tellurophenes. <i>Inorganic Chemistry</i> , 2013, 52, 13779-13790.	1.9	62
6683	Rotational spectroscopy of pyridazine and its isotopologs from 235–360 GHz: Equilibrium structure and vibrational satellites. <i>Journal of Chemical Physics</i> , 2013, 139, 224304.	1.2	45
6684	Quantum effects and anharmonicity in the H_2-Li^+ -benzene complex: A model for hydrogen storage materials. <i>Journal of Chemical Physics</i> , 2013, 139, 234305.	1.2	10
6685	Synthesis of Conjugated Polymers Containing DIBAC-Derived Triazole Monomers. <i>Macromolecules</i> , 2013, 46, 9593-9598.	2.2	13
6686	Preparation, Characterization, and Reactivity of Dinitrogen Molybdenum Complexes with Bis(diphenylphosphino)amine Derivative Ligands that Form a Unique 4-Membered $P=N=P$ Chelate Ring. <i>Inorganic Chemistry</i> , 2013, 52, 182-195.	1.9	51
6687	Accurate treatment of two-dimensional non-separable hindered internal rotors. <i>Journal of Chemical Physics</i> , 2013, 138, 134112.	1.2	42
6688	Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter. <i>Dalton Transactions</i> , 2013, 42, 8820.	1.6	33
6689	Speciation of $[Cp^*_2M_2O_5]$ in Polar and Donor Solvents. <i>Chemistry - A European Journal</i> , 2013, 19, 3969-3985.	1.7	3
6690	The structure of minimal magnetite cluster. <i>Russian Journal of General Chemistry</i> , 2013, 83, 1493-1500.	0.3	4
6691	Do halogen and methyl substituents have electronic effects on the structures of simple disilanes? An experimental and theoretical study of the molecular structures of the series $X_3SiSiMe_3$ ($X=H, F, Cl$ and) Tj ETQq1.1.0.784314 rgBT		
6692	Structures of a_n Ions Derived from Protonated Pentaglycine and Pentaalanine: Results from IRMPD Spectroscopy and DFT Calculations. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 1957-1968.	1.2	13
6693	Computational determination of the pigment binding motif in the chlorosome protein a of green sulfur bacteria. <i>Photosynthesis Research</i> , 2013, 118, 231-247.	1.6	4
6694	Adsorption and surface diffusion of silicon growth species in silicon carbide chemical vapour deposition processes studied by quantum-chemical computations. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	11
6695	First-principles electronic structure study of rhizoferrin and its Fe(III) complexes. <i>BioMetals</i> , 2013, 26, 1003-1012.	1.8	2
6696	Calculation of Molecular Thermochemical Data and Their Availability in Databases. <i>Green Energy and Technology</i> , 2013, , 515-547.	0.4	2
6697	Toward extension of the gas-phase basicity scale by novel pyridine containing guanidines. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 113-122.	0.7	20

#	ARTICLE	IF	CITATIONS
6698	Shedding Light on Structure-Property Relationships for Conjugated Microporous Polymers: The Importance of Rings and Strain. <i>Macromolecules</i> , 2013, 46, 7696-7704.	2.2	44
6699	The nature of the M-NO bond in [M(Imidazole)(PPIX)(L)] _q complexes (M=Fe ²⁺ , Ru ²⁺ ; L=NO ⁺ , NO and) <i>J. Phys. Chem. B</i> , 2013, 117, 10534-10543.	1.2	3
6700	Counteranion and Solvent Assistance in Ruthenium-Mediated Alkyne to Vinylidene Isomerizations. <i>Inorganic Chemistry</i> , 2013, 52, 8919-8932.	1.9	36
6701	Ruthenium-Catalyzed Hydrogenation of Oxygen-Functionalized Aromatic Compounds in Water. <i>ChemCatChem</i> , 2013, 5, 3241-3248.	1.8	12
6702	Side chain fluorination and anion effect on the structure of 1-butyl-3-methylimidazolium ionic liquids. <i>Journal of Chemical Physics</i> , 2013, 139, 084502.	1.2	63
6703	Side Chain Flexibility in Perfluorosulfonic Acid Ionomers: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10534-10543.	1.1	13
6704	Oxo-Functionalization and Reduction of the Uranyl Ion through Lanthanide-Element Bond Homolysis: Synthetic, Structural, and Bonding Analysis of a Series of Singly Reduced Uranyl-Rare Earth Complexes. <i>Journal of the American Chemical Society</i> , 2013, 135, 3841-3854.	6.6	107
6705	Spectroscopic properties of N1,N5-bis[pyridine-2-methylene]-thiocarbohydrazone and its corresponding zinc (II) and nickel (II) metal complexes: A DFT and TD-DFT study. <i>Synthetic Metals</i> , 2013, 175, 174-182.	2.1	4
6706	Ab Initio Calculation of Molecular Aggregation Effects: A Coumarin-343 Case Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11072-11085.	1.1	15
6707	Toward Reliable Prediction of the Energy Ladder in Multichromophoric Systems: A Benchmark Study on the FMO Light-Harvesting Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4928-4938.	2.3	52
6708	Synthesis, single crystal structure and performance of N-substituted derivatives of dinitroimidazole. <i>New Journal of Chemistry</i> , 2013, 37, 2837.	1.4	17
6709	Isolation and X-ray structures of four Rh(PCP) complexes including a Rh(I) dioxygen complex with a short O-O bond. <i>Polyhedron</i> , 2013, 58, 106-114.	1.0	8
6710	Stereoselective 1,3-dipolar cycloadditions of nitrones derived from amino acids. Asymmetric synthesis of N-(alkoxycarbonylmethyl)-3-hydroxypyrrolidin-2-ones. <i>Tetrahedron</i> , 2013, 69, 9381-9390.	1.0	11
6711	1,3-Dipolar cycloadditions of Stone-Wales defective single-walled carbon nanotubes: A theoretical study. <i>Journal of Computational Chemistry</i> , 2013, 34, 2223-2232.	1.5	18
6712	Reactivity of iridium(I) PNP amido complexes toward protonation and oxidation. <i>Journal of Organometallic Chemistry</i> , 2013, 744, 35-40.	0.8	17
6713	Silver(I) complexes with symmetrical Schiff bases: Synthesis, structural characterization, DFT studies and antimycobacterial assays. <i>Polyhedron</i> , 2013, 62, 104-109.	1.0	22
6714	Near-Infrared Laser Induced Conformational Change of Alanine in Low-Temperature Matrixes and the Tunneling Lifetime of Its Conformer VI. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1952-1962.	1.1	59
6715	Photoelectron spectroscopic and density functional theoretical studies of the 2'-deoxycytidine homodimer radical anion. <i>Journal of Chemical Physics</i> , 2013, 139, 075101.	1.2	5

#	ARTICLE	IF	CITATIONS
6716	Atmospheric Significance of Water Clusters and Ozone-Water Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10381-10396.	1.1	101
6717	Resonance Stabilized Perfluorinated Ionomers for Alkaline Membrane Fuel Cells. <i>Macromolecules</i> , 2013, 46, 7826-7833.	2.2	90
6718	Ring-Expansion Reaction of Isatins with Ethyl Diazoacetate Catalyzed by Dirhodium(II)/DBU Metal-Organic System: En Route to Viridicatin Alkaloids. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 6280-6290.	1.2	18
6719	Mechanism of the Gold(III)-Catalyzed Isomerization of Substituted Allenes to Conjugated Dienes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2013, 78, 9715-9724.	1.7	21
6720	Synthesis and Structure of a Trinuclear Pd-Ag-Pd Carbene Acetato Complex. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2013, 639, 1237-1241.	0.6	5
6721	Influence of reactant type on the Sr incorporation grade and structural characteristics of Ba _{1-x} Sr _x TiO ₃ (x=0-1) grown by sol-gel-hydrothermal synthesis. <i>Ceramics International</i> , 2013, 39, 8823-8831.	2.3	42
6722	Computational Studies on the Excited States of Luminescent Platinum(II) Alkynyl Systems of Tridentate Pincer Ligands in Radiative and Nonradiative Processes. <i>Journal of the American Chemical Society</i> , 2013, 135, 15135-15143.	6.6	104
6723	Structural and Vibrational Properties of Imidazo[4,5-c]pyridine, a Structural Unit in Natural Products. <i>Journal of Natural Products</i> , 2013, 76, 1637-1646.	1.5	4
6724	Theoretical study of cyclometalated Ru(II) dyes: Implications on the open-circuit voltage of dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 272, 80-89.	2.0	5
6725	A theoretical study on magnetic properties of bis-TEMPO diradicals with possible application. <i>Computational and Theoretical Chemistry</i> , 2013, 1024, 15-23.	1.1	15
6726	Brightly Blue and Green Emitting Cu(I) Dimers for Singlet Harvesting in OLEDs. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11823-11836.	1.1	224
6727	Blue light emitting electrochemical cells incorporating triazole-based luminophores. <i>Journal of Materials Chemistry C</i> , 2013, 1, 7440.	2.7	68
6728	Full-colour luminescent compounds based on anthracene and 2,2'-dipyridylamine. <i>Journal of Materials Chemistry C</i> , 2013, 1, 7409.	2.7	25
6729	Optimization of RI-MP2 Auxiliary Basis Functions for 6-31G** and 6-311G** Basis Sets for First-, Second-, and Third-Row Elements. <i>Journal of Computational Chemistry</i> , 2013, 34, 2568-2575.	1.5	23
6730	Synthetic and DFT Studies Towards a Unified Approach to Phlegmarine Alkaloids: Aza-Michael Intramolecular Processes Leading to 5-Oxodecahydroquinolines. <i>Chemistry - A European Journal</i> , 2013, 19, 13881-13892.	1.7	24
6731	Solvation structure of iron group metal ion in TFSA-based ionic liquids investigated by Raman spectroscopy and DFT calculations. <i>Journal of Molecular Structure</i> , 2013, 1048, 59-63.	1.8	17
6732	Evaluation of density functional methods on the geometric and energetic descriptions of species involved in Cu+-promoted catalysis. <i>Journal of Molecular Modeling</i> , 2013, 19, 5457-5467.	0.8	8
6733	Boron complexes of redox-active diimine ligand. <i>Dalton Transactions</i> , 2013, 42, 7952.	1.6	30

#	ARTICLE	IF	CITATIONS
6734	Surface modification of the TiO ₂ nanoparticle surface enables fluorescence monitoring of aggregation and enhanced photoreactivity. Integrative Biology (United Kingdom), 2013, 5, 133-143.	0.6	8
6735	Diphenyltriacetylenes: novel nematic liquid crystal materials and analysis of their nematic phase-transition and birefringence behaviours. Journal of Materials Chemistry C, 2013, 1, 8094.	2.7	29
6736	Hydrothermal synthesis of an ortho-metallated Co(III) complex anchored by a carboxylate group with a selective oxidation catalytic property. Dalton Transactions, 2013, 42, 4313.	1.6	5
6737	A novel VIVO ^{III} pyrimidinone complex: synthesis, solution speciation and human serum protein binding. Dalton Transactions, 2013, 42, 11841.	1.6	38
6738	Two-step radical reactions that switch low multiplicity channels leading to the carbene and carbyne species detected for Ru(5F) + CH ₄ ⁿ F _n (n = 2-4) interactions under matrix isolation conditions. RSC Advances, 2013, 3, 11607.	1.7	10
6739	Diimine Complexes of Rhodium(I) and Iridium(I): Their Reactivity with Dioxygen and Dihydrogen. European Journal of Inorganic Chemistry, 2013, 2013, 4775-4788.	1.0	7
6740	Spectroscopic, radiochemical, and theoretical studies of the Ga ³⁺ + N ₂ hydroxyethyl piperazine ⁺ + CH ₂ ethanesulfonic acid (HEPES buffer) system: evidence for the formation of Ga ³⁺ •HEPES complexes in ⁶⁸ Ga labeling reactions. Contrast Media and Molecular Imaging, 2013, 8, 265-273.	0.4	21
6741	Synthesis and Characterization of Luminescent Cyclometalated Platinum(II) Complexes of 1,3-Bis(Hetero)azolylbenzenes with Tunable Color for Applications in Organic Light-Emitting Devices through Extension of π Conjugation by Variation of the Heteroatom. Chemistry - A European Journal, 2013, 19, 13910-13924.	1.7	50
6742	Ab Initio Study of ² H Nuclear Quadrupole Coupling Constants in Deuterated Crystalline Oxalic Acid Dehydrated Polymorphs. Molecular Crystals and Liquid Crystals, 2013, 575, 188-201.	0.4	1
6743	Ab initio study of the circular intensity difference in electric-field-induced second harmonic generation of chiral natural amino acids. Physical Chemistry Chemical Physics, 2013, 15, 1198-1207.	1.3	13
6744	A simple and rapid route to novel tetra(4-thiaalkyl)ammonium bromides. RSC Advances, 2013, 3, 24612.	1.7	11
6745	Emission spectroscopy of uranium(IV) compounds: a combined synthetic, spectroscopic and computational study. RSC Advances, 2013, 3, 4350.	1.7	57
6746	The reduction of carbon dioxide in iron biocatalyst catalytic hydrogenation reaction: a theoretical study. Dalton Transactions, 2013, 42, 11186.	1.6	16
6747	Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. Physical Chemistry Chemical Physics, 2013, 15, 7567.	1.3	31
6748	Investigation of the surface chemistry of phosphine-stabilized ruthenium nanoparticles – an advanced solid-state NMR study. Physical Chemistry Chemical Physics, 2013, 15, 17383.	1.3	29
6749	Computational study of the hydrodefluorination of fluoroarenes at [Ru(NHC)(PR ₃) ₂ (CO)(H) ₂]: predicted scope and regioselectivities. Dalton Transactions, 2013, 42, 7386.	1.6	42
6750	Computational study of the double C-Cl bond activation of dichloromethane and phosphinealkylation at [CoCl(PR ₃) ₃] ₃ . Dalton Transactions, 2013, 42, 4208-4217.	1.6	19
6751	Naturally and synthetically linked lys48 diubiquitin: a QM/MM study. RSC Advances, 2013, 3, 16122.	1.7	14

#	ARTICLE	IF	CITATIONS
6752	How do perfluorinated alkanolic acids elicit cytochrome P450 to catalyze methane hydroxylation? An MD and QM/MM study. <i>RSC Advances</i> , 2013, 3, 2995.	1.7	21
6753	Role of Formation of Statistical Aggregates in Chlorophyll Fluorescence Concentration Quenching. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3976-3982.	1.2	22
6754	Ultrafast Energy Transfer in Divinylbiphenyl and Divinylstilbene Copolymers Bridged by Silylene. <i>Journal of Physical Chemistry C</i> , 2013, 117, 64-70.	1.5	7
6755	Detecting low-level flexibility using residual dipolar couplings: a study of the conformation of cellobiose. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18223.	1.3	8
6756	Assessment of Kohn-Sham density functional theory and Møller-Plesset perturbation theory for ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13664.	1.3	98
6757	Reactivity differences between 2,4- and 2,5-disubstituted zirconacyclopentadienes: a highly selective and general approach to 2,4-disubstituted phospholes. <i>Dalton Transactions</i> , 2013, 42, 10997.	1.6	20
6758	Mechanistic insights into iron catalyzed dehydrogenation of formic acid: β -hydride elimination vs. direct hydride transfer. <i>Dalton Transactions</i> , 2013, 42, 11987.	1.6	58
6759	On the nature of the photochemical reaction of polypyridyl Ru(II) complexes leading to sunlight-to-chemical energy conversion: density functional analysis. <i>RSC Advances</i> , 2013, 3, 9414.	1.7	0
6760	An extrapolation method for the efficient calculation of molecular response properties within Born-Oppenheimer molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9392.	1.3	1
6761	Synthesis and structures of tridentate β -diketiminato zinc phenoxides as catalysts for immortal ring-opening polymerization of lactide. <i>Catalysis Science and Technology</i> , 2013, 3, 3268.	2.1	24
6762	A theoretical study of hydration effects on structural stability and hydrogen-bonding dynamics of 2'-deoxyguanosine 5'-monophosphate with different negative charges. <i>Canadian Journal of Chemistry</i> , 2013, 91, 169-175.	0.6	0
6763	Mechanisms for the Formation of Acenes from β -Diketones by Bisdecarbonylation. <i>Journal of Organic Chemistry</i> , 2013, 78, 1851-1857.	1.7	18
6764	A new scheme for significant enhancement of the second order nonlinear optical response from molecules to ordered aggregates. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1810.	1.3	24
6765	Tuning structure and properties of Pd and Pt camphor derived complexes. <i>Inorganica Chimica Acta</i> , 2013, 395, 169-175.	1.2	9
6766	A silver complex with tryptophan: Synthesis, structural characterization, DFT studies and antibacterial and antitumor assays in vitro. <i>Journal of Molecular Structure</i> , 2013, 1031, 125-131.	1.8	33
6767	Understanding C-H Bond Activation on a Diruthenium(I) Platform. <i>Organometallics</i> , 2013, 32, 340-349.	1.1	20
6768	Three-coordinate Nickel(I) Complexes Stabilised by Six-, Seven- and Eight-membered Ring Heterocyclic Carbenes: Synthesis, EPR/DFT Studies and Catalytic Activity. <i>Chemistry - A European Journal</i> , 2013, 19, 2158-2167.	1.7	89
6769	Exo/endo Selectivity of the Ring-Closing Enyne Methathesis Catalyzed by Second Generation Ru-Based Catalysts. Influence of Reactant Substituents. <i>ACS Catalysis</i> , 2013, 3, 206-218.	5.5	31

#	ARTICLE	IF	CITATIONS
6770	Small Changes Have Consequences: Lessons from Tetrabenzyltitanium and η^5 -zirconium Surface Organometallic Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 964-973.	1.7	24
6771	Polycyclic phosphonic acid derivatives obtained by a [4+2] cycloaddition strategy using phosphonodienes. <i>Tetrahedron</i> , 2013, 69, 1138-1147.	1.0	17
6772	Mechanisms for Solvatochromic Shifts of Free-Base Porphine Studied with Polarizable Continuum Models and Explicit Solute-Solvent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 470-480.	2.3	17
6773	A Noninnocent Cyclooctadiene (COD) in the Reaction of an η^5 -Ir(COD)(OAc)-Precursor with Imidazolium Salts. <i>Organometallics</i> , 2013, 32, 192-201.	1.1	22
6774	Induced Optical Activity of DNA-Templated Cyanine Dye Aggregates: Exciton Coupling Theory and TD-DFT Studies. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5909-5918.	1.1	13
6775	A comparative study of the adsorption and oxidation of L-alanine and L-serine on Au(1 0 0), Au(1 1 1) and gold thin film electrodes in acid media. <i>Electrochimica Acta</i> , 2013, 89, 72-83.	2.6	31
6776	Tuning conformations of calix[4]tubes by weak intramolecular interactions. <i>New Journal of Chemistry</i> , 2013, 37, 416-424.	1.4	11
6777	Taming the shrew: [TMEDALi-Zn(C ₂ H ₄) ₂] as a model compound for anionic ethene polymerisation. <i>New Journal of Chemistry</i> , 2013, 37, 494-501.	1.4	5
6778	Interfacial States in Donor-Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 533-542.	2.3	45
6779	Parametrization and Benchmark of DFTB3 for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 338-354.	2.3	743
6780	Novel phospholyl(diphenylphosphino)methane-ruthenium complexes: unexpected non-assisted cis to trans isomerization of [RuCl ₂ (P ^o) ₂]. <i>Dalton Transactions</i> , 2013, 42, 75-81.	1.6	5
6781	Anion- π interactions in adducts of anionic guests with octahydroxy-pyridine[4]arene: theoretical and experimental elucidation. <i>New Journal of Chemistry</i> , 2013, 37, 356-365.	1.4	6
6782	Influence of the O-phosphorylation of serine, threonine and tyrosine in proteins on the amidic ¹⁵ N chemical shielding anisotropy tensors. <i>Journal of Biomolecular NMR</i> , 2013, 55, 59-70.	1.6	2
6783	Theoretical study of neutral and charged Sc ₃ (benzene) ₃ clusters. <i>Journal of Nanoparticle Research</i> , 2013, 15, 1.	0.8	7
6784	Conformational properties of 1-methyl-1-germacyclohexane: low-temperature NMR and quantum chemical calculations. <i>Structural Chemistry</i> , 2013, 24, 769-774.	1.0	8
6785	A General Mechanism for the Copper- and Silver-Catalyzed Olefin Aziridination Reactions: Concomitant Involvement of the Singlet and Triplet Pathways. <i>Journal of the American Chemical Society</i> , 2013, 135, 1338-1348.	6.6	160
6786	Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2013, 135, 3017-3026.	6.6	135
6787	Application of MCD spectroscopy and TD-DFT to endohedral metallofullerenes for characterization of their electronic transitions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3593.	1.3	18

#	ARTICLE	IF	CITATIONS
6788	Molecular rearrangement reactions in the gas phase triggered by electron attachment. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4754.	1.3	25
6789	Atomic orbital basis sets. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 273-295.	6.2	165
6790	Understanding Pd-Pd Bond Length Variation in (PNP)Pd(PNP) Dimers. <i>Inorganic Chemistry</i> , 2013, 52, 2317-2322.	1.9	15
6791	The Multiradical Character of One- and Two-Dimensional Graphene Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2581-2584.	7.2	197
6792	Iridium Dihydroxybipyridine Complexes Show That Ligand Deprotonation Dramatically Speeds Rates of Catalytic Water Oxidation. <i>Inorganic Chemistry</i> , 2013, 52, 9175-9183.	1.9	142
6793	Bipyridine and phenanthroline IR-spectral bands as indicators of metal spin state in hexacoordinated complexes of Fe, Ni and Co. <i>Dalton Transactions</i> , 2013, 42, 1787-1797.	1.6	82
6794	Factors that Influence Stereoselectivity in Proline-Catalyzed Mannich Reactions. <i>Asian Journal of Organic Chemistry</i> , 2013, 2, 85-90.	1.3	3
6795	Aldehyde-Assisted Hydrogen Transfer during the Formation of Hydride-Iridafurans from Alkynes and Aldehydes. <i>Chemistry - A European Journal</i> , 2013, 19, 1796-1809.	1.7	7
6796	Mechanism of Ketone Allylation with Allylboronates as Catalyzed by Zinc Compounds: A DFT Study. <i>Chemistry - A European Journal</i> , 2013, 19, 124-134.	1.7	12
6797	Giant Residual Dipolar ^{13}C - ^1H Couplings in High-Spin Organoiron Complexes: Elucidation of Their Structures in Solution by ^{13}C -NMR Spectroscopy. <i>Chemistry - A European Journal</i> , 2013, 19, 1599-1606.	1.7	27
6798	A Comparison of Primary and Secondary Hydrogen Abstraction from Organophosphates by Hydroxyl Radical. <i>International Journal of Chemical Kinetics</i> , 2013, 45, 187-201.	1.0	8
6799	Gaussian basis sets for molecular applications. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 21-34.	1.0	152
6800	Fluorescent BINOL-based sensor for thorium recognition and a density functional theory investigation. <i>Journal of Hazardous Materials</i> , 2013, 263, 638-642.	6.5	35
6801	A novel projection approximation algorithm for the fast and accurate computation of molecular collision cross sections (IV). Application to polypeptides. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 275-280.	0.7	57
6802	Biological activity of Pd(II) complexes with mono- and disubstituted pyridines: Experimental and theoretical studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 2765-2768.	1.0	7
6803	QSPR modeling of n-octanol/air partition coefficients and liquid vapor pressures of polychlorinated dibenzo-p-dioxins. <i>Chemosphere</i> , 2013, 91, 229-232.	4.2	18
6804	NHC-copper(I) bifluoride complexes: α -Auto-activating catalysts. <i>Journal of Organometallic Chemistry</i> , 2013, 730, 95-103.	0.8	28
6805	DFT study on the reaction of the β -amino acid anion catalyzed by the aldehyde: Decarboxylation vs. intramolecular CO ₂ transfer. <i>Computational and Theoretical Chemistry</i> , 2013, 1006, 1-8.	1.1	2

#	ARTICLE	IF	CITATIONS
6806	A novel projection approximation algorithm for the fast and accurate computation of molecular collision cross sections (II). Model parameterization and definition of empirical shape factors for proteins. <i>International Journal of Mass Spectrometry</i> , 2013, 345-347, 89-96.	0.7	66
6807	Synthesis of diiron η^4 -allenyl complexes by electrophilic addition to propen-2-yl-dimetallacyclopentenone species: A joint experimental and DFT study. <i>Journal of Organometallic Chemistry</i> , 2013, 731, 61-66.	0.8	3
6808	Critical Evaluation of Implicit Solvent Models for Predicting Aqueous Oxidation Potentials of Neutral Organic Compounds. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5046-5058.	2.3	105
6809	New Diruthenium Bis-alkynyl Compounds as Potential Ditopic Linkers. <i>Organometallics</i> , 2013, 32, 6461-6467.	1.1	5
6810	Cyclization of acyl radical onto NC bond: Application in the synthesis of β -lactam. <i>Computational and Theoretical Chemistry</i> , 2013, 1008, 83-89.	1.1	2
6811	Rationalization of the Barrier Height for <i>p</i> -Z-styrene Epoxidation by Iron(IV)-Oxo Porphyrin Cation Radicals with Variable Axial Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 7968-7979.	1.9	66
6812	Charge Transfer and Polarization for Chloride Ions Bound in ClC Transport Proteins: Natural Bond Orbital and Energy Decomposition Analyses. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16029-16043.	1.2	13
6813	Reduction of N ₂ by H ₂ to NH ₃ and N ₂ H ₄ using [MoL] (L=triamidoamine) and organic co-catalysts: A theoretical approach. <i>Journal of Molecular Catalysis A</i> , 2013, 370, 140-144.	4.8	14
6814	Photochemical functionalization of allyl benzoates by C-H insertion. <i>Tetrahedron</i> , 2013, 69, 6065-6069.	1.0	3
6815	Similarities and differences of serotonin and its precursors in their interactions with model membranes studied by molecular dynamics simulation. <i>Journal of Molecular Structure</i> , 2013, 1045, 124-130.	1.8	18
6816	Exploring the capabilities of TDDFT calculations to explain the induced chirality upon a binding process: A simple case, 3-carboxycoumarin. <i>Journal of Molecular Structure</i> , 2013, 1036, 341-349.	1.8	11
6817	Theoretical study on the mechanism of reaction of CHF ₂ with NO ₂ . <i>Computational and Theoretical Chemistry</i> , 2013, 1010, 1-10.	1.1	3
6818	Carbamazepine polymorphs: Theoretical and experimental vibrational spectroscopy studies. <i>Vibrational Spectroscopy</i> , 2013, 65, 12-23.	1.2	37
6819	John Pople: The Man and His Science. <i>ACS Symposium Series</i> , 2013, , 301-315.	0.5	0
6820	Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation. <i>Journal of the American Chemical Society</i> , 2013, 135, 3887-3896.	6.6	89
6821	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4735.	1.3	44
6822	Tricarbonylrhenium complexes from 2-pyridyl-1,2,3-triazole ligands bearing a 4-substituted phenyl arm: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2013, 42, 7019.	1.6	48
6823	Synthesis, Photochromic, and Computational Studies of Dithienylethene-Containing β -Diketonate Derivatives and Their Near-Infrared Photochromic Behavior Upon Coordination of a Boron(III) Center. <i>Chemistry - A European Journal</i> , 2013, 19, 3467-3476.	1.7	58

#	ARTICLE	IF	CITATIONS
6824	Polymerization of cyclic esters using N-heterocyclic carbene carboxylate catalysts. <i>Polymer Chemistry</i> , 2013, 4, 2414.	1.9	43
6825	Calculation of wavefunctions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. Part I. Application of the Huzinaga equation. <i>Journal of Computational Chemistry</i> , 2013, 34, 854-861.	1.5	7
6826	Calculation of wavefunctions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. II. Application of the local basis equation. <i>Journal of Computational Chemistry</i> , 2013, 34, 862-869.	1.5	5
6827	Ab Initio Calculation of the IR Spectrum of PTFE: Helical Symmetry and Defects. <i>Journal of Physical Chemistry B</i> , 2013, 117, 706-718.	1.2	60
6828	Picosecond TRIR Studies of $M_3(CO)_{12}$ (M = Fe, Os) Clusters in Solution. <i>Organometallics</i> , 2013, 32, 2178-2186.	1.1	8
6829	Pattern Formation Due to Fluorination on Graphene Fragments: Structures, Hopping Behavior, and Magnetic Properties. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8506-8511.	1.1	14
6830	Stabilization of metastable hydrogen trioxide (HOOOH) and the hydrotrioxyl radical (HOOO) by complexation with sulfuric acid. A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2013, 1010, 19-24.	1.1	11
6831	Stabilization of oxidovanadium(IV) by organic radicals. <i>Dalton Transactions</i> , 2013, 42, 4586.	1.6	22
6832	Increasing the Efficiency of the Transannular Diels-Alder Strategy via Palladium(II)-Catalyzed Macrocyclizations. <i>Organic Letters</i> , 2013, 15, 582-585.	2.4	24
6833	Hydrogen Bonding and Proton Transfer to Ruthenium Hydride Complex CpRuH(dppe): Metal and Hydride Dichotomy. <i>Inorganic Chemistry</i> , 2013, 52, 1787-1797.	1.9	20
6834	Spectroscopic and Theoretical Study of the Grafting Modes of Phosphonic Acids on ZnO Nanorods. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5364-5372.	1.5	45
6835	Some Pictures of Alcoholic Dancing: From Simple to Complex Hydrogen-Bonded Networks Based on Polyalcohols. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4680-4690.	1.5	18
6836	Computational chemical analysis of unconjugated bilirubin anions and insights into pKa values clarification. <i>Journal of Chemical Physics</i> , 2013, 138, 035101.	1.2	8
6837	Doped Polycyclic Aromatic Hydrocarbons as Building Blocks for Nanoelectronics: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2013, 78, 1894-1902.	1.7	32
6838	Theoretical Design of Molecular Electrocatalysts with Flexible Pendant Amines for Hydrogen Production and Oxidation. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 542-546.	2.1	32
6839	An Interplay Between Infrared Multiphoton Dissociation Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry and Density Functional Theory Computations in the Characterization of a Tripodal Quinolin-8-Olate Gd(III) Complex. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 589-601.	1.2	0
6840	X-ray observation of a helium atom and placing a nitrogen atom inside He@C60 and He@C70. <i>Nature Communications</i> , 2013, 4, 1554.	5.8	55
6841	Hybrid density functional-molecular mechanics calculations for core-electron binding energies of glycine in water solution. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 244-254.	1.3	15

#	ARTICLE	IF	CITATIONS
6842	Nickel(II) and Palladium(II) Complexes with Chelating N-Heterocyclic Carbene Amidate Ligands: Interplay between Normal and Abnormal Coordination Modes. <i>Organometallics</i> , 2013, 32, 1913-1923.	1.1	34
6843	Chiral Fluorinated β -Sulfonyl Carbanions: Enantioselective Synthesis and Electrophilic Capture, Racemization Dynamics, and Structure. <i>Chemistry - A European Journal</i> , 2013, 19, 3869-3897.	1.7	33
6844	Noniterative Multireference Coupled Cluster Methods on Heterogeneous CPU-GPU Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1949-1957.	2.3	37
6845	Detection of Nitric Oxide and Nitroxyl with Benzoesorufin-Based Fluorescent Sensors. <i>Inorganic Chemistry</i> , 2013, 52, 3285-3294.	1.9	79
6846	Ligand Perturbations on Fluorescence of Dinuclear Platinum Complexes of 5,12-Diethynyltetracene: A Spectroscopic and Computational Study. <i>Organometallics</i> , 2013, 32, 1620-1629.	1.1	27
6847	Molecular structure and spectroscopy of divalent first row transition metals, Mn-Zn, with salicylaldiminate ligands. <i>Polyhedron</i> , 2013, 54, 300-308.	1.0	7
6848	pH-Dependent Reduction Potentials and Proton-Coupled Electron Transfer Mechanisms in Hydrogen-Producing Nickel Molecular Electrocatalysts. <i>Inorganic Chemistry</i> , 2013, 52, 3643-3652.	1.9	50
6849	Tuned and Balanced Redistributed Charge Scheme for Combined Quantum Mechanical and Molecular Mechanical (QM/MM) Methods and Fragment Methods: Tuning Based on the CM5 Charge Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1036-1042.	2.3	20
6850	Attractive electron-electron interactions within robust local fitting approximations. <i>Journal of Computational Chemistry</i> , 2013, 34, 1486-1496.	1.5	67
6851	Monomeric Rhodium(II) Complexes Supported by a Diarylamido/Bis(phosphine) PNP Pincer Ligand and Their Reactivity Toward Dihydrogen. <i>Organometallics</i> , 2013, 32, 2050-2058.	1.1	32
6852	New Parameterization Scheme of DFT-D for Graphitic Materials. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2844-2853.	1.1	13
6853	Theoretical studies on the spectroscopic properties of a series of palladium (II) complexes with 1-allyl-3-(2-pyridyl)thiourea. <i>Synthetic Metals</i> , 2013, 167, 51-63.	2.1	6
6854	Siamese-Twin Porphyrin: A Pyrazole-Based Expanded Porphyrin of Persistent Helical Conformation. <i>Chemistry - A European Journal</i> , 2013, 19, 5868-5880.	1.7	34
6855	Water square (uudd) in novel CuII framework structures built from isomeric (aminomethyl)pyridines and oxalate: Synthesis, structure, spectral and DFT studies. <i>Polyhedron</i> , 2013, 54, 164-172.	1.0	9
6856	Shape-Programmed Nanofabrication: Understanding the Reactivity of Dichalcogenide Precursors. <i>ACS Nano</i> , 2013, 7, 3616-3626.	7.3	67
6857	Decamethylscandocinium-hydrido-(perfluorophenyl)borate: fixation and tandem tris(perfluorophenyl)borane catalysed deoxygenative hydrosilation of carbon dioxide. <i>Chemical Science</i> , 2013, 4, 2152.	3.7	132
6858	Polymerizing Base Sensitive Cyclic Carbonates Using Acid Catalysis. <i>ACS Macro Letters</i> , 2013, 2, 306-312.	2.3	83
6859	Regioselective Ring-Emitting Esterification on Azacyclohexane Quaternary Salts: A DFT and Synthetic Study for Covalent Fixation of Electrostatic Polymer Self-Assemblies. <i>Journal of Organic Chemistry</i> , 2013, 78, 3086-3094.	1.7	9

#	ARTICLE	IF	CITATIONS
6860	Coupled Cluster Theories for Strongly Correlated Molecular Systems. Springer Series in Solid-state Sciences, 2013, , 237-271.	0.3	2
6861	Fluorescence Enhancement of Pyrene Chromophores Induced by Alkyl Groups through π - π Conjugation: Systematic Synthesis of Primary, Secondary, and Tertiary Alkylated Pyrenes at the 1, 3, 6, and 8 Positions and Their Photophysical Properties. Journal of Organic Chemistry, 2013, 78, 3196-3207.	1.7	99
6862	9,10-Phenanthrenesemiquinone radical complexes of ruthenium(III), osmium(III) and rhodium(III) and redox series. Dalton Transactions, 2013, 42, 6538.	1.6	20
6863	Selective enrichment of phosphopeptides by a metal-organic framework. Analytical Methods, 2013, 5, 2379.	1.3	36
6864	Catalytic Cycle for N \equiv CN Bond Cleavage by Molybdenum Silyl Catalyst: A DFT Study. Organometallics, 2013, 32, 2725-2735.	1.1	12
6865	On the Electronic Structure of <i>cis</i> -mer-[RuCl ₃ (1 <i>H</i> -indazole) ₂ (NO)], a Hypothetical Metabolite of the Antitumor Drug Candidate KP1019: An Experimental and DFT Study. European Journal of Inorganic Chemistry, 2013, 2013, 2505-2519.	1.0	18
6866	A Systematic Approach for Understanding Slater-Gaussian Functions in Computational Chemistry. Journal of Chemical Education, 2013, 90, 609-612.	1.1	6
6867	Highly efficient iridium(III) phosphors with phenoxy-substituted ligands and their high-performance OLEDs. Journal of Materials Chemistry C, 2013, 1, 808-821.	2.7	66
6868	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
6869	A DFT Study on the Structural and Antioxidant Properties of Three Flavonols. Food Biophysics, 2013, 8, 90-94.	1.4	17
6870	Synthesis, Physical Properties, and Anion Recognition of Two Novel Larger Azaacenes: Benzannelated Hexazaheptacene and Benzannelated Δ^2 -dihydrohexazaheptacene. Chemistry - an Asian Journal, 2013, 8, 1574-1578.	1.7	113
6871	Theoretical Studies of the Ground and Excited State Structures of Stilbene. Journal of Physical Chemistry A, 2013, 117, 9424-9434.	1.1	19
6872	Unimolecular Photoconversion of Multicolor Luminescence on Hierarchical Self-Assemblies. Journal of the American Chemical Society, 2013, 135, 5175-5182.	6.6	144
6873	Ruthenium Complexes with Chiral Bis-Pinene Ligands: an Array of Subtle Structural Diversity. Inorganic Chemistry, 2013, 52, 4985-4992.	1.9	7
6874	Advanced chemical recycling of poly(ethylene terephthalate) through organocatalytic aminolysis. Polymer Chemistry, 2013, 4, 1610-1616.	1.9	136
6875	Syntheses, photophysical, electroluminescence and computational studies of rhenium(I) diimine triarylamine-containing alkynyl complexes. New Journal of Chemistry, 2013, 37, 1753.	1.4	27
6876	Ring-opening polymerization of racemic β -butyrolactone promoted by rare earth trisborohydride complexes towards a PHB-diol: an experimental and DFT study. Polymer Chemistry, 2013, 4, 3077.	1.9	20
6877	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760.	2.3	243

#	ARTICLE	IF	CITATIONS
6878	Luminescent Platinum(II) Complexes of 1,3-Bis(<i>N</i> -alkylbenzimidazol-2-yl)benzene-Type Ligands with Potential Applications in Efficient Organic Light-Emitting Diodes. <i>Chemistry - A European Journal</i> , 2013, 19, 6385-6397.	1.7	80
6879	Thiophene-Fused Bisdehydro[12]annulene That Undergoes Transannular Alkyne Cycloaddition by Either Light or Heat. <i>Journal of the American Chemical Society</i> , 2013, 135, 1731-1734.	6.6	29
6880	A joint experimental/theoretical investigation of the MMA polymerization initiated by yttrium phenoxyamine complexes. <i>Dalton Transactions</i> , 2013, 42, 9226.	1.6	4
6881	Tensor representation techniques in post-Hartree-Fock methods: matrix product state tensor format. <i>Molecular Physics</i> , 2013, 111, 2398-2413.	0.8	15
6882	Computational Study of the Initial Stage of Diborane Pyrolysis. <i>Inorganic Chemistry</i> , 2013, 52, 5962-5969.	1.9	12

6883 Reactivity Studies of Iridium Pyridylidenes

#	ARTICLE	IF	CITATIONS
6896	Pt(II) complexes with (N,N- λ^2) or (C,N,E)- λ^3 (E=N,S) ligands: Cytotoxic studies, effect on DNA tertiary structure and structure-activity relationships. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 4210-4217.	1.4	22
6897	Structure and dynamics of solvent shells around photoexcited metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6268.	1.3	17
6898	Computational Investigations on Base-Catalyzed Diaryl Ether Formation. <i>Journal of Organic Chemistry</i> , 2013, 78, 5436-5443.	1.7	20
6899	A new type of metal chelate affinity chromatography using trivalent lanthanide ions for phosphopeptide enrichment. <i>Analyst</i> , 2013, 138, 2995.	1.7	43
6900	Understanding the Density Functional Dependence of DFT-Calculated Electronic Couplings in Organic Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 919-924.	2.1	79
6901	λ^1 -Monoacylated and $\lambda^1, \lambda^1\lambda^2$ - and $\lambda^1, \lambda^2\lambda^2$ -Diacylated Dipyrrins as Highly Sensitive Fluorescence "Turn-on" Zn ²⁺ Probes. <i>Journal of Organic Chemistry</i> , 2013, 78, 5328-5338.	1.7	129
6902	Doubly electron-attached and doubly ionized equation-of-motion coupled-cluster methods with 4-particle-2-hole and 4-hole-2-particle excitations and their active-space extensions. <i>Journal of Chemical Physics</i> , 2013, 138, 194102.	1.2	71
6903	Two-photon-induced singlet fission in rubrene single crystal. <i>Journal of Chemical Physics</i> , 2013, 138, 184508.	1.2	30
6904	Were Reactions of Triplet Silylenes Observed?. <i>Journal of the American Chemical Society</i> , 2013, 135, 9032-9040.	6.6	21
6905	Ultrafast Excited-State Dynamics of <i>ortho</i> -Terphenyl and 1,2-Diphenylcyclohexene: The Role of Ethylenic Twisting in the Nonadiabatic Photocyclization of Stilbene Analogs. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1895-1900.	2.1	13
6906	Cyclometalated Iridium Complexes of Bis(Aryl) Phosphine Ligands: Catalytic C-H/C-D Exchanges and C-C Coupling Reactions. <i>Inorganic Chemistry</i> , 2013, 52, 6694-6704.	1.9	32
6907	Screening metal-organic frameworks for selective noble gas adsorption in air: effect of pore size and framework topology. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9093.	1.3	92
6908	A generalized any-particle propagator theory: Prediction of proton affinities and acidity properties with the proton propagator. <i>Journal of Chemical Physics</i> , 2013, 138, 194108.	1.2	28
6909	Global optimization of clusters using electronic structure methods. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2091-2109.	1.0	184
6910	Synthesis and Comparison of Transition Metal Complexes of Abnormal and Normal Tetrazolyidenes: A Neglected Ligand Species. <i>Inorganic Chemistry</i> , 2013, 52, 7031-7044.	1.9	25
6911	Interplay between 1,3-Butadien-1,4-diyl and 2-Buten-1,4-dicarbene Derivatives: The Quest for Nucleophilic Carbenes. <i>Journal of the American Chemical Society</i> , 2013, 135, 8022-8030.	6.6	18
6912	Benchmarking of London Dispersion-Accounting Density Functional Theory Methods on Very Large Molecular Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1580-1591.	2.3	362
6913	The reaction of NH-indazoles with 1-fluoro-2,4-dinitrobenzene: the unusual formation of benzotriazole-N-oxides. <i>New Journal of Chemistry</i> , 2013, 37, 2384.	1.4	5

#	ARTICLE	IF	CITATIONS
6914	Excitation of the six lowest electronic transitions in water by 90 eV electrons. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2013, 46, 125201.	0.6	33
6915	Synthesis and characterization of new electron acceptor perylene diimide molecules for photovoltaic applications. <i>Dyes and Pigments</i> , 2013, 99, 329-338.	2.0	56
6916	Discovery of new heterocycles with activity against human neutrophil elastase based on a boron promoted one-pot assembly reaction. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 4465.	1.5	31
6917	A new palladium(II)-allyl complex containing a thioether-triazole ligand as active catalyst in Suzuki-Miyaura reaction. Use of tetraalkylammonium salts as promoters: Influence of the salt anion and cation on the catalytic activity. <i>Inorganica Chimica Acta</i> , 2013, 405, 188-195.	1.2	23
6918	Sourcing the affinity of flavonoids for the glycogen phosphorylase inhibitor site via crystallography, kinetics and QM/MM-PBSA binding studies: Comparison of chrysin and flavopiridol. <i>Food and Chemical Toxicology</i> , 2013, 61, 14-27.	1.8	29
6919	The conversion of protonated cytosine-SO ₃ ⁻ to uracil-SO ₃ ⁻ : Insights into the novel induced hydrolytic deamination through bisulfite catalysis. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9034.	1.3	9
6920	Atmospheric degradation of 2,3,7,8-tetrachlorinated dibenzo-p-dioxins in the presence of NO ₃ at night. <i>Canadian Journal of Chemistry</i> , 2013, 91, 398-405.	0.6	2
6921	Chirality Control for in Situ Preparation of Gold Nanoparticle Superstructures Directed by a Coordinatable Organogelator. <i>Journal of the American Chemical Society</i> , 2013, 135, 9174-9180.	6.6	68
6922	Syntheses and Photophysical Investigations of Cr(III) Hexadentate Iminopyridine Complexes and Their Tris(Bidentate) Analogues. <i>Inorganic Chemistry</i> , 2013, 52, 1368-1378.	1.9	27
6923	Colorimetric and Ratiometric Near-Infrared Fluorescent Cyanide Chemodosimeter Based on Phenazine Derivatives. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 1317-1326.	4.0	187
6924	Electrochemiluminescent Ruthenium(II) N-Heterocyclic Carbene Complexes: a Combined Experimental and Theoretical Study. <i>Inorganic Chemistry</i> , 2013, 52, 7448-7459.	1.9	82
6925	Structural and Mechanistic Basis of the Fast Metathesis Initiation by a Six-Coordinated Ruthenium Catalyst. <i>Organometallics</i> , 2013, 32, 3625-3630.	1.1	39
6926	Oxidovanadium Catechol Complexes: Radical versus Non-Radical States and Redox Series. <i>Inorganic Chemistry</i> , 2013, 52, 7417-7430.	1.9	25
6927	Fascinating Role of the Number of f Electrons in Dipolar and Octupolar Contributions to Quadratic Hyperpolarizability of Trinuclear Lanthanides-Biscopper Schiff Base Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 7550-7556.	1.9	10
6928	Computational Prediction of Structures and Optical Excitations for Nanoscale Ultrasmall ZnS and CdSe Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3581-3596.	2.3	51
6929	Amplified Spontaneous Emission in Pentathienoacene Dioxides by Direct Optical Pump and by Energy Transfer: Correlation with Photophysical Parameters. <i>Advanced Optical Materials</i> , 2013, 1, 588-599.	3.6	11
6930	Reactivity of Auranofin with Selenols and Thiols – Implications for the Anticancer Activity of Gold(I) Compounds. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 2718-2727.	1.0	25
6931	New Implicit Solvation Models for Dispersion and Exchange Energies. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5812-5820.	1.1	29

#	ARTICLE	IF	CITATIONS
6932	Insights into the Photochemical Disproportionation of Transition Metal Dimers on the Picosecond Time Scale. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3777-3785.	1.1	7
6933	Mechanism of AMPPD Chemiluminescence in a Different Voice. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2300-2312.	2.3	44
6934	Phenomenon of Quantum Entanglement in a System Composed of Two Minimal Protocells. <i>Origins of Life and Evolution of Biospheres</i> , 2013, 43, 49-66.	0.8	4
6935	A silver complex with ibuprofen: Synthesis, solid state characterization, DFT calculations and antibacterial assays. <i>Journal of Molecular Structure</i> , 2013, 1049, 1-6.	1.8	34
6936	Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2790-2799.	1.1	55
6937	Rational Design of Double-Check Mercury Ion Chemosensors Based on Photochromic Compounds. <i>Israel Journal of Chemistry</i> , 2013, 53, 288-293.	1.0	18
6938	Orbital Analysis and Excited-State Calculations in an Energy-Based Fragmentation Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3350-3363.	2.3	9
6939	Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2110-2142.	1.0	1,426
6940	Enantiopure isoplagiochin C by directed deracemization through axis-to-axis chirality transfer. <i>Tetrahedron: Asymmetry</i> , 2013, 24, 575-581.	1.8	2
6941	Synthesis, Characterization, Photoluminescence, and Simulations of a CCC-NHC-Supported Pt ₂ Ag ₂ Mixed-Metal Cluster Containing a PtAg ₂ Metallacyclopropane. <i>Organometallics</i> , 2013, 32, 752-761.	1.1	41
6942	Molecular structure and tautomers of [30]trithia-2,3,5,10,12,13,15,20,22,23,25,30-dodecaazahexaphyrin. <i>Journal of Porphyrins and Phthalocyanines</i> , 2013, 17, 220-228.	0.4	14
6943	Aromatic Claisen Rearrangements of <i>O</i> -Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2823-2831.	1.2	18
6944	Synthesis, characterization and photovoltaic properties of poly(cyclopentadithiophene-alt-isoindigo). <i>Polymer Chemistry</i> , 2013, 4, 5351.	1.9	20
6945	Computational Design of Two-Photon Fluorescent Probes for a Zinc Ion Based on a Salen Ligand. <i>Inorganic Chemistry</i> , 2013, 52, 5702-5713.	1.9	25
6946	Reactions of Acids with Naphthyridine-Functionalized Ferrocenes: Protonation and Metal Extrusion. <i>Inorganic Chemistry</i> , 2013, 52, 1432-1442.	1.9	5
6947	Relationship between stabilization energy and thermophysical properties of different imidazolium ionic liquids: DFT studies. <i>Computational and Theoretical Chemistry</i> , 2013, 1015, 27-33.	1.1	30
6948	Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. <i>Chemistry of Materials</i> , 2013, 25, 2254-2263.	3.2	141
6949	Theoretical Study of Reactivity of Ge(II)-hydride Compound: Comparison with Rh(I)-Hydride Complex and Prediction of Full Catalytic Cycle by Ge(II)-hydride. <i>Journal of the American Chemical Society</i> , 2013, 135, 8955-8965.	6.6	41

#	ARTICLE	IF	CITATIONS
6950	Interactions between halide anions and a molecular hydrophobic interface. <i>Faraday Discussions</i> , 2013, 160, 255-270.	1.6	47
6951	Methane CH Activation by Palladium Complexes with Chelating Bis(NHC) Ligands: A DFT Study. <i>Organometallics</i> , 2013, 32, 3469-3480.	1.1	66
6952	Cholesterol- and Estradiol-Appended Alkynylplatinum(II) Complexes as Supramolecular Gelators: Synthesis, Characterization, Photophysical and Gelation Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 9987-9994.	1.7	27
6953	Realistic Energy Surfaces for Real-World Systems: An IMOMO CCSD(T):DFT Scheme for Rhodium-Catalyzed Hydroformylation with the δ -PDPon Ligand. <i>Chemistry - A European Journal</i> , 2013, 19, 16272-16281.	1.7	25
6954	Second-Sphere Interactions between the C93-Y157 Cross-Link and the Substrate-Bound Fe Site Influence the O ₂ Coupling Efficiency in Mouse Cysteine Dioxygenase. <i>Biochemistry</i> , 2013, 52, 9104-9119.	1.2	49
6955	Computational Study of the Migration of Rhenium from One Enantioface of an Olefin to the Other Facilitated by (C-H)···Re Interactions. <i>Organometallics</i> , 2013, 32, 7141-7152.	1.1	5
6956	Spectroscopic and Computational Characterization of the NO Adduct of Substrate-Bound Fe(II) Cysteine Dioxygenase: Insights into the Mechanism of O ₂ Activation. <i>Biochemistry</i> , 2013, 52, 6040-6051.	1.2	32
6957	Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15792-15803.	1.2	19
6958	Phosphorescence Color Tuning of Cyclometalated Iridium Complexes by <i>o</i> -Carborane Substitution. <i>Inorganic Chemistry</i> , 2013, 52, 160-168.	1.9	118
6959	Clarification on the Decarboxylation Mechanism in KasA Based on the Protonation State of Key Residues in the Acyl-Enzyme State. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8095-8104.	1.2	8
6960	Photoexcitation and Charge-Transfer-to-Solvent Relaxation Dynamics of the $\langle \text{CH}_3 \rangle$ Complex. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7595-7605.	1.1	8
6961	Piezoelectric Effects of Applied Electric Fields on Hydrogen-Bond Interactions: First-Principles Electronic Structure Investigation of Weak Electrostatic Interactions. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1365-1370.	2.1	35
6962	On the Track to Silica-Supported Tungsten Oxo Metathesis Catalysts: Input from $\langle \text{O} \rangle$ Solid-State NMR. <i>Inorganic Chemistry</i> , 2013, 52, 10119-10130.	1.9	40
6963	Experimental and Theoretical Studies on the Fragmentation of Gas-Phase Uranyl ²⁺ , Neptunyl ²⁺ , and Plutonyl ²⁺ Diglycolamide Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10544-10550.	1.1	33
6964	<i>N</i> -Alkylpyrrolidine-Alane Compounds for Energy Applications. <i>Journal of Physical Chemistry C</i> , 2013, 117, 2628-2634.	1.5	11
6965	Understanding Selectin Counter-Receptor Binding from Electrostatic Energy Computations and Experimental Binding Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16443-16454.	1.2	15
6966	Jet-Cooled Spectroscopy of the $\dot{\text{I}}$ -Methylbenzyl Radical: Probing the State-Dependent Effects of Methyl Rocking Against a Radical Site. <i>Journal of Physical Chemistry A</i> , 2013, 117, 13465-13480.	1.1	17
6967	Mechanistic Examination of C ¹² -C ¹³ Bond Cleavages of Tryptophan Residues during Dissociations of Molecular Peptide Radical Cations. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1059-1068.	1.1	15

#	ARTICLE	IF	CITATIONS
6968	Novel Approach to Excited-State Calculations of Large Molecules Based on Divide-and-Conquer Method: Application to Photoactive Yellow Protein. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5565-5573.	1.2	36
6969	<i>In Silico</i> Categorization of <i>In Vivo</i> Intrinsic Clearance Using Machine Learning. <i>Molecular Pharmaceutics</i> , 2013, 10, 1318-1321.	2.3	11
6970	Nonstatistical Dynamic Effects in the Thermal C ² →C ⁶ Diels-Alder Cyclization of Enyne Allenes. <i>Journal of Organic Chemistry</i> , 2013, 78, 1451-1462.	1.7	18
6971	Theoretical Investigation of Phosphinidene Oxide Polypyridine Ruthenium(II) Complexes: Toward the Design of a New Class of Photochromic Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12821-12830.	1.1	14
6972	Stereodynamics of Nitrogen Chiral Centers in azap ³ -Cyclodipeptides. <i>Chirality</i> , 2013, 25, 341-349.	1.3	4
6973	A Case for Soft Error Detection and Correction in Computational Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3995-4005.	2.3	15
6974	Enhancement of Lithium Ion Mobility in Ionic Liquid Electrolytes in Presence of Additives. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25343-25351.	1.5	61
6975	Extension of the AMBER Force Field for Nitroxide Radicals and Combined QM/MM/PCM Approach to the Accurate Determination of EPR Parameters of DMPO-H in Solution. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3626-3636.	2.3	8
6976	Oxidative Additions of Aryl Halides to Palladium Proceed through the Monoligated Complex. <i>ChemCatChem</i> , 2013, 5, 3604-3609.	1.8	79
6977	Fragmentation, structure, and energetics of small sodium formate clusters: Evidence for strong influence of entropic effects. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 292-302.	0.7	4
6978	Structural Consequences of the N7 and C8 Translocation on the Metal Binding Behavior of Adenine. <i>Inorganic Chemistry</i> , 2013, 52, 1916-1925.	1.9	7
6979	Ruthenium-Catalyzed Transvinylolation - New Insights. <i>Advanced Synthesis and Catalysis</i> , 2013, 355, 2845-2859.	2.1	22
6980	Adsorption behavior of Co and C ₂ H ₂ on the graphite basal surface: A quantum chemistry study. <i>Journal of Structural Chemistry</i> , 2013, 54, 850-856.	0.3	1
6981	Adsorption behavior and electronic properties of Pd _n (n = 10) clusters on silicon carbide nanotubes: a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 085302.	0.7	1
6982	Electron-Induced Degradation of 8-Bromo-2-deoxyadenosine 3',5'-Diphosphate, a DNA Radiosensitizing Nucleotide. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8681-8688.	1.2	23
6983	Theoretical Investigation of Lactide Ring-Opening Polymerization Induced by a Dinuclear Indium Catalyst. <i>Organometallics</i> , 2013, 32, 6950-6956.	1.1	54
6984	Hydrogen Atom in Water from Ambient to High Temperatures. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16530-16541.	1.2	6
6985	Molecular orbital energy level modulation through incorporation of selenium and fluorine into conjugated polymers for organic photovoltaic cells. <i>Journal of Materials Chemistry A</i> , 2013, 1, 13422.	5.2	31

#	ARTICLE	IF	CITATIONS
6986	Conformational Properties of 1-Halogenated-1-Silacyclohexanes, $C_5H_{10}SiHX$ (X = Tj, ET, Q, O, O, rg, BT) / Overlock Spectroscopy, and Quantum-Chemical Calculations. <i>Organometallics</i> , 2013, 32, 6996-7005.	1.1	27
6987	Toward the Understanding of Radical Reactions: Experimental and Computational Studies of Titanium(III) Diamine Bis(phenolate) Complexes. <i>Inorganic Chemistry</i> , 2013, 52, 9427-9439.	1.9	20
6988	Determining Equilibrium Fluctuations Using Temperature-Dependent 2D-IR. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15346-15355.	1.2	17
6989	Novel Chemistry for the Selective Oxidation of Benzyl Alcohol by Graphene Oxide and N-Doped Graphene. <i>Organic Letters</i> , 2013, 15, 5920-5923.	2.4	32
6990	Aluminum Hydride Separation Using <i>N</i> -Alkylmorpholine. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14983-14991.	1.5	5
6991	Methane Adsorption on Aggregates of Fullerenes: Site-Selective Storage Capacities and Adsorption Energies. <i>ChemSusChem</i> , 2013, 6, 1235-1244.	3.6	21
6992	Electropolymerized Three-Dimensional Randomly Branched EDOT-Containing Copolymers. <i>Langmuir</i> , 2013, 29, 15463-15473.	1.6	21
6993	Alternant conjugated oligomers with tunable and narrow HOMO-LUMO gaps as sustainable nanowires. <i>RSC Advances</i> , 2013, 3, 25881.	1.7	55
6994	How Does the Environment Affect the Absorption Spectrum of the Fluorescent Protein mKeima?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1731-1742.	2.3	24
6995	Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9518-9531.	1.2	43
6996	Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Comparison between Calculated and Observed Properties. <i>Energy & Fuels</i> , 2013, 27, 702-710.	2.5	94
6997	Probing Isotope Shifts in ^{103}Rh and ^{195}Pt NMR Spectra with Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8054-8064.	1.1	9
6998	Rhodium(I) Silyl Complexes for C-F Bond Activation Reactions of Aromatic Compounds: Experimental and Computational Studies. <i>Organometallics</i> , 2013, 32, 3795-3807.	1.1	55
6999	Linear and Nonlinear Optical Properties of Ramified Hexaazatriphenylenes: Charge Transfer Contributions to the Octupolar Response. <i>Journal of Physical Chemistry C</i> , 2013, 117, 626-632.	1.5	18
7000	QM/MM Structural and Spectroscopic Analysis of the Di-iron(II) and Di-iron(III) Ferroxidase Site in M Ferritin. <i>Inorganic Chemistry</i> , 2013, 52, 8551-8563.	1.9	10
7001	Azaisoquinolinones: N Positions Tell You Different Stories in Their Optical Properties. <i>Journal of Organic Chemistry</i> , 2013, 78, 12760-12768.	1.7	21
7002	Pseudopotentials for hybridized carbon atoms. <i>Journal of Computational Chemistry</i> , 2013, 34, 49-59.	1.5	1
7003	Variationally determined electronic states for the theoretical analysis of intramolecular interaction. II. Qualitative nature of the $Pi\text{-}O$ bond in phosphine oxides. <i>Journal of Computational Chemistry</i> , 2013, 34, 149-161.	1.5	11

#	ARTICLE	IF	CITATIONS
7004	Energy Level Modulation of HOMO, LUMO, and Band-Gap in Conjugated Polymers for Organic Photovoltaic Applications. <i>Advanced Functional Materials</i> , 2013, 23, 439-445.	7.8	152
7005	Pestalotiopensâ€¦A and B: Stereochemically Challenging Flexible Sesquiterpeneâ€Cyclopaldic Acid Hybrids from <i>Pestalotiopsis</i> sp.. <i>Chemistry - A European Journal</i> , 2013, 19, 15556-15564.	1.7	56
7006	Communication: A Jastrow factor coupled cluster theory for weak and strong electron correlation. <i>Journal of Chemical Physics</i> , 2013, 139, 181101.	1.2	46
7007	The Jastrow antisymmetric geminal power in Hilbert space: Theory, benchmarking, and application to a novel transition state. <i>Journal of Chemical Physics</i> , 2013, 139, 194105.	1.2	64
7008	Flexible nuclear screening approximation to the two-electron spin-orbit coupling based on ab initio parameterization. <i>Journal of Chemical Physics</i> , 2013, 139, 204106.	1.2	8
7009	Dynamic scaffold of chiral binaphthol derivatives with the alkynylplatinum(II) terpyridine moiety. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 7986-7991.	3.3	65
7010	Accurate basis set truncation for wavefunction embedding. <i>Journal of Chemical Physics</i> , 2013, 139, 024103.	1.2	79
7011	Thermodynamic Study of Hydrolysis Reactions in Aqueous Solution from Ab Initio Potential and Molecular Dynamics Simulations. <i>Journal of Chemistry</i> , 2013, 2013, 1-8.	0.9	1
7012	The Influence of Alkoxy Substitutions on the Properties of Diketopyrrolopyrrole-Phenyl Copolymers for Solar Cells. <i>Materials</i> , 2013, 6, 3022-3034.	1.3	8
7013	General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: Theory and benchmarks. <i>Journal of Chemical Physics</i> , 2013, 139, 134105.	1.2	117
7014	Dynamical second-order Bethe-Salpeter equation kernel: A method for electronic excitation beyond the adiabatic approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 154109.	1.2	23
7015	Mono- and di-nuclear photoluminescent complexes of zinc(ii), cadmium(ii) and mercury(ii) of a chiral diimine ligand. <i>Dalton Transactions</i> , 2013, 42, 13026.	1.6	6
7016	On the basis set convergence of electron-electron entanglement measures: helium-like systems. <i>Frontiers in Chemistry</i> , 2013, 1, 24.	1.8	13
7017	Disposal of Dangerous Chemicals in Urban Areas and Mega Cities. <i>NATO Science for Peace and Security Series C: Environmental Security</i> , 2013, , .	0.1	10
7018	STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF THIOPHENE AND THIENOTHIOPHENE CONTAINING DIKETO-PYRROLO-PYRROLES (DPPs) IN POLAR APROTIC SOLVENTS. <i>Journal of Molecular and Engineering Materials</i> , 2013, 01, 1250003.	0.9	3
7019	Accuracy and Applicability of the New Exchange Correlation Functionals for Reproduction of the Infrared Spectra of Butyl Acrylate and Butyl Methacrylate Molecules. <i>Organic Chemistry International</i> , 2013, 2013, 1-12.	1.0	3
7020	Open-shell pair interaction energy decomposition analysis (PIEDA): Formulation and application to the hydrogen abstraction in tripeptides. <i>Journal of Chemical Physics</i> , 2013, 138, 074111.	1.2	39
7021	Linear-scaling symmetry-adapted perturbation theory with scaled dispersion. <i>Journal of Chemical Physics</i> , 2013, 139, 184104.	1.2	19

#	ARTICLE	IF	CITATIONS
7022	Theoretical study of the electronic excitations of free-base porphyrin-Ar ₂ van der Waals complexes. <i>Journal of Chemical Physics</i> , 2013, 139, 074303.	1.2	4
7023	Synthesis of 2-Azido-4-nitroimidazole and Its Derivatives for High-Energy Materials. <i>Chinese Journal of Chemistry</i> , 2013, 31, 1539-1545.	2.6	5
7024	Lewis Bases Trigger Intramolecular CH-Bond Activation: (tBu ₃ SiO) ₂ W=NtBu [r _l har ₂] (tBu ₃ SiO)(¹⁸ O, ¹³ C-tBu ₂ SiOCMe ₂ CH ₂)HW=NtBu. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4056-4067.	1.0	6
7025	The accuracy of the Gaussian-and-finite-element-Coulomb (GFC) method for the calculation of Coulomb integrals. <i>Journal of Chemical Physics</i> , 2013, 139, 054114.	1.2	2
7026	Local unitary transformation method toward practical electron correlation calculations with scalar relativistic effect in large-scale molecules. <i>Journal of Chemical Physics</i> , 2013, 139, 034109.	1.2	29
7027	Theoretical study on the mechanism of Pd(OAc) ₂ catalyzed dehydrogenative cross-coupling of two heteroarenes. <i>RSC Advances</i> , 2013, 3, 20772.	1.7	5
7028	Born-Oppenheimer molecular dynamics and electronic properties of chlorophyll-c2 in liquid methanol. <i>Journal of Chemical Physics</i> , 2013, 138, 225102.	1.2	8
7029	Efficient distance-including integral screening in linear-scaling Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2013, 138, 014101.	1.2	66
7030	Structural Fluctuation of Disilanyl Double-Pillared Bisheteroarenes. <i>Chemistry - an Asian Journal</i> , 2013, 8, 1177-1181.	1.7	5
7031	<i>In-Silico</i> Calculations as a Helpful Tool for Designing New Extractants in Liquid-Liquid Extraction. <i>Solvent Extraction and Ion Exchange</i> , 2013, 31, 499-518.	0.8	5
7032	Extending molecular simulation time scales: Parallel in time integrations for high-level quantum chemistry and complex force representations. <i>Journal of Chemical Physics</i> , 2013, 139, 074114.	1.2	18
7033	An oxorhenium(V) Schiff-base complex: synthesis, structure, spectroscopic characterization, electrochemistry, and DFT calculations. <i>Journal of Coordination Chemistry</i> , 2013, 66, 1178-1188.	0.8	10
7034	Molecular electrostatic potentials by systematic molecular fragmentation. <i>Journal of Chemical Physics</i> , 2013, 139, 184117.	1.2	13
7035	Laser-induced dissociation of singly protonated peptides at 193 and 266 nm within a hybrid linear ion trap mass spectrometer. <i>Rapid Communications in Mass Spectrometry</i> , 2013, 27, 1119-1127.	0.7	18
7036	A multi-state fragment charge difference approach for diabatic states in electron transfer: Extension and automation. <i>Journal of Chemical Physics</i> , 2013, 139, 154104.	1.2	44
7037	A combined molecular dynamics/micromechanics/finite element approach for multiscale constitutive modeling of nanocomposites with interface effects. <i>Applied Physics Letters</i> , 2013, 103, .	1.5	27
7038	Preliminary Theoretical Insights into Sml ₂ -Mediated Reactions: Activation of Ketones in THF. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 4042-4049.	1.0	19
7039	On the interactions between poly(ethylene oxide) and graphite oxide: A comparative study by different computational methods. <i>Journal of Chemical Physics</i> , 2013, 138, 094308.	1.2	7

#	ARTICLE	IF	CITATIONS
7040	Density functional theory study of the interaction of vinyl radical, ethyne, and ethene with benzene, aimed to define an affordable computational level to investigate stability trends in large van der Waals complexes. <i>Journal of Chemical Physics</i> , 2013, 139, 244306.	1.2	9
7041	A benchmark study of DFT methods on the electronic properties of lanthanofullerenes: a case study of Ce@C _{2v} (9)-C ₈₂ anion. <i>RSC Advances</i> , 2013, 3, 26252.	1.7	2
7043	DFT Study on the Recovery of Hoveyda's Grubbs-Type Catalyst Precursors in Enyne and Diene Ring-Closing Metathesis. <i>Chemistry - A European Journal</i> , 2013, 19, 14553-14565.	1.7	30
7044	CHEMICAL DESCRIPTION OF THE INTERACTION BETWEEN GLYCAN LIGAND AND SIGLEC-7 USING AB INITIO FMO METHOD AND CLASSICAL MD SIMULATION. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350060.	1.8	4
7045	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. <i>Journal of Chemical Physics</i> , 2013, 139, 214109.	1.2	29
7046	Tuning Redox Chemistry and Photophysics in Core-Substituted Tetraazaperopyrenes (TAPPs). <i>Chemistry - A European Journal</i> , 2013, 19, 13811-13822.	1.7	20
7047	COMPARATIVE INVESTIGATION OF THE EFFECT OF TYPE OF DENSITY FUNCTIONAL IN THE DETERMINATION OF GEOMETRICAL PARAMETERS IN A Cu COMPLEX. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350066.	1.8	2
7049	Synthesis, Characterization, and Mesomorphic Investigations of Calamitic Liquid Crystals of methyl 4-(4-(alkoxy)-2-hydroxybenzylideneamino) benzoates and Their Copper(II) and Nickel(II) Complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2013, 587, 1-17.	0.4	6
7050	Kinetic Evidence of an Apparent Negative Activation Enthalpy in an Organocatalytic Process. <i>Scientific Reports</i> , 2013, 3, 2557.	1.6	33
7051	Negative Charge and Solvent Effects on Electronic Excited-State Hydrogen Bonding of 2-Deoxycytidine 5'-Monophosphate (dCMP) in Aqueous Solution. <i>Bulletin of the Chemical Society of Japan</i> , 2013, 86, 586-593.	2.0	0
7052	Divide-and-Conquer Electronic-Structure Study on the Mechanism of the West Nile Virus NS3 Protease Inhibitor. <i>Bulletin of the Chemical Society of Japan</i> , 2013, 86, 67-74.	2.0	4
7053	C≡N Bond Cleavage by Iron Silyl Complex and Electronic Effect of the Group or Atom Attached to Cyano Group: A Theoretical DFT Study. <i>Bulletin of the Chemical Society of Japan</i> , 2013, 86, 273-275.	2.0	1
7054	Pyridine-Enhanced Head-to-Tail Dimerization of Terminal Alkynes by a Rhodium-N-Heterocyclic Carbene Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 15304-15314.	1.7	46
7055	Functionalized Bis(pentafluoroethyl)phosphanes: Improved Syntheses and Molecular Structures in the Gas Phase. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 3392-3404.	1.0	24
7056	Tuning the Hydrolytic Properties of Half-Sandwich-Type Organometallic Cations in Aqueous Solution. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 3090-3100.	1.0	21
7057	The Roles of Counterion and Water in a Stereoselective Cysteine-Catalyzed Rauhut's Currier Reaction: A Challenge for Computational Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 14245-14253.	1.7	33
7058	La ₂ @C _s (17490)-C ₇₆ : A New Non-IPR Dimetallic Metallofullerene Featuring Unexpectedly Weak Metal-Pentalene Interactions. <i>Chemistry - A European Journal</i> , 2013, 19, 17125-17130.	1.7	35
7059	Intramolecular versus intermolecular electronic interactions between [5,6]-open and [6,6]-closed C ₆₀ adducts with exTTF. <i>Chemical Science</i> , 2013, 4, 3166.	3.7	11

#	ARTICLE	IF	CITATIONS
7060	A Novel Approach to the Detection and Characterization of PAH Cations and PAH-Photoproducts. Proceedings of the International Astronomical Union, 2013, 9, 286-290.	0.0	4
7061	ESI formation of a Meisenheimer complex from tetryl and its unusual dissociation. Journal of Mass Spectrometry, 2013, 48, 306-311.	0.7	8
7062	Interplay of π - π^* versus π - π Conjugation in the Excited States and Charged Defects of Branched Oligothiophenes as Models for Dendrimeric Materials. Chemistry - A European Journal, 2013, 19, 17165-17171.	1.7	8
7063	Oxido- and Sulfidoniobium(V)N,N-Diethylcarbamates: Synthesis, Characterization and DFT Study. European Journal of Inorganic Chemistry, 2013, 2013, 3112-3118.	1.0	11
7064	Complete π * intramolecular aromatic hydroxylation mechanism through O ₂ activation by a Schiff base macrocyclic dicopper(I) complex. Beilstein Journal of Organic Chemistry, 2013, 9, 585-593.	1.3	6
7065	Facile and Selective Synthetic Approach for Ruthenium Complexes Utilizing a Molecular Sieve Effect in the Supporting Ligand. Inorganics, 2013, 1, 32-45.	1.2	5
7066	Lanczos-driven coupled-cluster damped linear response theory for molecules in polarizable environments. Journal of Chemical Physics, 2014, 141, 244107.	1.2	19
7067	On the Use of Locally Dense Basis Sets in the Calculation of EPR Hyperfine Couplings: A Study on Model Systems for Bio-Inorganic Fe and Co Complexes. Current Inorganic Chemistry, 2014, 3, 270-283.	0.2	6
7068	A Theoretical Study of Ligand Effects on the Electronic Structures of Ligated Zinc Porphyrin using Density Functional Theory. Journal of the Vacuum Society of Japan, 2014, 57, 102-110.	0.3	6
7070	Photosynthesis and Photo-Stability of Nucleic Acids in Prebiotic Extraterrestrial Environments. Topics in Current Chemistry, 2014, 356, 123-164.	4.0	23
7071	Does NHC Directly Participate in the CO ₂ Insertion into the U ^{III} -N Bond? A Density Functional Theory Study. Organometallics, 2014, 33, 7007-7010.	1.1	10
7072	The Fourier space restricted Hartree-Fock method for the electronic structure calculation of linear poly(tetrafluoroethylene). Science China Chemistry, 2014, 57, 1355-1362.	4.2	1
7073	Exchange coupling and magnetic blocking in dilanthanide complexes bridged by the multi-electron redox-active ligand 2,3,5,6-tetra(2-pyridyl)pyrazine. Chemical Science, 2014, 5, 4701-4711.	3.7	151
7074	Synthesis of Bright Alkenyl-1,2,4-triazoles: A Theoretical and Photophysical Study. ChemPlusChem, 2014, 79, 1489-1497.	1.3	4
7075	Doubly electron-attached and doubly ionised equation-of-motion coupled-cluster methods with full and active-space treatments of 4-particle-2-hole and 4-hole-2-particle excitations: the role of orbital choices. Molecular Physics, 2014, 112, 868-885.	0.8	21
7076	The Reduction-Coupled Oxo Activation (ROA) Mechanism Responsible for the Catalytic Selective Activation and Functionalization of n-Butane to Maleic Anhydride by Vanadium Phosphate Oxide. Topics in Catalysis, 2014, 57, 1171-1187.	1.3	39
7077	Catalytic Hydrocarbon Oxidation by Palladium-bis-NHC-Complexes. Topics in Catalysis, 2014, 57, 1372-1376.	1.3	14
7078	Complexes of platinum and palladium with β^2 -diketones and DMSO: Synthesis, characterization, molecular modeling, and biological studies. Journal of Molecular Structure, 2014, 1075, 370-376.	1.8	26

#	ARTICLE	IF	CITATIONS
7079	Design and Applications of Nanomaterials for Sensors. Challenges and Advances in Computational Chemistry and Physics, 2014, , .	0.6	6
7080	A computational study on the formation of pyridin-2(1H)-one and pyridine-2(1H)-thione from the reaction of cobaltacyclopentadiene with isocyanate and isothiocyanate. Journal of Organometallic Chemistry, 2014, 770, 101-115.	0.8	8
7081	A computational study of hexachlorobenzene-soil organic matter-interactions. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450009.	1.8	6
7082	Conjugation in and Optical Properties of 1-<i>R</i>-1,2-Diphospholes and 1-<i>R</i>-Phospholes. Journal of Physical Chemistry A, 2014, 118, 12168-12177.	1.1	30
7083	N,S,Pa€Hybrid Donorâ€“Acceptor Organic Dyes for Dyeâ€“Sensitized Solar Cell: Synthesis, Optical Properties, and Photovoltaic Performances. Heteroatom Chemistry, 2014, 25, 533-547.	0.4	21
7084	Formation of cyanates in low-valent uranium chemistry: a synergistic experimental/theoretical study. Dalton Transactions, 2014, 43, 11202-11208.	1.6	18
7085	An unusual mechanism for HOMOâ€“LUMO gap narrowing in a minimal near-IR dye generated by the deprotonation of bis(dicyanomethylene)indan. Chemical Physics Letters, 2014, 608, 355-359.	1.2	5
7086	Electron-induced single strand break in the nucleotide of 5- and 6-bromouridine. A DFT study. Chemical Physics Letters, 2014, 612, 289-294.	1.2	14
7087	Synthesis and photoinduced electron transfer in platinum(<sc>ii</sc>) bis(N-(4-ethynylphenyl)carbazole)bipyridine fullerene complexes. Dalton Transactions, 2014, 43, 17624-17634.	1.6	14
7088	Exploration of zeroth-order wavefunctions and energies as a first step toward intramolecular symmetry-adapted perturbation theory. Journal of Chemical Physics, 2014, 140, 154107.	1.2	15
7089	An ESR and DFT study of hydration of the 2â€“deoxyuridine-5-yl radical: a possible hydroxyl radical intermediate. Chemical Communications, 2014, 50, 14605-14608.	2.2	15
7090	New Unsymmetrically Benzene-Fused Bis (Tetrathiafulvalene): Synthesis, Characterization, Electrochemical Properties and Electrical Conductivity of Their Materials. International Journal of Molecular Sciences, 2014, 15, 4550-4564.	1.8	5
7091	Formation, isomerization, and dissociation of $\hat{\mu}$ - and $\hat{\pm}$ -carbon-centered tyrosylglycylglycine radical cations. Physical Chemistry Chemical Physics, 2014, 16, 24235-24243.	1.3	9
7092	Modeling nuclear resonance vibrational spectroscopic data of binuclear nonheme iron enzymes using density functional theory. Canadian Journal of Chemistry, 2014, 92, 975-978.	0.6	7
7093	A combined resonance enhanced multiphoton ionization and ab initio study of the first absorption band of 1,2,4,5-tetrafluorobenzene, pentafluorobenzene, and hexafluorobenzene. Journal of Chemical Physics, 2014, 141, 154310.	1.2	4
7094	FTIR/PCA study of propanol in argon matrix: The initial stage of clustering and conformational transitions. Low Temperature Physics, 2014, 40, 1077-1082.	0.2	15
7095	Why do the [PhSiO_{1.5}]_{8,10,12} cages self-brominate primarily in the ortho position? Modeling reveals a strong cage influence on the mechanism. Physical Chemistry Chemical Physics, 2014, 16, 25760-25764.	1.3	18
7096	Electronic Structure of Covalently Linked Zinc Bacteriochlorin Molecular Arrays: Insights into Molecular Design for NIR Light Harvesting. Journal of Physical Chemistry A, 2014, 118, 9901-9913.	1.1	10

#	ARTICLE	IF	CITATIONS
7097	A combined MD/QM and experimental exploration of conformational richness in branched oligothiophenes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24841-24852.	1.3	13
7098	On the Mechanism of the Palladium Bis(NHC) Complex Catalyzed CH Functionalization of Propane: Experiment and DFT Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 14872-14879.	1.7	36
7099	How does the increment of hetero-cyclic conjugated moieties affect electro-optical and charge transport properties of novel naphtha-difuran derivatives? A computational approach. <i>Journal of Molecular Modeling</i> , 2014, 20, 2547.	0.8	7
7100	Semi-quantitative assessment of the intersystem crossing rate: an extension of the El-Sayed rule to the emissive transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26184-26192.	1.3	108
7101	How to Chemically Tailor Metal-Porphyrin-Like Active Sites on Carbon Nanotubes and Graphene for Minimal Overpotential in the Electrochemical Oxygen Evolution and Oxygen Reduction Reactions. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29482-29491.	1.5	36
7102	Does decarboxylation make 2,5-dihydroxybenzoic acid special in matrix-assisted laser desorption/ionization?. <i>Rapid Communications in Mass Spectrometry</i> , 2014, 28, 1082-1088.	0.7	10
7103	Efficient anharmonic vibrational spectroscopy for large molecules using local-mode coordinates. <i>Journal of Chemical Physics</i> , 2014, 141, 104105.	1.2	102
7104	Recommending Hartree-Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14612-14626.	1.2	53
7105	The Synthesis of Highly Active Iridium(II) Complexes and their Application in Catalytic Hydrogen Isotope Exchange. <i>Advanced Synthesis and Catalysis</i> , 2014, 356, 3551-3562.	2.1	107
7106	Accurate and systematically improvable density functional theory embedding for correlated wavefunctions. <i>Journal of Chemical Physics</i> , 2014, 140, 18A507.	1.2	127
7107	Reactivity of a Series of Isostructural Cobalt Pincer Complexes with CO ₂ , CO, and H ₂ . <i>Inorganic Chemistry</i> , 2014, 53, 13031-13041.	1.9	41
7108	FOHI-D: An iterative Hirshfeld procedure including atomic dipoles. <i>Journal of Chemical Physics</i> , 2014, 140, 144104.	1.2	14
7109	A direct evidence of vibrationally delocalized response at ice surface. <i>Journal of Chemical Physics</i> , 2014, 141, 18C503.	1.2	10
7110	Efficient algorithms for semiclassical instanton calculations based on discretized path integrals. <i>Journal of Chemical Physics</i> , 2014, 141, 024101.	1.2	14
7111	TDDFT Assessment of Functionals for Optical O ⁺ O Transitions in Small Radicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11033-11046.	1.1	15
7112	Electronic excited states of chromium and vanadium bisarene complexes revisited: interpretation of the absorption spectra on the basis of TD DFT calculations. <i>Dalton Transactions</i> , 2014, 43, 17703-17711.	1.6	4
7113	A DFT-based model for calculating solvolytic reactivity. The nucleofugality of aliphatic carboxylates in terms of N _f parameters. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 5698.	1.5	17
7114	Anomalous One-Electron Processes in the Chemistry of Uranium Nitrogen Multiple Bonds. <i>Inorganic Chemistry</i> , 2014, 53, 9129-9139.	1.9	57

#	ARTICLE	IF	CITATIONS
7115	Shared-memory parallelization of a local correlation multi-reference CI program. <i>Computer Physics Communications</i> , 2014, 185, 3175-3188.	3.0	8
7116	Reactions between cold methyl halide molecules and alkali-metal atoms. <i>Journal of Chemical Physics</i> , 2014, 140, 014303.	1.2	3
7117	Theoretical Study on the Hydration Structure of Divalent Radium Ion Using Fragment Molecular Orbital-Molecular Dynamics (FMO-MD) Simulation. <i>Journal of Solution Chemistry</i> , 2014, 43, 1669-1675.	0.6	15
7118	Influence of the environment on protein bond energies. <i>Chemical Physics Letters</i> , 2014, 615, 75-82.	1.2	0
7119	Complete active space second-order perturbation theory with cumulant approximation for extended active-space wavefunction from density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2014, 141, 174111.	1.2	110
7120	Total Synthesis of (±)-Oxalicumone C and Chiral Resolution and Elucidation of Its Absolute Configuration. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 7788-7792.	1.2	11
7121	Unprecedented Chemical Reactivity of a Paramagnetic Endohedral Metallofullerene La@C ₈₂ that Leads Hydrogen Addition in the 1,3-Dipolar Cycloaddition Reaction. <i>Journal of the American Chemical Society</i> , 2014, 136, 17537-17546.	6.6	5
7122	Nonorthogonal molecular orbital method: Single-determinant theory. <i>Journal of Chemical Physics</i> , 2014, 140, 204111.	1.2	4
7123	Testing time-dependent density functional theory with depopulated molecular orbitals for predicting electronic excitation energies of valence, Rydberg, and charge-transfer states and potential energies near a conical intersection. <i>Journal of Chemical Physics</i> , 2014, 141, 104106.	1.2	13
7124	A Series of Uranium (IV, V, VI) Tritylimido Complexes, Their Molecular and Electronic Structures and Reactivity with CO ₂ . <i>Inorganic Chemistry</i> , 2014, 53, 13142-13153.	1.9	40
7125	The one-electron oxidation of a dithiolate molecule: The importance of chemical intuition. <i>Journal of Chemical Physics</i> , 2014, 140, 18A519.	1.2	8
7126	Low-energy elastic electron scattering by acetaldehyde. <i>Physical Review A</i> , 2014, 89, .	1.0	10
7127	Metal-Free Stabilization of Monomeric Antimony(I): A Carbene-Supported Stibinidene. <i>Chemistry - A European Journal</i> , 2014, 20, 8914-8917.	1.7	43
7128	Mechanistic Insight into the Photoredox Catalysis of Anti-Markovnikov Alkene Hydrofunctionalization Reactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 17024-17035.	6.6	268
7129	The theoretical estimation of C-H, N-H, O-H and S-H acids in dimethylsulfoxide solution. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 926-934.	0.9	10
7130	Structure and Vibrational Analyses of LiP15. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 5135-5144.	1.0	12
7131	Molecular dynamics simulations of ion solvation by flexible boundary QM/MM: On the partial charge transfer between QM and MM subsystems. <i>Journal of Computational Chemistry</i> , 2014, 35, 1778-1788.	1.5	19
7132	Geometric Matching Principle for Adsorption Selectivity of Ionic Liquids: A Simple Method into the Fascinating World of Shape-Controlled Chemistry. <i>Chemistry - A European Journal</i> , 2014, 20, 9012-9017.	1.7	11

#	ARTICLE	IF	CITATIONS
7133	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part II: Solution Phase. <i>ChemPhysChem</i> , 2014, 15, 3246-3257.	1.0	27
7134	Binding of Scandium Ions to Metalloporphyrin-Flavin Complexes for Long-Lived Charge Separation. <i>Chemistry - A European Journal</i> , 2014, 20, 15518-15532.	1.7	7
7135	Seleno groups control the energy-level alignment between conjugated organic molecules and metals. <i>Journal of Chemical Physics</i> , 2014, 140, 014705.	1.2	11
7136	Lanthanide-IMAC enrichment of carbohydrates and polyols. <i>Biomedical Chromatography</i> , 2014, 28, 412-418.	0.8	4
7137	Fullerene modification of gold electrodes and gold nanoparticles based on application of aromatic thioacetate-functionalized C ₆₀ . <i>RSC Advances</i> , 2014, 4, 64310-64318.	1.7	12
7138	Robust and efficient variational fitting of Fock exchange. <i>Journal of Chemical Physics</i> , 2014, 141, 124114.	1.2	58
7139	Phosphorescent C ^{SC*} Cyclometalated Pt(II) Dibenzofuranyl-NHC Complexes - An Auxiliary Ligand Study. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 256-264.	1.0	45
7140	Intermolecular Interaction of [60]Fullerene with Tröger's Base Analogues. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2014, 22, 66-74.	1.0	2
7141	The Diverse Manifold of Electronic States Generated by a Single Carbon Defect in a Graphene Sheet: Multireference Calculations Using a Pyrene Defect Model. <i>ChemPhysChem</i> , 2014, 15, 3334-3341.	1.0	10
7142	Phosphorescent Iridium(III) Complexes of Cyclometalated 5-Aryl-1 <i>H</i> -1,2,4-Triazole Ligands: Structural, Computational, Spectroscopic, and Device Studies. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27763-27771.	1.5	18
7143	Vibrational Study of SO ₂ Adsorption on Pt/SiO ₂ . <i>Journal of Physical Chemistry C</i> , 2014, 118, 29713-29723.	1.5	10
7144	Efficiency of perturbation-selection and its orbital dependence in the SAC-CI calculations for valence excitations of medium-size molecules. <i>Journal of Computational Chemistry</i> , 2014, 35, 2163-2176.	1.5	20
7145	Binding of Mazindol and Analogs to the Human Serotonin and Dopamine Transporters. <i>Molecular Pharmacology</i> , 2014, 85, 208-217.	1.0	22
7146	Computational Insight into the Mechanism of Nickel-Catalyzed Reductive Carboxylation of Styrenes using CO ₂ . <i>Organometallics</i> , 2014, 33, 7147-7156.	1.1	43
7147	Theoretical Analysis of Cobalt Handman Porphyrins: Ligand Dearomatization and Mechanistic Implications for Hydrogen Evolution. <i>ACS Catalysis</i> , 2014, 4, 4516-4526.	5.5	90
7148	NLO-X (X = O, S, Se, Te): New Gaussian basis sets for prediction of linear and nonlinear electric properties. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 796-804.	1.0	9
7149	Calculated Temperature Development of the Relative Stabilities of Yb@C ₈₂ Isomers. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2014, 22, 147-154.	1.0	11
7150	DFT study of the effect of solvent on the H-atom transfer involved in the scavenging of the free radicals $\dot{\text{a}}\text{-HO}_2$ and $\dot{\text{a}}\text{-O}_2\dot{\text{a}}^{\cdot}$ by caffeic acid phenethyl ester and some of its derivatives. <i>Journal of Molecular Modeling</i> , 2014, 20, 2509.	0.8	21

#	ARTICLE	IF	CITATIONS
7151	Computational Inhibition Studies of the Human Proteasome by Argyrinin-Based Analogues with Subunit Specificity. <i>Chemical Biology and Drug Design</i> , 2014, 84, 99-107.	1.5	9
7152	Surface Hopping Dynamics with DFT Excited States. <i>Topics in Current Chemistry</i> , 2014, 368, 415-444.	4.0	53
7153	Theoretical investigation of the degradation mechanisms in host and guest molecules used in OLED active layers. <i>Proceedings of SPIE</i> , 2014, , .	0.8	0
7154	The positions of inner hydroxide groups and aluminium ions in exfoliated kaolinite as indicators of the external chemical environment. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25830-25839.	1.3	11
7155	Computational Approaches to Homogeneous Gold Catalysis. <i>Topics in Current Chemistry</i> , 2014, 357, 213-283.	4.0	28
7156	The ground state and electronic structure of Gd@C82: A systematic theoretical investigation of first principle density functionals. <i>Journal of Chemical Physics</i> , 2014, 141, 244306.	1.2	22
7157	Armed-Disarmed Concept in the Synthesis of Glycosidic Bond. , 2014, , 117-179.		0
7158	8th Congress on Electronic Structure: Principles and Applications (ESPA 2012). <i>Highlights in Theoretical Chemistry</i> , 2014, , .	0.0	0
7159	Synthesis and Characterization of Novel Re(BIAN)(CO) ₃ Cl Derivatives Including the First Example of a Water-soluble Tricarbonyl Rhenium(I) Complex with Bis(imino)acenaphthene Ligands. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014, 69, 691-698.	0.3	7
7160	Cyanide and Azide Anion Complexation by a Bidentate Stibonium-Borane Lewis Acid. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2014, 69, 1199-1205.	0.3	21
7161	Study of a Conformational Equilibrium of Lisinopril by HPLC, NMR, and DFT. <i>International Journal of Analytical Chemistry</i> , 2014, 2014, 1-8.	0.4	3
7162	Rigid biimidazole ancillary ligands as an avenue to bright deep blue cationic iridium($\langle \text{sc} \rangle \text{iii} \langle / \text{sc} \rangle$) complexes. <i>Faraday Discussions</i> , 2014, 174, 165-182.	1.6	26
7163	Chemical and structural analysis related to defects in nanocrystalline Ba _{1-x} Sr _x TiO ₃ grown via hydrothermal sol-gel. <i>Ceramics International</i> , 2014, 40, 4975-4984.	2.3	11
7164	Acetamide as the model of the peptide bond: Nonadiabatic photodynamical simulations in the gas phase and in the argon matrix. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 136-143.	1.1	4
7165	A complete series of halocarbonyl molybdenum PNP pincer complexes - Unexpected differences between NH and NMe spacers. <i>Journal of Organometallic Chemistry</i> , 2014, 760, 74-83.	0.8	29
7166	A DFT study on doping assisted changing of B80 electronic structure: Promising candidates for NH ₃ sensor. <i>Sensors and Actuators B: Chemical</i> , 2014, 191, 457-463.	4.0	25
7167	Aggregation behavior of anionic surface active ionic liquids with double hydrocarbon chains in aqueous solution: Experimental and theoretical investigations. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2014, 453, 53-61.	2.3	36
7168	Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 158-166.	1.1	6

#	ARTICLE	IF	CITATIONS
7169	Selective fluorescent sensors for malate anion using the complex of phenanthroline-based Eu(III) in aqueous solution. <i>Sensors and Actuators B: Chemical</i> , 2014, 201, 131-137.	4.0	23
7170	The Second-Order Polarization Propagator Approximation (SOPPA) method coupled to the polarizable continuum model. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 54-60.	1.1	9
7171	CO bonding in FeN ₄ complexes and the effect of the macrocycle ligand: A DFT study. <i>Polyhedron</i> , 2014, 67, 36-43.	1.0	11
7172	Synthesis, characterization and theoretical study of 2-azido-4-nitroimidazole-based energetic salts. <i>Chinese Chemical Letters</i> , 2014, 25, 438-440.	4.8	7
7173	Mechanism and origins of enantioselectivity for [BMIM]Cl ionic liquids and ZnCl ₂ co-catalyzed coupling reaction of CO ₂ with epoxides. <i>Journal of Molecular Catalysis A</i> , 2014, 385, 133-140.	4.8	34
7174	Design, structural and spectroscopic elucidation, and the in vitro biological activities of new triorganotin dithiocarbamates – Part II. <i>Polyhedron</i> , 2014, 79, 161-169.	1.0	18
7175	Mechanism of addition-fragmentation reaction of thiocarbonyl compounds in free radical polymerization. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 39-45.	1.1	11
7176	Mechanism of Asymmetric Hydrogenation of α -Dehydroamino Acids Catalyzed by Rhodium Complexes: Large-Scale Experimental and Computational Study. <i>ACS Catalysis</i> , 2014, 4, 203-219.	5.5	43
7177	Theoretical investigation and design of high-efficiency dithiafulvenyl-based sensitizers for dye-sensitized solar cells: the impacts of elongating π -spacers and rigidifying dithiophene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9458.	1.3	40
7178	Reaction of Alkynes and Azides: Not Triazoles Through Copper Acetylides but Oxazoles Through Copper Nitrene Intermediates. <i>Chemistry - A European Journal</i> , 2014, 20, 3463-3474.	1.7	45
7179	Copper Active Sites in Biology. <i>Chemical Reviews</i> , 2014, 114, 3659-3853.	23.0	1,305
7180	Iron-sulfur bond covalency from electronic structure calculations for classical iron-sulfur clusters. <i>Journal of Computational Chemistry</i> , 2014, 35, 540-552.	1.5	24
7181	Geometrical and optical benchmarking of copper guanidine-quinoline complexes: Insights from TD-DFT and many-body perturbation theory. <i>Journal of Computational Chemistry</i> , 2014, 35, 1-17.	1.5	62
7182	Theoretical study of the interaction between X (H, F) and graphene. <i>Molecular Simulation</i> , 2014, 40, 306-312.	0.9	1
7183	Anchor Points Reactive Potential for Bond-Breaking Reactions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 924-933.	2.3	16
7184	Formation of water-chlorophyll clusters in dilute samples of chlorophyll-a in ether at low temperature. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2323-2330.	1.3	12
7185	New dinuclear copper(I) metallacycles containing bis-Schiff base ligands fused with two 1,2,4-triazole rings: Synthesis, characterization, molecular structures and theoretical calculations. <i>Polyhedron</i> , 2014, 69, 188-196.	1.0	24
7186	How Do DFT-DCP, DFT-NL, and DFT-D3 Compare for the Description of London-Dispersion Effects in Conformers and General Thermochemistry?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 968-980.	2.3	81

#	ARTICLE	IF	CITATIONS
7187	Mixed-valence VIV/VV tetrametallate core {V ₄ N ₂ O ₁₄ } cluster containing tris(hydroxymethyl)aminomethane and acetylacetonate. <i>Inorganic Chemistry Communication</i> , 2014, 41, 72-75.	1.8	17
7188	Quantum chemical DFT study of the interaction between molecular oxygen and FeN ₄ complexes, and effect of the macrocyclic ligand. <i>Journal of Molecular Modeling</i> , 2014, 20, 2131.	0.8	9
7189	UV-vis absorption spectrum of a novel Ru(II) complex intercalated in DNA: [Ru(2,2'-bipy)(dppz)(2,2'-ArPy)] ⁺ . <i>Journal of Molecular Modeling</i> , 2014, 20, 2082.	0.8	16
7190	Prediction of SAMPL4 host-guest binding affinities using funnel metadynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 443-454.	1.3	20
7191	Theoretical studies of ground and excited states in a series of Zn(II) complexes, derived from thiourea and thiosemicarbazide. <i>European Physical Journal D</i> , 2014, 68, 1.	0.6	2
7192	Density functional studies of the stepwise substitution of pyridine, pyridazine, pyrimidine, pyrazine, and 1,3,5-triazine with BCO. <i>Journal of Molecular Modeling</i> , 2014, 20, 2079.	0.8	2
7193	Synthesis, redox properties, and basicity of substituted 1-aminoanthraquinones: spectroscopic, electrochemical, and computational studies in acetonitrile solutions. <i>Structural Chemistry</i> , 2014, 25, 625-634.	1.0	24
7194	<i>meso</i> -Ester and Carboxylic Acid Substituted BODIPYs with Far-Red and Near-Infrared Emission for Bioimaging Applications. <i>Chemistry - A European Journal</i> , 2014, 20, 2301-2310.	1.7	55
7195	Phenol-Quinone Tautomerism in (Arylazo)naphthols and the Analogous Schiff Bases: Benchmark Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 778-789.	1.1	23
7196	Efficient calculation of two-electron integrals for high angular basis functions. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 543-552.	1.0	16
7197	Selective Catalytic Deuterium Labeling of Alcohols during a Transfer Hydrogenation Process of Ketones Using D ₂ O as the Only Deuterium Source. Theoretical and Experimental Demonstration of a Ru-H/D+Exchange as the Key Step. <i>ACS Catalysis</i> , 2014, 4, 1040-1053.	5.5	44
7198	An extensible interface for QM/MM molecular dynamics simulations with AMBER. <i>Journal of Computational Chemistry</i> , 2014, 35, 95-108.	1.5	130
7199	Charge-Transfer Complex Formation in Gelation: The Role of Solvent Molecules with Different Electron-Donating Capacities. <i>Chemistry - A European Journal</i> , 2014, 20, 5721-5726.	1.7	44
7200	Tunable Fluorophores Based on <i>N</i> -Arylimino)pyrrolyl Chelates of Diphenylboron: Synthesis, Structure, Photophysical Characterization, and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2014, 20, 4126-4140.	1.7	36
7201	Heteronuclear NMR Spectroscopy as a Surface-Selective Technique: A Unique Look at the Hydroxyl Groups of γ -Alumina. <i>Chemistry - A European Journal</i> , 2014, 20, 4038-4046.	1.7	82
7202	Nickel(I) Monomers and Dimers with Cyclopentadienyl and Indenyl Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 5327-5337.	1.7	65
7203	Synthesis, physicochemical characterization, DFT calculation and biological activities of Fe(III) and Co(II)-omeprazole complexes. Potential application in the <i>Helicobacter pylori</i> eradication. <i>Journal of Molecular Structure</i> , 2014, 1061, 5-13.	1.8	16
7204	Electronic structure of fullerene-squaraine complexes for photovoltaic devices. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 237-242.	1.1	7

#	ARTICLE	IF	CITATIONS
7205	Reactivity of Coordinatively Unsaturated Bis(N-heterocyclic carbene) Pt(II) Complexes toward H ₂ . Crystal Structure of a 14-Electron Pt(II) Hydride Complex. <i>Inorganic Chemistry</i> , 2014, 53, 4257-4268.	1.9	25
7206	New zirconium complexes supported by N-heterocyclic carbene (NHC) ligands: Synthesis and assessment of hydroamination catalytic properties. <i>Journal of Organometallic Chemistry</i> , 2014, 760, 60-66.	0.8	21
7207	Adaptive multiconfigurational wave functions. <i>Journal of Chemical Physics</i> , 2014, 140, 124114.	1.2	92
7208	Structural and optical properties of new cyclometalated Ru(II) derived compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 760, 248-259.	0.8	15
7209	Double-Hybrid Density Functionals Free of Dispersion and Counterpoise Corrections for Non-Covalent Interactions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3175-3182.	1.1	23
7210	Facile Synthesis of Dibenzopentalene Dianions and Their Application as New "Extended Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 7571-7575.	1.7	14
7211	Design of Weak Donor Alkyl Functionalized Push Pull Pyrene Dyes Exhibiting Enhanced Fluorescence Quantum Yields and Unique On/Off Switching Properties. <i>Chemistry - an Asian Journal</i> , 2014, 9, 1797-1807.	1.7	30
7212	Benchmarking Hydrogen and Carbon NMR Chemical Shifts at HF, DFT, and MP2 Levels. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 572-578.	2.3	152
7214	Near-IR Sensitization of Dye-Sensitized Solar Cells Using Thiocyanate-Free Cyclometalated Ruthenium(II) Complexes Having a Pyridylquinoline Ligand. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1303-1311.	1.0	21
7215	A New Family of Doubly Cyclopalladated Diimines. A Remarkable Effect of the Linker between the Metalated Units on Their Cytotoxicity. <i>Organometallics</i> , 2014, 33, 2862-2873.	1.1	21
7216	Ruthenium, Rhodium, Osmium, and Iridium Complexes of Osazones (Osazones = Bis-Arylhydrazones of) <i>Tj ETQq0 0 0 rgBT /Overlock 10</i>	1.9	12
7217	Synthesis of Highly Reactive Polyisobutylene Catalyzed by EtAlCl ₂ /Bis(2-chloroethyl) Ether Soluble Complex in Hexanes. <i>Macromolecules</i> , 2014, 47, 1959-1965.	2.2	43
7218	Comparison of the One-Electron Oxidations of CO-Bridged vs Unbridged Bimetallic Complexes: Electron-Transfer Chemistry of Os ₂ Cp ₂ (CO) ₄ and Os ₂ Cp [*] ₂ (1/4-CO) ₂ (CO) ₂ (Cp =) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 57 Td (Î<sub>2</sub>)</i>	1.1	57
7219	Organometallics, 2014, 33, 4716-4728. A new fluorescent probe for Zn ²⁺ with red emission and its application in bioimaging. <i>Dalton Transactions</i> , 2014, 43, 8048-8053.	1.6	37
7221	Tribenzylamine C-H Activation and Intermolecular Hydrogen Transfer Promoted by WCl ₆ . <i>Inorganic Chemistry</i> , 2014, 53, 3832-3838.	1.9	16
7222	Mechanistic Insights into Ruthenium-Catalyzed Production of H ₂ and CO ₂ from Methanol and Water: A DFT Study. <i>ACS Catalysis</i> , 2014, 4, 1129-1133.	5.5	85
7223	Cyclodimerization versus Polymerization of Methyl Methacrylate Induced by N-Heterocyclic Carbenes: A Combined Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2014, 20, 3989-3997.	1.7	37
7224	Synthesis and Some Properties of Transition Metal Complexes Based on the Octathiophophetane Ammonium Salts. <i>Heteroatom Chemistry</i> , 2014, 25, 434-441.	0.4	1

#	ARTICLE	IF	CITATIONS
7225	Synthesis and photovoltaic properties of new [1,2,5]thiadiazolo[3,4-c]pyridine-based organic Broadly absorbing sensitizers for dye-sensitized solar cells. <i>Tetrahedron</i> , 2014, 70, 3901-3908.	1.0	25
7226	A fast metal-metal bonded water oxidation catalyst. <i>Journal of Catalysis</i> , 2014, 315, 25-32.	3.1	20
7227	Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 715-721.	1.0	9
7228	Roles of water molecules in trapping carbon dioxide molecules inside the interlayer space of graphene oxides. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9656-9666.	1.3	29
7229	Palladium(II) Complexes with N-Heteroaromatic Bidentate Hydrazone Ligands: The Effect of the Chelate Ring Size and Lipophilicity on in vitro Cytotoxic Activity. <i>Chemical Biology and Drug Design</i> , 2014, 84, 333-341.	1.5	14
7230	Aluminum-Stabilized Low-Spin Iron(II) Hydrido Complexes of 1,4,7-Trimethyl-1,4,7-triazacyclononane. <i>Inorganic Chemistry</i> , 2014, 53, 5100-5108.	1.9	8
7231	Using Room Temperature Current Noise To Characterize Single Molecular Spectra. <i>ACS Nano</i> , 2014, 8, 2111-2117.	7.3	5
7232	Choosing RASSCF orbital active spaces for multiple electronic states. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 14-19.	1.1	22
7233	Comprehensive physicochemical studies of a new hybrid material: 2-Amino-4-methyl-3-nitropyridinium hydrogen oxalate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 117, 434-441.	2.0	6
7234	Synthesis, characterization and mesomorphic investigations of ester-substituted aroylhydrazones possessing a lateral hydroxyl group. <i>Polyhedron</i> , 2014, 74, 99-112.	1.0	8
7235	What are the spectroscopic properties of HFC-32? Answers from DFT. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1472-1485.	1.0	16
7236	EDOT-Based Copolymers with Pendant Anthraquinone Units: Analysis of Their Optoelectronic Properties within the Double-Cable Context. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9899-9910.	1.5	2
7237	Yttrium and lanthanide complexes of β^2 -dialdehydes: synthesis, characterization, luminescence and electrochemistry of coordination compounds with the conjugate base of bromomalonaldehyde. <i>Dalton Transactions</i> , 2014, 43, 9303.	1.6	7
7238	DFT Study on Mechanism of N-Alkylation of Amino Derivatives with Primary Alcohols Catalyzed by Copper(II) Acetate. <i>ACS Catalysis</i> , 2014, 4, 2231-2240.	5.5	36
7239	Sensitivity of ab Initio vs Empirical Methods in Computing Structural Effects on NMR Chemical Shifts for the Example of Peptides. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 122-133.	2.3	20
7240	Double Role of the Hydroxy Group of Phosphoryl in Palladium(II)-Catalyzed ortho-Olefination: A Combined Experimental and Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2014, 79, 80-87.	1.7	35
7241	A new size extensive multireference perturbation theory. <i>Journal of Computational Chemistry</i> , 2014, 35, 121-129.	1.5	13
7242	Synthesis and characterization of ferrocenyl camphor compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 760, 108-114.	0.8	7

#	ARTICLE	IF	CITATIONS
7243	Theoretical and Experimental Study of Inclusion Complexes Formed by Isoniazid and Modified β -Cyclodextrins: ^1H NMR Structural Determination and Antibacterial Activity Evaluation. Journal of Physical Chemistry B, 2014, 118, 81-93.	1.2	34
7244	Benzo[1,2-b:4,5-b \prime]dithiophene and benzotriazole based small molecule for solution-processed organic solar cells. Organic Electronics, 2014, 15, 405-413.	1.4	42
7245	Electron-Transfer Processes in 3,4-Diferrocenylpyrroles: Insight into a Missing Piece of the Polyferrocenyl-Containing Pyrroles Family. Organometallics, 2014, 33, 145-157.	1.1	37
7246	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	1.3	398
7247	Blue phosphorescent nitrile containing C^*C cyclometalated NHC platinum(II) complexes. Dalton Transactions, 2014, 43, 3297-3305.	1.6	46
7248	Computational Insights on the Geometrical Arrangements of Cu(II) with a Mixed-Donor N_3S_3 Macrobicyclic Ligand. Inorganic Chemistry, 2014, 53, 512-521.	1.9	6
7249	Computational modelling of donor-acceptor conjugated polymers through engineered backbone manipulations based on a thiophene-quinoxaline alternating copolymer. Journal of Materials Chemistry A, 2014, 2, 2202-2212.	5.2	24
7250	Topology of the electron density of multicenter bonding in the anion TCNE_2^{2-} . Structural Chemistry, 2014, 25, 679-682.	1.0	1
7251	Acetaldehyde adsorption and condensation on anatase TiO_2 : Influence of acetaldehyde dimerization. Journal of Molecular Catalysis A, 2014, 381, 77-88.	4.8	20
7252	Structure-property relationships of oligothiophene-isoindigo polymers for efficient bulk-heterojunction solar cells. Energy and Environmental Science, 2014, 7, 361-369.	15.6	108
7253	Dicobalt- μ_4 -oxo Polyoxometalate Compound, $[(\text{I}^{\pm})_2\text{P}_2\text{W}_{17}\text{O}_{61}\text{Co}_2\text{O}]^{14-}$: A Potent Species for Water Oxidation, C^-H Bond Activation, and Oxygen Transfer. Inorganic Chemistry, 2014, 53, 1779-1787.	1.9	30
7254	Synthesis, Characterization, and Photophysical Properties of Bodipy-Spirooxazine and -Spiropyran Conjugates: Modulation of Fluorescence Resonance Energy Transfer Behavior via Acidochromic and Photochromic Switching. ACS Applied Materials & Interfaces, 2014, 6, 1550-1562.	4.0	75
7255	Synthesis of new wide nematic diaryl-diacetylenes containing thiophene-based heteromonocyclic and heterobicyclic structures, and their birefringence properties. Liquid Crystals, 2014, 41, 642-651.	0.9	29
7256	Gold complexes with benzimidazole derivatives: synthesis, characterization and biological studies. BioMetals, 2014, 27, 183-194.	1.8	22
7257	Experimental and Theoretical Study on Palladium-Catalyzed C^-P Bond Formation via Direct Coupling of Triarylbismuths with $\text{P}(\text{O})^-\text{H}$ Compounds. Journal of Organic Chemistry, 2014, 79, 608-617.	1.7	76
7258	QSAR, docking, dynamic simulation and quantum mechanics studies to explore the recognition properties of cholinesterase binding sites. Chemico-Biological Interactions, 2014, 209, 1-13.	1.7	30
7259	The Triplet-Singlet Gap in the m -Xylylene Radical: A Not So Simple One. Journal of Chemical Theory and Computation, 2014, 10, 335-345.	2.3	56
7260	Potential Energy Curves via Double Ionization Potential Calculations: Example of HF Molecule. Advances in Quantum Chemistry, 2014, , 153-172.	0.4	2

#	ARTICLE	IF	CITATIONS
7261	Conjugated polymers based on benzodithiophene and fluorinated quinoxaline for bulk heterojunction solar cells: thiophene versus thieno[3,2-b]thiophene as π -conjugated spacers. <i>Polymer Chemistry</i> , 2014, 5, 2083.	1.9	68
7262	Dihydrogen Bonding in Complex $(PP)_3RuH(\bar{I})_1-BH_4$ Featuring Two Proton-Accepting Hydride Sites: Experimental and Theoretical Studies. <i>Inorganic Chemistry</i> , 2014, 53, 1080-1090.	1.9	21
7263	Systematic Approach to Conformational Sampling for Assigning Absolute Configuration Using Vibrational Circular Dichroism. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 477-494.	2.9	47
7264	Configuration Interaction-Corrected Tamm-Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 322-328.	2.1	45
7265	Nanostructured films of in situ deprotected thioacetyl-functionalized C60-fullerenes on a gold surface. <i>Journal of Materials Chemistry A</i> , 2014, 2, 2353.	5.2	20
7266	Synthesis, characterisation and some chemistry of C- and B-substituted carboxylic acids of cobalt bis(dicarbollide). <i>Dalton Transactions</i> , 2014, 43, 5106.	1.6	17
7267	Exfoliation of Graphite with Triazine Derivatives under Ball-Milling Conditions: Preparation of Few-Layer Graphene via Selective Noncovalent Interactions. <i>ACS Nano</i> , 2014, 8, 563-571.	7.3	241
7268	The nature of vertical excited states of dyes containing metals for DSSC applications: insights from TD-DFT and density based indexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14435.	1.3	57
7269	Calculations of One-Electron Redox Potentials of Oxoiron(IV) Porphyrin Complexes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 243-251.	2.3	47
7270	A combined experimental and computational study of fluxional processes in sigma amine-borane complexes of rhodium and iridium. <i>Dalton Transactions</i> , 2014, 43, 11118-11128.	1.6	26
7271	Calculating core-level excitations and X-ray absorption spectra of medium-sized closed-shell molecules with the algebraic diagrammatic construction scheme for the polarization propagator. <i>Journal of Computational Chemistry</i> , 2014, 35, 1900-1915.	1.5	131
7272	Efficient Implementation of Local Excitation Approximation for Treating Excited States of Molecules in Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5308-5317.	2.3	7
7273	Theoretical investigation of the effect of the solvent, hydrogen bond and amino group on the isomerization of Rhodamines. <i>Computational and Theoretical Chemistry</i> , 2014, 1050, 1-6.	1.1	10
7274	Theoretical Investigations on the Mechanism of Dual 1,3-Dipolar Cycloaddition of CO_2 with Isocyanides and Alkynes. <i>Journal of Organic Chemistry</i> , 2014, 79, 10811-10819.	1.7	5
7275	Turn-on Phosphorescent Chemodosimeter for Hg^{2+} Based on a Cyclometalated Ir(III) Complex and Its Application in Time-Resolved Luminescence Assays and Live Cell Imaging. <i>Inorganic Chemistry</i> , 2014, 53, 11498-11506.	1.9	51
7276	Dinuclear Nickel Complexes in Five States of Oxidation Using a Redox-Active Ligand. <i>Inorganic Chemistry</i> , 2014, 53, 11770-11777.	1.9	102
7277	Momentum space analysis of the electronic structure of biphenyl. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 225102.	0.6	5
7278	Computational Chemistry Meets Experiments for Explaining the Behavior of Bibenzyl: A Thermochemical and Spectroscopic (Infrared, Raman, and NMR) Investigation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5586-5592.	2.3	22

#	ARTICLE	IF	CITATIONS
7279	A near-infrared "off" fluorescent and colourimetric cyanide chemodosimeter based on phenothiazine with applications in living cell imaging. <i>RSC Advances</i> , 2014, 4, 59809-59816.	1.7	14
7280	Rational modifications on champion porphyrin dye SM315 using different electron-withdrawing moieties toward high performance dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24994-25003.	1.3	40
7281	Synthesis of novel dispiropyrrolothiazoles by three-component 1,3-dipolar cycloaddition and evaluation of their antimycobacterial activity. <i>RSC Advances</i> , 2014, 4, 59462-59471.	1.7	33
7282	Quantum Mechanics/Molecular Mechanics Modeling of Photoelectron Spectra: The Carbon 1s Core "Electron Binding Energies of Ethanol" Water Solutions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13217-13225.	1.2	14
7283	Monitoring of Reaction Intermediates in the Gas Phase: Ruthenium-Catalyzed C-C Coupling. <i>Organometallics</i> , 2014, 33, 6868-6878.	1.1	22
7284	Electron correlation in solids via density embedding theory. <i>Journal of Chemical Physics</i> , 2014, 141, 054113.	1.2	75
7285	Equation of motion coupled cluster methods for electron attachment and ionization potential in fullerenes C ₆₀ and C ₇₀ . <i>Journal of Chemical Physics</i> , 2014, 141, 074304.	1.2	16
7286	C-C Stretching Raman Spectra and Stabilities of Hydrocarbon Molecules in Natural Gas Hydrates: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11641-11651.	1.1	27
7287	Why Does the Coordination Mode of Physiological Bis(L-histidinato)copper(II) Differ in the Gas Phase, Crystal Lattice, and Aqueous Solutions? A Quantum Chemical Study. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 198-212.	1.0	6
7288	Electronic Structure of the Positive Radical of ¹³ C-Labeled Poly(3-Octylthienylene Vinylene) Polymer. <i>Applied Magnetic Resonance</i> , 2014, 45, 827-839.	0.6	2
7289	Toward force fields for atomistic simulations of iridium-containing complexes. <i>Journal of Computational Chemistry</i> , 2014, 35, 18-29.	1.5	5
7290	A Comprehensive Mechanistic Picture of the Isomerizing Alkoxyacylation of Plant Oils. <i>Journal of the American Chemical Society</i> , 2014, 136, 16871-16881.	6.6	114
7291	A Computational Study on a Strategy for Isolating a Stable Cyclopentadienyl Cation. <i>Chemistry - A European Journal</i> , 2014, 20, 14132-14138.	1.7	13
7292	Entropically Favored Adsorption of Cellulosic Molecules onto Carbon Materials through Hydrophobic Functionalities. <i>ChemSusChem</i> , 2014, 7, 1443-1450.	3.6	91
7293	Understanding the Guanidine-Like Cationic Moiety for Optimal Binding into the DNA Minor Groove. <i>ChemMedChem</i> , 2014, 9, 2065-2073.	1.6	15
7294	Insights into the Electronic Structure of Cu ^{II} Bound to an Imidazole Analogue of Westiellamide. <i>Inorganic Chemistry</i> , 2014, 53, 12323-12336.	1.9	14
7295	Computational Mechanistic Study of Fe-Catalyzed Hydrogenation of Esters to Alcohols: Improving Catalysis by Accelerating Precatalyst Activation with a Lewis Base. <i>ACS Catalysis</i> , 2014, 4, 4377-4388.	5.5	91
7296	The effect of diffuse basis functions on valence bond structural weights. <i>Molecular Physics</i> , 2014, 112, 654-660.	0.8	4

#	ARTICLE	IF	CITATIONS
7297	Effect of Including Torsional Parameters for Histidine-Metal Interactions in Classical Force Fields for Metalloproteins. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13106-13111.	1.2	13
7298	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. <i>Organometallics</i> , 2014, 33, 6065-6075.	1.1	31
7299	Importance of Ligand Exchanges in Pd(II)-Brønsted Acid Cooperative Catalytic Approach to Spirocyclic Rings. <i>Journal of the American Chemical Society</i> , 2014, 136, 15998-16008.	6.6	61
7300	PITOMBA: Parameter Interface for Oligosaccharide Molecules Based on Atoms. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5068-5080.	2.3	20
7301	Interaction Energy of Large Molecules from Restrained Denominator MP2-F12. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4857-4861.	2.3	12
7302	Spectroscopic and quantum-chemical investigations of chloro-bis-bipyridyl complexes of ruthenium(II) with 4-substituted pyridine ligands. <i>Optics and Spectroscopy (English Translation of Optika i Tj ETQq1 1 0.784314.rgBT /Overlock 10</i>		
7303	Transfer of the chelating ligands in the systems $[LAuCl_2]^{+}[PdCl_4]^{2-}$: Synthesis and structure of the salt $(NH_4)_0.20[(Bipy)AuCl_2]1.04[(Bipy)PdCl_2]0.96[AuCl_4]0.76[PdCl_4]0.24$. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2014, 40, 477-483.	0.3	1
7304	Direct Observation of Metal Ketenes Formed by Photoexcitation of a Fischer Carbene using Ultrafast Infrared Spectroscopy. <i>Organometallics</i> , 2014, 33, 6149-6153.	1.1	10
7305	DFT Virtual Screening Identifies Rhodium Amidinate Complexes As Potential Homogeneous Catalysts for Methane-to-Methanol Oxidation. <i>ACS Catalysis</i> , 2014, 4, 4455-4465.	5.5	24
7306	Synthesis, biological evaluation and SAR studies of novel bicyclic antitumor platinum(IV) complexes. <i>European Journal of Medicinal Chemistry</i> , 2014, 83, 374-388.	2.6	21
7307	Highly diastereoselective 1,3-dipolar cycloadditions of chiral non-racemic nitrones to 1,2-diaza-1,3-dienes: an experimental and computational investigation. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8888-8901.	1.5	14
7308	Reduction of an Fe(i) mesityl complex induced by β -acid ligands. <i>Dalton Transactions</i> , 2014, 43, 9032.	1.6	11
7309	Roles of carboxylate donors in O-O bond scission of peroxodi-iron(III) to high-spin oxodi-iron(IV) with a new carboxylate-containing dinucleating ligand. <i>Chemical Science</i> , 2014, 5, 2282-2292.	3.7	19
7310	Fluorine-free blue-green emitters for light-emitting electrochemical cells. <i>Journal of Materials Chemistry C</i> , 2014, 2, 5793-5804.	2.7	60
7311	Direct experimental and computational evidence for the dihydride pathway in TangPHOS-Rh catalysed asymmetric hydrogenation. <i>Dalton Transactions</i> , 2014, 43, 1785-1790.	1.6	21
7312	Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Push-Pull Substituted Azobenzene. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12518-12530.	1.2	18
7313	A Dissociative Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation and Infrared Experiments Reveal Characteristics of the Strongly Hydrolytic Arsenic(III). <i>Inorganic Chemistry</i> , 2014, 53, 11861-11870.	1.9	10
7314	Molecular design of organic sensitizers absorbing over a broadened visible region for dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 57916-57922.	1.7	5

#	ARTICLE	IF	CITATIONS
7315	New sulfone-based electron-transport materials with high triplet energy for highly efficient blue phosphorescent organic light-emitting diodes. <i>Journal of Materials Chemistry C</i> , 2014, 2, 10129-10137.	2.7	31
7316	Ruthenium, osmium and rhodium complexes of 1,4-diaryl 1,4-diazabutadiene: radical versus non-radical states. <i>Dalton Transactions</i> , 2014, 43, 13731-13741.	1.6	11
7317	Homoleptic and heteroleptic Au(i) complexes containing the new [Co ₅ C(CO) ₁₂] ⁺ cluster as ligand. <i>Dalton Transactions</i> , 2014, 43, 9633.	1.6	18
7318	On the factors that control the reactivity of meta-benzynes. <i>Chemical Science</i> , 2014, 5, 2205-2215.	3.7	24
7319	Role of hydrogen bonds in molecular packing of photoreactive crystals: templating photodimerization of protonated stilbazoles in crystalline state with a combination of water molecules and chloride ions. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 1509-1520.	1.6	15
7320	The reasons for ligand-dependent quantum yields and spectroscopic properties of platinum(II) complexes based on tetradentate O ⁻ N ⁻ C ⁻ N ligands: a DFT and TD-DFT study. <i>Dalton Transactions</i> , 2014, 43, 2849-2858.	1.6	7
7321	Out of cross-conjugation: the unexpected structure of tetrazinones. <i>RSC Advances</i> , 2014, 4, 47762-47768.	1.7	3
7322	Well-Defined Supported Mononuclear Tungsten Oxo Species as Olefin Metathesis Pre-Catalysts. <i>ACS Catalysis</i> , 2014, 4, 4232-4241.	5.5	38
7323	Catalytic kinetic resolution of a dynamic racemate: highly stereoselective β -lactone formation by N-heterocyclic carbene catalysis. <i>Chemical Science</i> , 2014, 5, 1974-1982.	3.7	68
7324	Tautomeric preference in polymorphs and pseudopolymorphs of succinylsulfathiazole: fast evaporation screening and thermal studies. <i>CrystEngComm</i> , 2014, 16, 4706-4714.	1.3	18
7325	Femtosecond Stimulated Raman Spectroscopy of the Cyclobutane Thymine Dimer Repair Mechanism: A Computational Study. <i>Journal of the American Chemical Society</i> , 2014, 136, 14801-14810.	6.6	31
7326	Synthesis, crystal structure, and optical characteristics of [Pd ₂ Hg ₄ Cl ₆ {Te(DMB)} ₆] \cdot 2DMF, [HgClTe(DMB)] ₄ , and the ring-forming cluster [Pd ₁₂ (TePh) ₂₄] \cdot 2DMF. <i>New Journal of Chemistry</i> , 2014, 38, 2394-2399.	1.4	19
7327	Electrodeposition and Properties of Donor-Acceptor Double-Cable Polythiophene with High Content of Pendant Fulleropyrrolidine Moieties. <i>Electrochimica Acta</i> , 2014, 148, 145-152.	2.6	10
7328	Two-Photon and Time-Resolved Fluorescence Spectroscopy as Probes for Structural Determination in Amyloid- β Peptides and Aggregates. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2351-2359.	1.2	22
7329	Evaluation of CM5 Charges for Condensed-Phase Modeling. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2802-2812.	2.3	54
7330	Conformation-Controlled Sorption Properties and Breathing of the Aliphatic Al-MOF [Al(OH)(CDC)]. <i>Inorganic Chemistry</i> , 2014, 53, 4610-4620.	1.9	74
7331	Protonation of Nickel- α -Iron Hydrogenase Models Proceeds after Isomerization at Nickel. <i>Journal of the American Chemical Society</i> , 2014, 136, 12385-12395.	6.6	29
7332	Torque-selective Ring Opening of Fused Cyclobutenamides: Evidence for a <i>cis,trans</i> -Cyclooctadienone Intermediate. <i>Journal of the American Chemical Society</i> , 2014, 136, 9802-9805.	6.6	27

#	ARTICLE	IF	CITATIONS
7333	The study of sodium dodecyl sulfate self-assembly behavior at three different concentrations in the presence and absence of lysozyme: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2014, 199, 184-189.	2.3	11
7334	Optimization of an AMBER Force Field for the Artificial Nucleic Acid, LNA, and Benchmarking with NMR of L(CAAU). <i>Journal of Physical Chemistry B</i> , 2014, 118, 1216-1228.	1.2	32
7335	Ni ^{II} , Cu ^{II} and Zn ^{II} complexes with a sterically hindered scorpionate ligand (Tpms ^{Ph}) and catalytic application in the diastereoselective nitroaldol (Henry) reaction. <i>Dalton Transactions</i> , 2014, 43, 15192-15200.	1.6	31
7336	Structures and properties of coordination polymers involving asymmetric biphenyl-3,2,5-tricarboxylate. <i>CrystEngComm</i> , 2014, 16, 10006-10016.	1.3	16
7337	Synthesis and characterisation of chelated cationic Re ^I (CO) ₃ bis(NHC)(WCA) complexes. <i>Dalton Transactions</i> , 2014, 43, 2259-2271.	1.6	18
7338	DFT study on the reaction mechanism of the ring closing enyne metathesis (RCEYM) catalyzed by molybdenum alkylidene complexes. <i>Dalton Transactions</i> , 2014, 43, 4573-4586.	1.6	18
7339	Spin density distribution after electron transfer from triethylamine to an [Ir(ppy) ₂ (bpy)] ⁺ photosensitizer during photocatalytic water reduction. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4789.	1.3	40
7340	The activation of N-glycosidic bond cleavage performed by base-excision repair enzyme hOGG1; theoretical study of the role of Lys 249 residue in activation of G, OxoG and FapyG. <i>RSC Advances</i> , 2014, 4, 44043-44051.	1.7	6
7341	Making Oxidation Potentials Predictable: Coordination of Additives Applied to the Electronic Fine Tuning of an Iron(II) Complex. <i>Inorganic Chemistry</i> , 2014, 53, 11573-11583.	1.9	29
7342	The radiosensitivity of 5- and 6-bromocytidine derivatives – electron induced DNA degradation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19424.	1.3	11
7343	Lewis acidic stiborafluorenes for the fluorescence turn-on sensing of fluoride in drinking water at ppm concentrations. <i>Chemical Science</i> , 2014, 5, 1886-1893.	3.7	111
7344	Towards a quantitative understanding of palladium metal scavenger performance: an electronic structure calculation approach. <i>Dalton Transactions</i> , 2014, 43, 469-478.	1.6	10
7345	Energy Offset Between Silicon Quantum Structures: Interface Impact of Embedding Dielectrics as Doping Alternative. <i>Advanced Materials Interfaces</i> , 2014, 1, 1400359.	1.9	32
7346	Linear Coordination Fullerene C ₆₀ Polymer [{Ni(Me ₃ P) ₂ }(I ^{1/4} -I ²)-C ₆₀]} Bridged by Zerovalent Nickel Atoms. <i>Inorganic Chemistry</i> , 2014, 53, 11960-11965.	1.9	35
7347	Effect of molecular vibrations on the MD/QC-simulated absorption spectra. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 261-270.	1.0	12
7348	Zethrene biradicals: How pro-aromaticity is expressed in the ground electronic state and in the lowest energy singlet, triplet, and ionic states. <i>Journal of Chemical Physics</i> , 2014, 140, 054706.	1.2	28
7349	A Density-Functional Study on the Change of Q/B-Band Intensity Ratio of Zinc Tetraphenylporphyrin in Solvents. <i>Journal of the Physical Society of Japan</i> , 2014, 83, 084802.	0.7	3
7350	Synthesis, cytotoxic and hydrolytic studies of titanium complexes anchored by a tripodal diamine bis(phenolate) ligand. <i>Dalton Transactions</i> , 2014, 43, 17422-17433.	1.6	21

#	ARTICLE	IF	CITATIONS
7351	P ^α H activation of secondary phosphanes on a parent amido diiridium complex. Dalton Transactions, 2014, 43, 1609-1619.	1.6	18
7352	The one-electron reduction of dithiolate and diselenolate ligands. Physical Chemistry Chemical Physics, 2014, 16, 10897.	1.3	11
7353	Influence of primary and auxiliary ligand on spectroscopic properties and luminescent efficiency of organoplatinum(ⁱⁱ) complexes bearing functionalized cyclometalated C ^N C ligands. Dalton Transactions, 2014, 43, 14029.	1.6	10
7354	Computational insights into carbon ^α carbon homocoupling reactions mediated by organolanthanide(ⁱⁱⁱ) complexes. Dalton Transactions, 2014, 43, 4520.	1.6	10
7355	Chain of dimers to assembly of trimers: temperature and ligand influenced formation of novel supramolecular assemblies of Cu(ⁱⁱ) with isomeric (aminomethyl) pyridines and azide. New Journal of Chemistry, 2014, 38, 3529.	1.4	19
7356	Photovoltaic properties of bis(octyloxy)benzo-[c][1,2,5]thiadiazole sensitizers based on an N,N-diphenylthiophen-2-amine donor. Journal of Materials Chemistry C, 2014, 2, 4063-4072.	2.7	18
7357	Cationic iridium(ⁱⁱⁱ) complexes bearing ancillary 2,5-dipyridyl(pyrazine) (2,5-dpp) and 2,2 [′] :5 [′] :2 ^{′′} :2 ^{′′′} -terpyridine (2,5-tpy) ligands: synthesis, optoelectronic characterization and light-emitting electrochemical cells. Dalton Transactions, 2014, 43, 13672-13682.	1.6	39
7358	Ramsey terms for two-, three-, and four-bond coupling involving ¹⁵ N and ¹⁷ O in hydrogen-bonded and nonhydrogen-bonded systems: are coupling constants sensitive to RAHBs?. Molecular Physics, 2014, 112, 107-116.	0.8	12
7359	All-atom molecular dynamics simulation of HPMA polymers. RSC Advances, 2014, 4, 7003.	1.7	3
7360	The ^α innocent ^α role of Sc ³⁺ on a non-heme Fe catalyst in an O ₂ environment. Dalton Transactions, 2014, 43, 11190.	1.6	2
7361	Aggregation-induced chiral symmetry breaking of a naphthalimide ^α cyanostilbene dyad. Physical Chemistry Chemical Physics, 2014, 16, 23854-23860.	1.3	16
7362	High efficiency solution-processed two-dimensional small molecule organic solar cells obtained via low-temperature thermal annealing. Journal of Materials Chemistry A, 2014, 2, 15904-15911.	5.2	48
7363	Electron induced single strand break and cyclization: a DFT study on the radiosensitization mechanism of the nucleotide of 8-bromoguanine. Physical Chemistry Chemical Physics, 2014, 16, 6568-6574.	1.3	17
7364	Through-space charge transfer and emission color tuning of di-o-carborane substituted benzene. Dalton Transactions, 2014, 43, 4978.	1.6	66
7365	Intermolecular charge transfer enhances two-photon absorption in yellow fluorescent protein. Physical Chemistry Chemical Physics, 2014, 16, 5958.	1.3	46
7366	Yttrium and lanthanide complexes of ^β 2-dialdehydes: synthesis, characterization and luminescence of coordination compounds with the conjugate base of nitromalonaldehyde. Dalton Transactions, 2014, 43, 10120.	1.6	6
7367	Unusual IR ring mode splittings for pyridinium species in H ₃ PW ₁₂ O ₄₀ heteropolyacid: involvement of the ^γ NH internal mode. RSC Advances, 2014, 4, 19159-19164.	1.7	2
7368	Introducing ^α LICA-FUKUI ^α software: reactivity-index calculations. Journal of Molecular Modeling, 2014, 20, 2492.	0.8	96

#	ARTICLE	IF	CITATIONS
7369	Catalyst selective and regiodivergent O- to C- or N-carboxyl transfer of pyrazolyl carbonates: synthetic and computational studies. <i>Chemical Science</i> , 2014, 5, 3651.	3.7	27
7370	Theoretical studies of cyclic adenosine monophosphate dependent protein kinase: native enzyme and ground-state and transition-state analogues. <i>Dalton Transactions</i> , 2014, 43, 3039-3043.	1.6	5
7371	Oxido-molybdenum complexes obtained by Cl/O interchange between MoCl_5 and carboxylic acids: a crystallographic, spectroscopic and computational study. <i>Dalton Transactions</i> , 2014, 43, 16416-16423.	1.6	9
7372	Oxidovanadium(IV), oxido-molybdenum(VI) and cobalt(III) complexes of o-phenylenediamine derivatives: oxidative dehydrogenation and photoluminescence. <i>Inorganic Chemistry Frontiers</i> , 2014, 1, 331-341.	3.0	5
7373	Electrochemical reactions of lithium-sulfur batteries: an analytical study using the organic conversion technique. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9344-9350.	1.3	120
7374	Catalytic Copper-Mediated Ring Opening and Functionalization of Benzoxazoles. <i>ACS Catalysis</i> , 2014, 4, 4215-4222.	5.5	16
7375	A new insight into the 5-carboxycytosine and 5-formylcytosine under typical bisulfite conditions: a deamination mechanism study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3573.	1.3	9
7376	A dominant homolytic Cl bond cleavage with low-spin triplet-state $\text{Fe}^{\text{IV}}\text{O}$ formed is revealed in the mechanism of heme-dependent chlorite dismutase. <i>Dalton Transactions</i> , 2014, 43, 973-981.	1.6	21
7377	Syntheses of mono- and diacylated bipyrrroles with rich substitution modes and development of a prodigiosin derivative as a fluorescent Zn(II) probe. <i>RSC Advances</i> , 2014, 4, 6133.	1.7	23
7378	Kinetic study on the aromatic nucleophilic substitution reaction of 3,6-dichloro-1,2,4,5-tetrazine by biothiols. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 670-675.	0.9	10
7379	Modulation of structural, energetic and electronic properties of DNA and size-expanded DNA bases upon binding to gold clusters. <i>RSC Advances</i> , 2014, 4, 29642-29651.	1.7	6
7380	Thiocyanate Complexes of Uranium in Multiple Oxidation States: A Combined Structural, Magnetic, Spectroscopic, Spectroelectrochemical, and Theoretical Study. <i>Inorganic Chemistry</i> , 2014, 53, 8624-8637.	1.9	28
7381	Mechanism of N-heterocyclic carbene-catalyzed chemical fixation of CO_2 with aziridines: a theoretical study. <i>RSC Advances</i> , 2014, 4, 17236-17244.	1.7	24
7382	Refinements to the Utah-Washington Mechanism of Electron Capture Dissociation. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7892-7901.	1.2	22
7383	Heteroleptic Cyclometalated Iridium(III) Complexes Supported by Triarylborolpicolinate Ligand: Ratiometric Turn-On Phosphorescence Response upon Fluoride Binding. <i>Inorganic Chemistry</i> , 2014, 53, 8672-8680.	1.9	43
7384	Spectroscopic and Computational Investigation of Iron(III) Cysteine Dioxygenase: Implications for the Nature of the Putative Superoxo-Fe(III) Intermediate. <i>Biochemistry</i> , 2014, 53, 5759-5770.	1.2	26
7385	A Theoretically-Guided Optimization of a New Family of Modular P,S-Ligands for Iridium-Catalyzed Hydrogenation of Minimally Functionalized Olefins. <i>Chemistry - A European Journal</i> , 2014, 20, 12201-12214.	1.7	41
7386	Extended coupled cluster method for potential energy surface: A decoupled approach. <i>Chemical Physics Letters</i> , 2014, 612, 209-213.	1.2	1

#	ARTICLE	IF	CITATIONS
7387	Unexpected DNA Affinity and Sequence Selectivity through Core Rigidity in Guanidinium-Based Minor Groove Binders. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7663-7672.	2.9	28
7388	Generation of Dihydrogen Molecule and Hydrosilylation of Carbon Dioxide Catalyzed by Zinc Hydride Complex: Theoretical Understanding and Prediction. <i>Inorganic Chemistry</i> , 2014, 53, 8485-8493.	1.9	43
7389	Diels-Alder Reaction on Free C ₆₈ Fullerene and Endohedral Sc ₃ N@C ₆₈ Fullerene Violating the Isolated Pentagon Rule: Importance of Pentagon Adjacency. <i>Chemistry - an Asian Journal</i> , 2014, 9, 2604-2611.	1.7	20
7390	Shining a Light on <i>s</i> -Triazine-Based Polymers. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4314-4324.	1.5	45
7391	Femtosecond Spectroscopy of Superfluorescent Fluorenyl Benzothiadiazoles with Large Two-Photon and Excited-State Absorption. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13790-13800.	1.5	20
7392	Photo-stable substituted dihydroindolo[2,3-b]carbazole-based organic dyes: tuning the photovoltaic properties by optimizing the structure for panchromatic DSSCs. <i>Tetrahedron</i> , 2014, 70, 8122-8128.	1.0	12
7393	Chiral transition-metal complexes as Brønsted-acid catalysts for the asymmetric Friedel-Crafts hydroxyalkylation of indoles. <i>Dalton Transactions</i> , 2014, 43, 11260-11268.	1.6	23
7394	Relaxation Pathways of Photoexcited Iodide-Methanol Clusters: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4494-4501.	1.1	3
7395	Investigation of the Cycloisomerization of 1,6-Enynes Catalyzed by Gold Nanoparticles with First-Principles Calculations: Mechanism and Selectivity. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18510-18520.	1.5	13
7396	The nature of persistent conformational chirality, racemization mechanisms, and predictions in diarylether heptanoid cyclophane natural products. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 3303-3309.	1.5	10
7397	Reactivity of Saturated Hydrocarbon Anchoring Arms on Si(100) upon White Light Photoactivation: Experimental Evidence and Theoretical Insights. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22509-22521.	1.5	0
7398	Bifunctional Porphyrin Catalysts for the Synthesis of Cyclic Carbonates from Epoxides and CO ₂ : Structural Optimization and Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2014, 136, 15270-15279.	6.6	404
7399	Multi-scale theoretical investigation of molecular hydrogen adsorption over graphene: coronene as a case study. <i>RSC Advances</i> , 2014, 4, 54447-54453.	1.7	40
7400	Polarisation charge switching through the motion of metal atoms trapped in fullerene cages. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23869-23873.	1.3	12
7401	Why Bistetracenes Are Much Less Reactive Than Pentacenes in Diels-Alder Reactions with Fullerenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 10743-10751.	6.6	52
7402	Insight into the Efficiency of Cinnamyl-Supported Precatalysts for the Suzuki-Miyaura Reaction: Observation of Pd(I) Dimers with Bridging Allyl Ligands During Catalysis. <i>Journal of the American Chemical Society</i> , 2014, 136, 7300-7316.	6.6	115
7403	Computational Exploration of Alternative Catalysts for Olefin Purification: Cobalt and Copper Analogues Inspired by Nickel Bis(dithiolene) Electrocatalysis. <i>Inorganic Chemistry</i> , 2014, 53, 9679-9691.	1.9	18
7404	Two-Photon Absorption in Fluorescent Protein Chromophores: TDDFT and CC2 Results. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3260-3269.	2.3	33

#	ARTICLE	IF	CITATIONS
7405	Acceleration of an Aromatic Claisen Rearrangement via a Designed Spirolygozyme Catalyst that Mimics the Ketosteroid Isomerase Catalytic Dyad. <i>Journal of the American Chemical Society</i> , 2014, 136, 3817-3827.	6.6	27
7406	A significant role of Arg41 residue in the enzymatic reaction of haloacid dehalogenase I-DEX YL studied by QM/MM method. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2014, 110, 23-31.	1.8	8
7407	Tuning the First Hyperpolarizabilities of Boron Nitride Nanotubes. <i>ACS Photonics</i> , 2014, 1, 928-935.	3.2	14
7408	Synthesis, Characterization, and Linkage Isomerism in Mononuclear Ruthenium Complexes Containing the New Pyrazolate-Based Ligand Hpbl. <i>Inorganic Chemistry</i> , 2014, 53, 8025-8035.	1.9	8
7409	A general, recursive, and open-ended response code. <i>Journal of Computational Chemistry</i> , 2014, 35, 622-633.	1.5	34
7410	DFT Mechanistic Study of RuII-Catalyzed Amide Synthesis from Alcohol and Nitrile Unveils a Different Mechanism for Borrowing Hydrogen. <i>ACS Catalysis</i> , 2014, 4, 2854-2865.	5.5	27
7411	On the Road to MM ² X Polymers: Redox Properties of Heterometallic Ni ^{II} -Pt Paddlewheel Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 10553-10562.	1.9	6
7412	Esterification of Indoline-Based Small-Molecule Donors for Efficient Co-evaporated Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14785-14794.	1.5	15
7413	Revisiting Photoemission and Inverse Photoemission Spectra of Nickel Oxide from First Principles: Implications for Solar Energy Conversion. <i>Journal of Physical Chemistry B</i> , 2014, 118, 7963-7971.	1.2	39
7414	Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3669-3680.	2.3	334
7415	Hydration Energy from a Composite Method for Implicit Representation of Solvent. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 211-219.	2.3	46
7416	Systematic Study of Locally Dense Basis Sets for NMR Shielding Constants. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 146-152.	2.3	44
7417	Benchmarking dispersion and geometrical counterpoise corrections for cost-effective large-scale DFT calculations of water adsorption on graphene. <i>Journal of Computational Chemistry</i> , 2014, 35, 1789-1800.	1.5	24
7418	Deconstructing the Catalytic Efficiency of Peroxiredoxin-5 Peroxidatic Cysteine. <i>Biochemistry</i> , 2014, 53, 6113-6125.	1.2	63
7419	Photophysical properties and photochemistry of substituted cinnamates and cinnamic acids for UVB blocking: effect of hydroxy, nitro, and fluoro substitutions at ortho, meta, and para positions. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 583-594.	1.6	28
7420	Shedding Light on the Photophysical Properties of Iridium(III) Complexes with N-Heterocyclic Carbene Ligands from a Theoretical Viewpoint. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5058-5067.	1.1	9
7421	A unifying mechanism for the rearrangement of vinyl allene oxide geometric isomers to cyclopentenones. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7694-7701.	1.5	8
7422	Does the Preferred Mechanism of a Catalytic Transformation Depend on the Density Functional? Ethylene Hydrosilylation by a Metal Complex as a Case Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3004-3013.	1.1	6

#	ARTICLE	IF	CITATIONS
7423	Is the contribution of cis and trans protonated 5-methylcytosine-SO ₃ ⁺ isomers equal in the conversion to thymine-SO ₃ ⁺ under bisulfite conditions? A theoretical perspective. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16264-16277.	1.3	4
7424	Catalyst activation and the dimerization energy of alkylaluminium compounds. <i>Journal of Organometallic Chemistry</i> , 2014, 772-773, 161-171.	0.8	59
7425	Analytic cubic and quartic force fields using density-functional theory. <i>Journal of Chemical Physics</i> , 2014, 140, 034103.	1.2	38
7426	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 52, 30-35.	1.3	26
7427	The conformational behavior, geometry and energy parameters of Menshutkin-like reaction of O-isopropylidene-protected glycofuranoid mesylates in view of DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 52, 91-102.	1.3	4
7428	Thermodynamic properties of the methyl esters of p-hydroxy and p-methoxy benzoic acids. <i>Journal of Chemical Thermodynamics</i> , 2014, 78, 43-57.	1.0	23
7429	Computational study on intramolecular electron transfer in 1,3-dinitrobenzene radical anion. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 803-810.	0.9	5
7430	Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Ruthenium Vinylidene Complexes. <i>Organometallics</i> , 2014, 33, 2549-2560.	1.1	8
7431	Aerobic Carbon-Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide. <i>Journal of the American Chemical Society</i> , 2014, 136, 10941-10948.	6.6	77
7432	Landscapes of Four-Enantiomer Conical Intersections for Photoisomerization of Stilbene: CASSCF Calculation. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9021-9031.	1.1	21
7433	Alkenyl-substituted titanocene dichloride complexes: Stability studies, binding and cytotoxicity. <i>Journal of Organometallic Chemistry</i> , 2014, 769, 46-57.	0.8	6
7434	DFT cluster model study of MoVO-type mixed-metal oxides. <i>Computational and Theoretical Chemistry</i> , 2014, 1045, 57-65.	1.1	7
7435	Regulation of the Rate of Dinucleation of a Monocopper(I) Complex Containing Bipyrimidine Rotary Units by Restricted Double Pyrimidine Rotation. <i>Inorganic Chemistry</i> , 2014, 53, 2831-2840.	1.9	14
7436	Unifying General and Segmented Contracted Basis Sets. Segmented Polarization Consistent Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1074-1085.	2.3	232
7437	C ⁺ C* Cyclometalated Platinum(II) NHC Complexes with β^2 -Ketoimine Ligands. <i>Organometallics</i> , 2014, 33, 898-908.	1.1	36
7438	High-Accuracy Vibrational Computations for Transition-Metal Complexes Including Anharmonic Corrections: Ferrocene, Ruthenocene, and Osmocene as Test Cases. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4565-4573.	2.3	46
7439	New Water Oxidation Chemistry of a Seven-Coordinate Ruthenium Complex with a Tetradentate Polypyridyl Ligand. <i>Inorganic Chemistry</i> , 2014, 53, 6904-6913.	1.9	48
7440	Symmetry Lowering in Triindoles: Impact on the Electronic and Photophysical Properties. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5470-5477.	1.5	27

#	ARTICLE	IF	CITATIONS
7441	Computational Insights on an Artificial Imine Reductase Based on the Biotin–Streptavidin Technology. <i>ACS Catalysis</i> , 2014, 4, 833-842.	5.5	27
7442	Germanium- and Silicon-Substituted Donor–Acceptor Type Copolymers: Effect of the Bridging Heteroatom on Molecular Packing and Photovoltaic Device Performance. <i>Advanced Energy Materials</i> , 2014, 4, 1400527.	10.2	46
7443	Mechanisms of large red-shift and intensity enhancement of absorption bands by π -bond breaking in a benzoporphyrin sensitizer for photodynamic therapy. <i>Journal of Porphyrins and Phthalocyanines</i> , 2014, 18, 513-518.	0.4	0
7444	Mechanistic Insights on Cooperative Asymmetric Multicatalysis Using Chiral Counterions. <i>Journal of Organic Chemistry</i> , 2014, 79, 7600-7606.	1.7	44
7445	A facile regioselective 1,3-dipolar cycloaddition protocol for the synthesis of new class of quinolinyl dispiro heterocycles. <i>Tetrahedron Letters</i> , 2014, 55, 5475-5480.	0.7	21
7446	Modulating the Electronic Structure of Chromophores by Chemical Substituents for Efficient Energy Transfer: Application to Fluorone. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6085-6091.	1.1	4
7447	Discovery and Mechanistic Studies of Facile N-Terminal C–C Bond Cleavages in the Dissociation of Tyrosine-Containing Peptide Radical Cations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4273-4281.	1.2	9
7448	Identifying Key Properties of Electrolytes for Light-Emitting Electrochemical Cells. <i>Chemistry of Materials</i> , 2014, 26, 5083-5088.	3.2	40
7449	Ab initio determination of the crystalline benzene lattice energy to sub-kilojoule/mole accuracy. <i>Science</i> , 2014, 345, 640-643.	6.0	230
7450	Self-Aggregation of New Alkylcarboxylate-Based Anionic Surface Active Ionic Liquids: Experimental and Theoretical Investigations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2758-2768.	1.2	51
7451	Benchmark Torsional Potentials of Building Blocks for Conjugated Materials: Bifuran, Bithiophene, and Biselenophene. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3647-3655.	2.3	41
7452	Excitation Energy Transfer in the Peridinin-Chlorophyll <i>a</i> -Protein Complex Modeled Using Configuration Interaction. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9141-9154.	1.2	19
7453	Electrocatalytic Oxygen Activation by Carbanion Intermediates of Nitrogen-Doped Graphitic Carbon. <i>Journal of the American Chemical Society</i> , 2014, 136, 3358-3361.	6.6	68
7454	Hydration of porphyrin and Mg–porphyrin: ab initio quantum mechanical charge field molecular dynamics simulations. <i>Molecular BioSystems</i> , 2014, 10, 117-127.	2.9	15
7455	Understanding the interaction of an antitumoral platinum(II) 7-azaindolate complex with proteins and DNA. <i>BioMetals</i> , 2014, 27, 1159-1177.	1.8	8
7456	Acid/Base Switching of the Tautomerism and Conformation of a Dioxoporphyrin for Integrated Binary Subtraction. <i>Chemistry - A European Journal</i> , 2014, 20, 12910-12916.	1.7	14
7457	Competitive Silyl–Prins Cyclization versus Tandem Sakurai–Prins Cyclization: An Interesting Substitution Effect. <i>Chemistry - A European Journal</i> , 2014, 20, 14112-14119.	1.7	33
7458	A New Tool To Guide Halofunctionalization Reactions: The Halenium Affinity ($\langle i \rangle \text{HalA} \langle /i \rangle$) Scale. <i>Journal of the American Chemical Society</i> , 2014, 136, 13355-13362.	6.6	77

#	ARTICLE	IF	CITATIONS
7459	CNN Pincer Ruthenium Catalysts for Hydrogenation and Transfer Hydrogenation of Ketones: Experimental and Computational Studies. <i>Chemistry - A European Journal</i> , 2014, 20, 13603-13617.	1.7	47
7460	Pd-Catalysed Mono- and Dicarboxylation of Aryl Iodides: Insights into the Mechanism and the Selectivity. <i>Chemistry - A European Journal</i> , 2014, 20, 10982-10989.	1.7	26
7461	Fragmentation of Peptide Radical Cations Containing a Tyrosine or Tryptophan Residue: Structural Features That Favor Formation of $[X + H]^+$ and $[Z + H]^+$ Ions. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6123-6133.	1.2	11
7462	Noninnocent Nature of Carbon Support in Metal/Carbon Catalysts: Etching/Pitting vs Nanotube Growth under Microwave Irradiation. <i>ACS Catalysis</i> , 2014, 4, 3806-3814.	5.5	49
7463	Dimers and Trimers of Diphosphenes: A Wealth of Cyclophosphanes. <i>Chemistry - A European Journal</i> , 2014, 20, 12607-12615.	1.7	25
7464	Solvatochromic Study of Highly Fluorescent Alkylated Isocyanonaphthalenes, Their π -Stacking, Hydrogen-Bonding Complexation, and Quenching with Pyridine. <i>ChemPhysChem</i> , 2014, 15, 3614-3625.	1.0	13
7465	Alkaline Stability of Benzyl Trimethyl Ammonium Functionalized Polyaromatics: A Computational and Experimental Study. <i>Chemistry of Materials</i> , 2014, 26, 5675-5682.	3.2	152
7466	Density functional theory study of transition metals doped B_{80} fullerene. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450050.	1.8	15
7467	Molecular Dynamics Simulations of DPPC/CTAB Monolayers at the Air/Water Interface. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11723-11737.	1.2	33
7468	Benchmarking of Density Functionals for the Accurate Description of Thiol-Disulfide Exchange. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4842-4856.	2.3	33
7469	Conformational Flexibility of Dibenzobarrelene-Based $PC(sp^3)_3P$ Pincer Iridium Hydride Complexes: The Role of Hemilabile Functional Groups and External Coordinating Solvents. <i>Organometallics</i> , 2014, 33, 5964-5973.	1.1	35
7470	Combined Experimental and Computational Approaches To Elucidate the Structures of Silver Clusters inside the ZSM-5 Cavity. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23874-23887.	1.5	23
7471	The issue of π -molecular radiators™ in microwave-assisted reactions. Computational calculations on ring closing metathesis (RCM). <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2436-2445.	1.5	19
7472	Piezoelectric Hydrogen Bonding: Computational Screening for a Design Rationale. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7404-7410.	1.1	28
7473	Mixed Ramp Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4369-4376.	2.3	17
7474	Theoretical Study of Neutral and Charged $Fe_7-(C_6H_6)_m$, $m = 1, 2$ Rice-Ball Clusters. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5548-5558.	1.1	10
7475	A DFT-D study on the electrochromic mechanism of ruthenium sulfoxide complexes. <i>RSC Advances</i> , 2014, 4, 45635-45640.	1.7	8
7476	C^N -Cyclometalated Platinum(II) Complexes with Sterically Demanding 1,2-Diarylimidazole Ligands. <i>Organometallics</i> , 2014, 33, 3464-3473.	1.1	22

#	ARTICLE	IF	CITATIONS
7477	Theoretical studies on the structures and detonation properties of nitro derivatives of symmetric benzo-dicycloureas. <i>Canadian Journal of Chemistry</i> , 2014, 92, 803-808.	0.6	4
7478	Exploring the Conformational Space of Cysteine by Matrix Isolation Spectroscopy Combined with Near-Infrared Laser Induced Conformational Change. <i>Journal of Physical Chemistry B</i> , 2014, 118, 2093-2103.	1.2	23
7479	Comparative study of Gaussian basis sets for calculation of core electron binding energies in first-row hydrides and glycine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	12
7480	NO adsorption and transformation on the BaO surfaces from density functional theory calculations. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
7481	Computational Investigation of [FeFe]-Hydrogenase Models: Characterization of Singly and Doubly Protonated Intermediates and Mechanistic Insights. <i>Inorganic Chemistry</i> , 2014, 53, 10301-10311.	1.9	30
7482	Synthesis and characterization of 5-amino-1,3,6-trinitro-1H-benzo[d]imidazol-2(3H)-one as an energetic material. <i>RSC Advances</i> , 2014, 4, 42215-42219.	1.7	1
7483	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic H ₂ Evolution. <i>Inorganic Chemistry</i> , 2014, 53, 10094-10100.	1.9	79
7484	Dipole-Mediated Rectification of Intramolecular Photoinduced Charge Separation and Charge Recombination. <i>Journal of the American Chemical Society</i> , 2014, 136, 12966-12973.	6.6	48
7485	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	56
7486	Calculation of the two-dimensional non-separable partition function for two molecular systems. <i>Journal of Molecular Modeling</i> , 2014, 20, 2190.	0.8	6
7487	A computational study on 4,7-di(furan-2-yl)benzo[c][1,2,5]thiadiazole monomer and its oligomers. <i>Journal of Molecular Modeling</i> , 2014, 20, 2269.	0.8	9
7488	Fingerprints in IR OH vibrational spectra of H ₂ O clusters from different H-bond conformations by means of quantum-chemical computations. <i>Journal of Molecular Modeling</i> , 2014, 20, 2281.	0.8	12
7489	Synthesis, Characterization, Self-Assembly, Gelation, Morphology and Computational Studies of Alkynylgold(III) Complexes of 2,6-Bis(benzimidazol-2-yl)pyridine Derivatives. <i>Chemistry - A European Journal</i> , 2014, 20, 9930-9939.	1.7	33
7490	Proton-Coupled Electron Transfer in Molecular Electrocatalysis: Theoretical Methods and Design Principles. <i>Inorganic Chemistry</i> , 2014, 53, 6427-6443.	1.9	163
7491	The cavity electromagnetic field within the polarizable continuum model of solvation: An application to the real-time time dependent density functional theory. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 112-119.	1.1	19
7492	Mechanistic Insight into the (NHC)copper(I)-Catalyzed Hydrosilylation of Ketones. <i>Organometallics</i> , 2014, 33, 1953-1963.	1.1	70
7493	C- and N-Coupled Dimers of 2-Aminotetraphenylporphyrins: Regiocontrolled Synthesis, Spectroscopic Properties, and Quantum-Chemical Calculations. <i>Chemistry - A European Journal</i> , 2014, 20, 3998-4006.	1.7	26
7494	Identifying atomic sites in N-doped pristine and defective graphene from ab initio core level binding energies. <i>Carbon</i> , 2014, 76, 155-164.	5.4	14

#	ARTICLE	IF	CITATIONS
7495	Ligand-Assisted Acyl Migration in Au-Catalyzed Isomerization of Propargylic Ester to Diketone: A DFT Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 5652-5663.	1.7	17
7496	Synthesis and photochromism of a spirooxazine derivative featuring a carbazole moiety: Fast thermal bleaching and excellent fatigue resistance. <i>Dyes and Pigments</i> , 2014, 107, 174-181.	2.0	19
7497	Tunable Fictitious Substituent Effects on the π - π^* Interactions of Substituted Sandwich Benzene Dimers. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3344-3350.	1.1	9
7498	Affinity of HIV-1 antibody 2G12 with monosaccharides: A theoretical study based on explicit and implicit water models. <i>Computational Biology and Chemistry</i> , 2014, 49, 36-44.	1.1	8
7499	Molecular properties of excited electronic state: Formalism, implementation, and applications of analytical second energy derivatives within the framework of the time-dependent density functional theory/molecular mechanics. <i>Journal of Chemical Physics</i> , 2014, 140, 18A506.	1.2	11
7500	Standard molar enthalpy of formation of methoxyacetophenone isomers. <i>Journal of Chemical Thermodynamics</i> , 2014, 74, 22-31.	1.0	11
7501	Radioiodinated Benzyloxybenzene Derivatives: A Class of Flexible Ligands Target to β -Amyloid Plaques in Alzheimer's Brains. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 6030-6042.	2.9	34
7502	Spectroelectrochemical and DFT Study of Thiourea Adsorption on Gold Electrodes in Acid Media. <i>Journal of Physical Chemistry C</i> , 2014, 118, 19070-19084.	1.5	17
7503	New Insights into the Adsorption of Aurocyanide Ion on Activated Carbon Surface: Electron Microscopy Analysis and Computational Studies Using Fullerene-like Models. <i>Langmuir</i> , 2014, 30, 7703-7709.	1.6	11
7504	A concise method to prepare linear 2,3-diazaoligoacene derivatives. <i>Tetrahedron Letters</i> , 2014, 55, 4346-4349.	0.7	17
7505	Mechanism of Cu/Pd-Catalyzed Decarboxylative Cross-Couplings: A DFT Investigation. <i>Journal of the American Chemical Society</i> , 2014, 136, 10007-10023.	6.6	88
7506	Design and Synthesis of Bipyridine Platinum(II) Bisalkynyl Fullerene Donor-Acceptor Triads with Ultrafast Charge Separation. <i>Journal of the American Chemical Society</i> , 2014, 136, 10041-10052.	6.6	82
7507	Intermolecular interactions between a Ru complex and organic dyes in cosensitized solar cells: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16166.	1.3	12
7508	Cationic Half-Sandwich Iron(II) and Iron(III) Complexes with N-Heterocyclic Carbene Ligands. <i>Organometallics</i> , 2014, 33, 5670-5677.	1.1	31
7509	Nature of Zr-Monosubstituted Monomeric and Dimeric Polyoxometalates in Water Solution at Different pH Conditions: Static Density Functional Theory Calculations and Dynamic Simulations. <i>Inorganic Chemistry</i> , 2014, 53, 778-786.	1.9	22
7510	A Practical Computational Approach to Study Molecular Instability Using the Pseudo-Jahn-Teller Effect. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1824-1833.	2.3	17
7511	Lead-iodide nanowire perovskite with methylviologen showing interfacial charge-transfer absorption: a DFT analysis. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17955-17959.	1.3	23
7512	Electronic Structures of Platinum(II) Complexes with 2-Arylpyridine and 1,3-Diketone Ligands: A Relativistic Density Functional Study on Photoexcitation and Phosphorescent Properties. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12443-12449.	1.5	10

#	ARTICLE	IF	CITATIONS
7513	Tailoring fluorescent strigolactones for in vivo investigations: a computational and experimental study. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2960-2968.	1.5	28
7514	Novel dihydrate formation in p-nitrophenylglyoxal. <i>Structural Chemistry</i> , 2014, 25, 1513-1520.	1.0	2
7515	Wavefunction and reactivity study of benzo[a]pyrene diol epoxide and its enantiomeric forms. <i>Structural Chemistry</i> , 2014, 25, 1521-1533.	1.0	370
7516	A density functional study of oxorhenium(V) complexes incorporating quinoline or isoquinoline carboxylic acids: structural, spectroscopic, and electronic properties. <i>Structural Chemistry</i> , 2014, 25, 1607-1623.	1.0	4
7517	Thermal Proton Transfer Reactions in Ultraviolet Matrix-Assisted Laser Desorption/Ionization. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 310-318.	1.2	54
7518	Brightly Luminescent Pt(II) Pincer Complexes with a Sterically Demanding Carboranyl-Phenylpyridine Ligand: A New Material Class for Diverse Optoelectronic Applications. <i>Journal of the American Chemical Society</i> , 2014, 136, 9637-9642.	6.6	165
7519	Electrochemical Solvent Reorganization Energies in the Framework of the Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2091-2102.	2.3	43
7520	Theoretical investigation of triphenylamine-based sensitizers with different π -spacers for DSSC. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 118, 1144-1151.	2.0	46
7521	Assignment of the Absolute Configuration and Total Synthesis of (+)-Caripyrin. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 4780-4784.	1.2	9
7522	Incorporating Cobalt Carbonyl Moieties onto Ethynylthiophene-Based Dithienylcyclopentene Switches. 1. Photochemistry. <i>Organometallics</i> , 2014, 33, 447-456.	1.1	15
7523	Role of Triplet States of Two Different Ligands in the Sensitized Emission of Ln ^{III} (Eu ^{III} , Tb ^{III}) in d ^f Hybrid Tetranuclear Heterometal (Zn ^{II} Ln ^{III}) ₂ . <i>Journal of the American Chemical Society</i> , 2014, 2014, 3101-3113.	1.5	30
7524	Rational design of catalysts for asymmetric diamination reaction using transition state modeling. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 2745-2753.	1.5	30
7525	The Protonation State of Catalytic Residues in the Resting State of KasA Revisited: Detailed Mechanism for the Activation of KasA by Its Own Substrate. <i>Biochemistry</i> , 2014, 53, 919-931.	1.2	11
7526	Origin of Red Shift in the Photoabsorption Peak in MEH-PPV Polymer. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13444-13450.	1.5	14
7527	Reducing CO ₂ to Methanol Using Frustrated Lewis Pairs: On the Mechanism of Phosphine-Borane-Mediated Hydroboration of CO ₂ . <i>Journal of the American Chemical Society</i> , 2014, 136, 10708-10717.	6.6	204
7528	Implementation of the diagonalization-free algorithm in the self-consistent field procedure within the four-component relativistic scheme. <i>Journal of Computational Chemistry</i> , 2014, 35, 1725-1737.	1.5	8
7529	Deep Red Phosphorescence of Cyclometalated Iridium Complexes by <i>o</i> -Carborane Substitution. <i>Inorganic Chemistry</i> , 2014, 53, 128-138.	1.9	99
7530	Theoretical assessment of the photosensitization mechanisms of porphyrin-ruthenium(II) complexes for the formation of reactive oxygen species. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 294, 68-74.	2.0	10

#	ARTICLE	IF	CITATIONS
7531	Photophysical Properties of Ruthenium(II) Polypyridyl DNA Intercalators: Effects of the Molecular Surroundings Investigated by Theory. <i>Chemistry - A European Journal</i> , 2014, 20, 12901-12909.	1.7	54
7532	C σ -H Bond Activation with Triel Metals: Indium and Gallium Zwitterions through Internal Hydride Abstraction in Rigid Salan Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 7706-7717.	1.7	8
7533	Structure and Stability of Lithium Superoxide Clusters and Relevance to Li ⁺ O ₂ Batteries. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 813-819.	2.1	74
7534	QM/MM-MD Simulations of Conjugated Polyelectrolytes: A Study of Luminescent Conjugated Oligothiophenes for Use as Biophysical Probes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3419-3428.	1.1	26
7535	Iron Catalysts Containing Amine(imine)diphosphine P-NH-N-P Ligands Catalyze both the Asymmetric Hydrogenation and Asymmetric Transfer Hydrogenation of Ketones. <i>Organometallics</i> , 2014, 33, 5791-5801.	1.1	94
7536	The Transmetalation Process in Suzuki-Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. <i>ChemCatChem</i> , 2014, 6, 3132-3138.	1.8	68
7537	Optimal Composition of Atomic Orbital Basis Sets for Recovering Static Correlation Energies. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2138-2148.	1.1	5
7538	Excited States of a Significantly Ruffled Porphyrin: Computational Study on Structure-Induced Rapid Decay Mechanism via Intersystem Crossing. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4184-4194.	1.1	18
7539	Determination of the Absolute Configuration of Perylene Quinone-Derived Mycotoxins by Measurement and Calculation of Electronic Circular Dichroism Spectra and Specific Rotations. <i>Chemistry - A European Journal</i> , 2014, 20, 11463-11470.	1.7	24
7540	Substrate-Dependent Mechanisms for the Gold(I)-Catalyzed Cycloisomerization of Silyl-Tethered Enynes: A Computational Study. <i>Organometallics</i> , 2014, 33, 4230-4239.	1.1	16
7541	How Sugars Pucker: Electronic Structure Calculations Map the Kinetic Landscape of Five Biologically Paramount Monosaccharides and Their Implications for Enzymatic Catalysis. <i>Journal of the American Chemical Society</i> , 2014, 136, 1008-1022.	6.6	134
7542	Coordinatively Unsaturated T-Shaped Platinum(II) Complexes Stabilized by Small N-Heterocyclic Carbene Ligands. <i>Synthesis and Cyclometalation. Organometallics</i> , 2014, 33, 3746-3756.	1.1	22
7543	Chromatographic Separation and Assignment of Absolute Configuration of Hydroxywarfarin Isomers. <i>Chirality</i> , 2014, 26, 95-101.	1.3	22
7544	Peptide Bond Formation via Glycine Condensation in the Gas Phase. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8583-8590.	1.2	17
7545	Elucidating Molecular Structures of Nonalkylated and Short-Chain Alkyl (<i>n</i> ≤ 5). <i>Tj ETQqO O O r g B T / O v e r l o c k 10 T f 50 192 T d ((</i>	3.2	53
7546	Mobility and Ultrahigh-Resolution Mass Spectrometries and Theoretical Collisional Cross-Section Calculations. <i>Analytical Chemistry</i> , 2014, 86, 3300-3307.	1.1	11
7547	Toward Enabling Large-Scale Open-Shell Equation-of-Motion Coupled Cluster Calculations: Triplet States of \dot{I}^2 -Carotene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9087-9093.	1.1	11
7547	The Lineshape of the Electronic Spectrum of the Green Fluorescent Protein Chromophore, Part I: Gas Phase. <i>ChemPhysChem</i> , 2014, 15, 3236-3245.	1.0	16
7548	Mechanism of N-H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium(I). <i>Organometallics</i> , 2014, 33, 715-721.	1.1	26

#	ARTICLE	IF	CITATIONS
7549	A Macrocyclic Chelator with Unprecedented Th ⁴⁺ Affinity. <i>Journal of the American Chemical Society</i> , 2014, 136, 9106-9115.	6.6	26
7550	Silver-Catalyzed Functionalization of Esters by Carbene Transfer: The Role of Ylide Zwitterionic Intermediates. <i>ChemCatChem</i> , 2014, 6, 2206-2210.	1.8	22
7551	Accurate Prediction of Hyperfine Coupling Constants in Muoniated and Hydrogenated Ethyl Radicals: <i>Ab Initio</i> Path Integral Simulation Study with Density Functional Theory Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2005-2015.	2.3	17
7552	The glycation site specificity of human serum transferrin is a determinant for transferrin's functional impairment under elevated glycaemic conditions. <i>Biochemical Journal</i> , 2014, 461, 33-42.	1.7	17
7553	Engineering Topochemical Polymerizations Using Block Copolymer Templates. <i>Journal of the American Chemical Society</i> , 2014, 136, 13381-13387.	6.6	65
7554	Synthesis, Characterization, and Reactivity of Furan- and Thiophene-Functionalized Bis(N-heterocyclic) Tj ETQq1 1 0,784314 rgBT /Over	1.9	15
7555	Properties and reactivities of nonheme iron(IV)=O versus iron(V)=O: long-range electron transfer versus hydrogen atom abstraction. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22611-22622.	1.3	7
7556	Enlarging the π System of Phosphorescent (C [*]) Cyclometalated Platinum(II) NHC Complexes. <i>Inorganic Chemistry</i> , 2014, 53, 6346-6356.	1.9	78
7557	1,3- β -Silyl-elimination in electron-deficient cationic systems. <i>Chemical Science</i> , 2014, 5, 3983.	3.7	20
7558	Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1164-1171.	2.3	48
7559	Dimetal hydride generated from dimetalated glycine: Formation mechanism and electronic structure. <i>International Journal of Mass Spectrometry</i> , 2014, 363, 32-39.	0.7	4
7560	Strychnobailonine, an Unsymmetrical Bisindole Alkaloid with an Unprecedented Skeleton from <i>Strychnos icaja</i> Roots. <i>Journal of Natural Products</i> , 2014, 77, 1078-1082.	1.5	19
7561	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. <i>Nature Chemistry</i> , 2014, 6, 623-628.	6.6	198
7562	Electron Localization Function Study on the Chemical Bonding in a Real Space for Tetrahedrane, Cubane, Adamantane, and Dodecahedrane and Their Perfluorinated Derivatives and Radical Anions. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4147-4156.	1.1	15
7563	Direct Dynamics Simulation of the Activation and Dissociation of 1,5-Dinitrobiuret (HDNB). <i>Journal of Physical Chemistry A</i> , 2014, 118, 2228-2236.	1.1	12
7564	Experimental and theoretical characterisation of phosphorescence from rhenium polypyridyl tricarbonyl complexes. <i>Polyhedron</i> , 2014, 67, 505-512.	1.0	20
7565	Terphenyl Complexes of Molybdenum and Tungsten with Quadruple Metal-Metal Bonds and Bridging Carboxylate Ligands. <i>Journal of the American Chemical Society</i> , 2014, 136, 9173-9180.	6.6	21
7566	Reaction pathways and roles of N-alkylmorpholine in Amine-alane transamination: A mechanistic study. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 5003-5009.	3.8	1

#	ARTICLE	IF	CITATIONS
7567	A new platinum complex with tryptophan: Synthesis, structural characterization, DFT studies and biological assays in vitro over human tumorigenic cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 209-215.	2.0	10
7568	Theoretical study of cellobiose hydrolysis to glucose in ionic liquids. <i>Chemical Physics Letters</i> , 2014, 603, 7-12.	1.2	26
7569	Substituent effects on electronic structure and spectral property of Zn(II) complexes based on the OONX ligands: DFT and TDDFT theoretical studies. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2014, 192, 7-12.	0.8	0
7570	Convergence of environment polarization effects in multiscale modeling of excitation energies. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 304-311.	1.1	36
7571	Structures, molecular orbitals and UV-vis spectra investigations on methyl 1-benzyl-1H-1,2,3-triazole-4-carboxylate: A computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 268-273.	2.0	3
7572	Ammonia and hydrazine synthesis from [N ₂ -W{(NHCH ₂ CH ₂) ₃ N}] and [AH]+[BH] ⁺ using Sivasankar catalytic cycle: DFT studies. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 73-78.	1.1	9
7573	Theoretical investigations of the structures and electronic spectra of Zn(II) and Ni(II) complexes with cyclohexylamine-N-dithiocarbamate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 122, 283-287.	2.0	10
7574	Mechanism of Mo-catalyzed C-S cleavage of thiophene. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 275-286.	0.8	5
7575	Ordered phases of ethylene adsorbed on charged fullerenes and their aggregates. <i>Carbon</i> , 2014, 69, 206-220.	5.4	14
7576	Effects of the basis set and of the exchange-correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 119, 34-41.	2.0	4
7577	Asymmetric hydrolytic kinetic resolution with recyclable polymeric Co(salen) complexes: a practical strategy in the preparation of (S)-metoprolol, (S)-toliprolol and (S)-alprenolol: computational rationale for enantioselectivity. <i>Catalysis Science and Technology</i> , 2014, 4, 3899-3908.	2.1	9
7578	Drug release by pH-responsive molecular tweezers: Atomistic details from molecular modeling. <i>Journal of Computational Chemistry</i> , 2014, 35, 1545-1551.	1.5	2
7579	Pyridinium-Fused Pyridinone: A Novel Turn-on-Fluorescent Chemodosimeter for Cyanide. <i>Chemistry - an Asian Journal</i> , 2014, 9, 121-125.	1.7	31
7580	25th Anniversary Article: Isoindigo-Based Polymers and Small Molecules for Bulk Heterojunction Solar Cells and Field Effect Transistors. <i>Advanced Materials</i> , 2014, 26, 1801-1826.	11.1	330
7581	Mechanism for Activation of the C≡N Bond of Nitriles by a Cationic CpRh ^{III} -Silyl Complex: A Systematic DFT Study. <i>Organometallics</i> , 2014, 33, 3030-3039.	1.1	17
7582	Tuning Excited States of Bipyridyl Platinum(II) Chromophores with π -Bonded Catecholate Organometallic Ligands: Synthesis, Structures, TD-DFT Calculations, and Photophysical Properties. <i>Inorganic Chemistry</i> , 2014, 53, 6624-6633.	1.9	26
7583	Understanding $\hat{1},\hat{1}^2$ -Unsaturated Imine Formation from Amine Additions to $\hat{1},\hat{1}^2$ -Unsaturated Aldehydes and Ketones: An Analytical and Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2014, 79, 5163-5172.	1.7	43
7584	Mechanism, Reactivity, and Selectivity in Rh(III)-Catalyzed Phosphoryl-Directed Oxidative C-H Activation/Cyclization: A DFT Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 5074-5081.	1.7	45

#	ARTICLE	IF	CITATIONS
7585	Effect of the Meso-Substituent in the Hückel-to-Möbius Topological Switches. <i>Journal of Organic Chemistry</i> , 2014, 79, 5036-5046.	1.7	27
7586	[4 + 2] Cycloaddition Reaction To Approach Diazatwistpentacenes: Synthesis, Structures, Physical Properties, and Self-assembly. <i>Journal of Organic Chemistry</i> , 2014, 79, 4438-4445.	1.7	72
7587	Anisotropic Dissymmetry Factor, $\langle i \rangle_g \langle i \rangle$: Theoretical Investigation on Single Molecule Chiroptical Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5046-5057.	1.1	61
7588	Theoretical Study of the Photochemical Initiation in Nitroxide-Mediated Photopolymerization. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4464-4470.	1.1	12
7589	Chemo-, Regio-, and Stereoselective Silver-Catalyzed Aziridination of Dienes: Scope, Mechanistic Studies, and Ring-Opening Reactions. <i>Journal of the American Chemical Society</i> , 2014, 136, 5342-5350.	6.6	89
7590	Quantum mechanical/effective fragment potential (QM/EFP) study of phosphate diester cleavage in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 5-12.	1.1	3
7591	2-Diphenylaminothiophene as the donor of porphyrin sensitizers for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2014, 38, 3227-3235.	1.4	47
7592	Chloride Ion-Aided Self-Assembly of Pseudocathrocholate Metal Tris-pyrazoloximates. <i>Inorganic Chemistry</i> , 2014, 53, 3062-3071.	1.9	30
7593	Catalytic C6 Functionalization of 2,3-Disubstituted Indoles by Scandium Triflate. <i>Journal of Organic Chemistry</i> , 2014, 79, 1047-1054.	1.7	71
7594	Urea-Catalyzed N-H Insertion Arylation Reactions of Nitrodiazoesters. <i>Journal of Organic Chemistry</i> , 2014, 79, 4832-4842.	1.7	24
7595	Theoretical Elucidation of the Mechanism of the Cycloaddition between Nitrone Ylides and Electron-Deficient Alkenes. <i>Journal of Organic Chemistry</i> , 2014, 79, 2189-2202.	1.7	15
7596	Combined Experimental and Computational Investigations of Rhodium- and Ruthenium-Catalyzed C-H Functionalization of Pyrazoles with Alkynes. <i>Journal of Organic Chemistry</i> , 2014, 79, 1954-1970.	1.7	75
7597	Quantification of Nonstatistical Dynamics in an Intramolecular Diels-Alder Cyclization without Trajectory Computation. <i>Journal of Organic Chemistry</i> , 2014, 79, 2368-2376.	1.7	15
7598	Identification of liquid-phase decomposition species and reactions for guanidinium azotetrazolate. <i>Thermochimica Acta</i> , 2014, 590, 51-65.	1.2	13
7599	Configurable photochromism of an unsymmetrical dithienylethene derivative by Cu ²⁺ ions or water. <i>Dyes and Pigments</i> , 2014, 111, 1-7.	2.0	15
7600	Catalytic Mechanisms of Direct Pyrrole Synthesis via Dehydrogenative Coupling Mediated by PNP-Ir or PNN-Ru Pincer Complexes: Crucial Role of Proton-Transfer Shuttles in the PNP-Ir System. <i>Journal of the American Chemical Society</i> , 2014, 136, 4974-4991.	6.6	171
7601	Modulating the Electronic Properties of Multimeric Thiophene Oligomers by Utilizing Carbon Nanotube Confinement. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5510-5522.	1.5	25
7602	Unravelling the S-O Linkage Photoisomerization Mechanisms in <i>cis</i> - and <i>trans</i> -[Ru(bpy) ₂ (DMSO) ₂] ²⁺ Using Density Functional Theory. <i>Inorganic Chemistry</i> , 2014, 53, 6752-6760.	1.9	32

#	ARTICLE	IF	CITATIONS
7603	Photochemistry of Chromium Arene Tricarbonyl Complexes with Tethered Pyridinyl and Propenyl Groups: Investigations of the Effect of Ring Size on Chelate Formation, Structure, and Linkage Isomerization. <i>Organometallics</i> , 2014, 33, 485-497.	1.1	14
7604	A Novel Square-Planar Ni(II) Complex with an Amino-Carboxamido-Dithiolato-Type Ligand as an Active-Site Model of NiSOD. <i>Inorganic Chemistry</i> , 2014, 53, 6512-6523.	1.9	29
7605	Site-specific polarizabilities from analytic linear-response theory. <i>Chemical Physics Letters</i> , 2014, 608, 24-27.	1.2	0
7606	A QSPR approach for the fast estimation of DFT/NBO partial atomic charges. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014, 134, 158-163.	1.8	20
7607	A theoretical study of temperature dependence of cluster formation from sulfuric acid and ammonia. <i>Chemical Physics</i> , 2014, 433, 60-66.	0.9	17
7608	New cyano-substituted organic dyes containing different electrophilic groups: aggregation-induced emission and large two-photon absorption cross section. <i>Tetrahedron</i> , 2014, 70, 7050-7056.	1.0	19
7609	A universal route to improving conjugated macromolecule photostability. <i>RSC Advances</i> , 2014, 4, 54919-54923.	1.7	23
7611	Syntheses of Geometrical Isomers for Comparison of Properties Caused by Steric and Electronic Effects in Carbonylruthenium(II) Complexes. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 1107-1115.	2.0	8
7612	Photochromic Reaction of Diarylethenes Having Phenol Moiety as an Aryl Ring. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 528-538.	2.0	16
7613	Theoretical Study on Intermolecular Interactions in Complexes of Cyclodextrins with Bile Acids: DFT and Ab Initio Fragment Molecular Orbital Calculations. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 258-266.	2.0	4
7614	Theoretical Study of the $\tilde{\epsilon} \rightarrow \tilde{\epsilon}^*$ Excited States of Oligoacenes: A Full $\tilde{\epsilon}$ -Valence DMRG-CASPT2 Study. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 1071-1073.	2.0	28
7615	A spectroscopic study of the optical properties of a nitrobenzoxadiazole derivative in solution: The role of specific interactions. <i>Chemical Physics Letters</i> , 2014, 610-611, 357-362.	1.2	3
7616	Iron(III)-Quantity-Dependent Aggregation-Dispersion Conversion of Functionalized Gold Nanoparticles. <i>Chemistry - A European Journal</i> , 2014, 20, 4032-4037.	1.7	17
7617	Low-energy elastic electron scattering from chloroethane, C ₂ H ₅ Cl. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 205202.	0.6	2
7618	PNOF5 calculations based on the ϵ -thermodynamic fragment energy method: C _n H _{2n+2} (n=1, 10) and (FH) _n (n=1, 8) as test cases. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	2
7619	Influence of Polarity and Activation Energy in Microwave-Assisted Organic Synthesis (MAOS). <i>ChemistryOpen</i> , 2015, 4, 308-317.	0.9	54
7620	Preliminary Characterization and In Vivo Studies of Structurally Identical ¹⁸ F- and ¹²⁵ I-Labeled Benzyloxybenzenes for PET/SPECT Imaging of β -Amyloid Plaques. <i>Scientific Reports</i> , 2015, 5, 12084.	1.6	14
7621	Quasipinning and selection rules for excitations in atoms and molecules. <i>Physical Review A</i> , 2015, 92, .	1.0	29

#	ARTICLE	IF	CITATIONS
7622	Ionization-site effects on the photofragmentation of chloro- and bromoacetic acid molecules. <i>Physical Review A</i> , 2015, 92, .	1.0	16
7623	A multi target approach to control chemical reactions in their inhomogeneous solvent environment. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 234003.	0.6	13
7624	Density Functional Theory Calculations for the Formation of Pentacoordinate Titanium α -Butoxide Derivatives. <i>Chemistry Letters</i> , 2015, 44, 1339-1341.	0.7	2
7625	Computational Studies of the Gas Phase Reactions of Ethers with Anions: Kinetic Barriers, Isotope Effects, Consecutive Eliminations and Site Selectivity. <i>European Journal of Mass Spectrometry</i> , 2015, 21, 141-147.	0.5	0
7626	Theoretical analysis of structures and electronic spectra in molecular cadmium chalcogenide clusters. <i>Journal of Chemical Physics</i> , 2015, 142, 234305.	1.2	18
7627	Analytic energy gradient of excited electronic state within TDDFT/MMpol framework: Benchmark tests and parallel implementation. <i>Journal of Chemical Physics</i> , 2015, 143, 134104.	1.2	25
7628	Spin-flip configuration interaction singles with exact spin-projection: Theory and applications to strongly correlated systems. <i>Journal of Chemical Physics</i> , 2015, 143, 144114.	1.2	27
7629	Design of exchange-correlation functionals through the correlation factor approach. <i>Journal of Chemical Physics</i> , 2015, 143, 144102.	1.2	30
7630	A study of potential energy curves from the model space quantum Monte Carlo method. <i>Journal of Chemical Physics</i> , 2015, 143, 214107.	1.2	20
7631	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. <i>Journal of Chemical Physics</i> , 2015, 143, 224107.	1.2	19
7632	Water network-mediated, electron-induced proton transfer in $[C_5H_5N \cdots (H_2O)_n]^+$ clusters. <i>Journal of Chemical Physics</i> , 2015, 143, 144305.	1.2	8
7633	The role of cytosine methylation on charge transport through a DNA strand. <i>Journal of Chemical Physics</i> , 2015, 143, 094306.	1.2	9
7634	Non-radiative relaxation of photoexcited chlorophylls: theoretical and experimental study. <i>Scientific Reports</i> , 2015, 5, 13625.	1.6	58
7635	On the use of different coordinate systems in mechanochemical force analyses. <i>Journal of Chemical Physics</i> , 2015, 143, 074118.	1.2	18
7636	Cross-strand disulfides in the non-hydrogen bonding site of antiparallel β -sheet (α CSDns): poised for biological switching. <i>RSC Advances</i> , 2015, 5, 86303-86321.	1.7	4
7637	A novel Gaussian-Sinc mixed basis set for electronic structure calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 064108.	1.2	11
7638	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. <i>Journal of Chemical Physics</i> , 2015, 143, 234103.	1.2	34
7639	Theoretical study on wettability of graphene/water interface. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	0

#	ARTICLE	IF	CITATIONS
7640	Iterative universal state selective correction for the Brillouin-Wigner multireference coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2015, 142, 114106.	1.2	6
7641	Chemical degradation mechanisms of membranes for alkaline membrane fuel cells. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	0
7642	Photodissociation at Various Wavelengths: Fragmentation Studies of Oxazine 170 Using Nanosecond Laser Pulses. <i>European Journal of Mass Spectrometry</i> , 2015, 21, 599-608.	0.5	4
7643	Fragment-based ¹³ C nuclear magnetic resonance chemical shift predictions in molecular crystals: An alternative to planewave methods. <i>Journal of Chemical Physics</i> , 2015, 143, 102809.	1.2	65
7644	Energetics, structure, and rovibrational spectroscopic properties of the sulfurous anions SNO ⁻ and OSN ⁻ . <i>Journal of Chemical Physics</i> , 2015, 143, 184301.	1.2	13
7645	Communication: Towards <i>ab initio</i> self-energy embedding theory in quantum chemistry. <i>Journal of Chemical Physics</i> , 2015, 143, 241102.	1.2	76
7646	Pseudo Jahn-Teller distortion for a tricyclic carbon sulfide (C ₆ S ₈) and its suppression in S-oxygenated dithiine (C ₄ H ₄ (SO ₂) ₂). <i>Chemical Physics</i> , 2015, 460, 101-105.	0.9	27
7647	Visualization of the four-component g-tensor density as a three-dimensional function. <i>Chemical Physics Letters</i> , 2015, 636, 46-50.	1.2	1
7648	Electronic and rovibrational quantum chemical analysis of C ₃ P ⁺ : the next interstellar anion?. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 453, 2825-2830.	1.6	13
7649	Tuning of the Electronic Properties of Armchair Graphene Nanoribbons through Functionalization: Theoretical Study of ¹ g _O ₂ Border Addition. <i>ChemPhysChem</i> , 2015, 16, 3030-3037.	1.0	2
7650	Nickel-Containing Keggin-Type Polyoxometalates as Hydrogen Evolution Catalysts: Photochemical Structure-Activity Relationships. <i>ChemPlusChem</i> , 2015, 80, 1389-1398.	1.3	45
7651	Application of a BOSS Gaussian interface for QM/MM simulations of H ₂ and methyl transfer reactions. <i>Journal of Computational Chemistry</i> , 2015, 36, 2064-2074.	1.5	12
7652	Experimentelle und theoretische Untersuchungen zur katalytischen asymmetrischen 4-Elektrocyclisierung von N-Heterocyclen. <i>Angewandte Chemie</i> , 2015, 127, 2801-2804.	1.6	15
7653	On the Critical Effect of the Metal (Mo vs. W) on the [3+2] Cycloaddition Reaction of M ₃ S ₄ Clusters with Alkynes: Insights from Experiment and Theory. <i>Chemistry - A European Journal</i> , 2015, 21, 14823-14833.	1.7	8
7655	Mechanistic Insights on the Iodine(III)-Mediated \hat{I}^{\pm} -Oxidation of Ketones. <i>Chemistry - A European Journal</i> , 2015, 21, 11206-11211.	1.7	64
7656	Controlled Redox Chemistry at Cerium within a Tripodal Nitroxide Ligand Framework. <i>Chemistry - A European Journal</i> , 2015, 21, 17850-17859.	1.7	50
7657	Asymmetric Base-Free Michael Addition at Room Temperature with Nickel-Based Bifunctional Amido-Functionalized N-Heterocyclic Carbene Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 1604-1615.	1.0	30
7658	Rh ^V -Nitrenoid as a Key Intermediate in Rh ^{III} -Catalyzed Heterocyclization by C ₁₂ H ₂ Activation: A Computational Perspective on the Cycloaddition of Benzamide and Diazo Compounds. <i>Chemistry - A European Journal</i> , 2015, 21, 9209-9218.	1.7	85

#	ARTICLE	IF	CITATIONS
7659	Preparation, Structural Determination, and Characterization of Electronic Properties of Bis-silylated and Bis-germylated Lu ₃ N@h-C ₈₀ . Chemistry - A European Journal, 2015, 21, 16411-16420.	1.7	13
7660	Effect of strain on gas-phase basicity of (E)-1-methyl-2-(1-methyl-2-adamantylidene)adamantane. Journal of Physical Organic Chemistry, 2015, 28, 447-451.	0.9	7
7661	Photochromic Dithienylethene-Containing Triarylborane Derivatives: Facile Approach to Modulate Photochromic Properties with Multi-addressable Functions. Chemistry - A European Journal, 2015, 21, 2182-2192.	1.7	31
7662	Highly Antiplasmodial Non-Natural Oxidative Products of Dioncophylline...A: Synthesis, Absolute Configuration, and Conformational Stability. Chemistry - A European Journal, 2015, 21, 14507-14518.	1.7	11
7663	Three-dimensional networks containing rectangular Sr ₄ and Ba ₄ units: Synthesis, structure, bonding, and potential application for Ne gas separation. International Journal of Quantum Chemistry, 2015, 115, 1501-1510.	1.0	6
7664	Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. Journal of Computational Chemistry, 2015, 36, 2158-2167.	1.5	10
7665	1,3-Butadienyl Dianions as Non-Innocent Ligands: Synthesis and Characterization of Aromatic Dilithio Rhodacycles. Angewandte Chemie - International Edition, 2015, 54, 9986-9990.	7.2	49
7666	Triesterase and Promiscuous Diesterase Activities of a Di-Co ^{II} -Containing Organophosphate Degrading Enzyme Reaction Mechanisms. Chemistry - A European Journal, 2015, 21, 3736-3745.	1.7	19
7667	Ruthenium(II) Complexes Containing Lutidine-Derived Pincer CNC Ligands: Synthesis, Structure, and Catalytic Hydrogenation of C≡N bonds. Chemistry - A European Journal, 2015, 21, 7540-7555.	1.7	49
7668	Extremely Facile Transformations of Tris(3,5-dimethylpyrazolyl)borate: a Bidentate Nitrogen Ligand and a C ₂ -Chiral Cation. European Journal of Inorganic Chemistry, 2015, 2015, 3232-3235.	1.0	2
7669	Mechanism of Thioether Oxidation over Di- and Tetrameric Ti and Ti-Containing Polyoxometalates. Chemistry - A European Journal, 2015, 21, 14496-14506.	1.7	27
7670	Synthesis and Photophysical, Electrochemical and Theoretical Study of Thiazole-Annulated Phthalocyanines. European Journal of Organic Chemistry, 2015, 2015, 7053-7068.	1.2	5
7671	Functionalization of C _n H _{2n+2} Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbon-Hydrogen Bonds. ChemCatChem, 2015, 7, 3254-3260.	1.8	23
7672	Microwave-Assisted Organocatalyzed Rearrangement of Propargyl Vinyl Ethers to Salicylaldehyde Derivatives: An Experimental and Theoretical Study. Chemistry - A European Journal, 2015, 21, 18280-18289.	1.7	14
7673	Theoretical Studies on the Asymmetric Baeyer-Villiger Oxidation Reaction of 4-Phenylcyclohexanone with m-CPBA Catalyzed by Chiral Scandium(III)-Dioxide Complexes. Chemistry - A European Journal, 2015, 21, 7264-7277.	1.7	16
7674	Synthesis of an Iridium Peroxido Complex and Its Reactivity Towards Brønsted Acids. European Journal of Inorganic Chemistry, 2015, 2015, 3157-3168.	1.0	10
7675	A Comparative Study of the Redox-Induced Linkage Isomerization of Ruthenium and Osmium Complexes. European Journal of Inorganic Chemistry, 2015, 2015, 5074-5080.	1.0	3
7676	A CASSCF/CASPT2 insight into excited-state intramolecular proton transfer of four imidazole derivatives. Journal of Computational Chemistry, 2015, 36, 2374-2380.	1.5	35

#	ARTICLE	IF	CITATIONS
7677	Contrasting electronic requirements for C≡H binding and C≡H activation in d ⁶ sandwich complexes of rhenium and tungsten. <i>Journal of Computational Chemistry</i> , 2015, 36, 1818-1830.	1.5	8
7678	Photomagnetic and nonlinear optical properties in <i>cis-trans</i> green fluoroprotein chromophore coupled Bis- <i>imino</i> nitroxide diradicals. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1561-1572.	1.0	12
7679	Mechanistic study on lowering the sensitivity of positive atmospheric pressure photoionization mass spectrometric analyses: size-dependent reactivity of solvent clusters. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 2095-2101.	0.7	16
7680	Assessment of Density-Functional Tight-Binding Ionization Potentials and Electron Affinities of Molecules of Interest for Organic Solar Cells Against First-Principles GW Calculations. <i>Computation</i> , 2015, 3, 616-656.	1.0	19
7681	On the Dehydrocoupling of Alkenylacetylenes Mediated by Various Samarocene Complexes: A Charming Story of Metal Cooperativity Revealing a Novel Dual Metal σ -Bond Metathesis Type of Mechanism (DM σ -BM). <i>Inorganics</i> , 2015, 3, 573-588.	1.2	2
7682	Metathetical Redox Reaction of (Diacetoxiido)arenes and Iodoarenes. <i>Molecules</i> , 2015, 20, 22635-22644.	1.7	20
7683	The Fourier Space Restricted Hartree-Fock Method for the Electronic Structure Calculation of One-Dimensionally Periodic Systems. <i>Advances in Quantum Chemistry</i> , 2015, 71, 153-194.	0.4	0
7684	Copper-Catalyzed Eglinton Oxidative Homocoupling of Terminal Alkynes: A Computational Study. <i>Journal of Chemistry</i> , 2015, 2015, 1-8.	0.9	11
7685	Electronic Structure and Circular Dichroism of Natural Alboatisins Isolated from Aerial Parts of <i>Isodon Albovillosus</i> : DFT and TDDFT Study. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 695-702.	0.6	4
7686	One and Multiple Bonds Interatomic Spin-Spin Coupling in σ -Cymene Ru(II) of 3,5-Dimethyl-, 3,5-Dicarboxylic-, and 5-Phenyl-pyrazole Derivatives. <i>Journal of Spectroscopy</i> , 2015, 2015, 1-11.	0.6	103
7687	Novel imidazolium and imidazolinium salts containing the 9-nickelafluorenyl anion synthesis, structures and reactivity. <i>Dalton Transactions</i> , 2015, 44, 7169-7176.	1.6	8
7688	Efficient electronic structure calculation for molecular ionization dynamics at high x-ray intensity. <i>Structural Dynamics</i> , 2015, 2, 041707.	0.9	47
7689	Electrochemical and Spectroelectrochemical Studies of Diphosphorylated Metalloporphyrins. Generation of a Phlorin Anion Product. <i>Inorganic Chemistry</i> , 2015, 54, 3501-3512.	1.9	46
7690	Mechanistic Investigations of the AuCl ₃ -Catalyzed Nitrene Insertion into an Aromatic C-H Bond of Mesitylene. <i>Journal of Organic Chemistry</i> , 2015, 80, 5795-5803.	1.7	10
7691	Density Functional Theory Based Analysis of Photoinduced Electron Transfer in a Triazacryptand Based K ⁺ Sensor. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2902-2907.	1.1	31
7692	Kinetics and Thermodynamics of the Reaction between the HO^\bullet Radical and Adenine: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6516-6527.	1.1	21
7693	A computational study of the effects of ancillary ligands on copper(σ) π -ethylene interaction. <i>New Journal of Chemistry</i> , 2015, 39, 5410-5419.	1.4	12
7694	Tethered Bisadducts of C ₆₀ and C ₇₀ with Addends on a Common Hexagonal Face and a 12-Membered Hole in the Fullerene Cage. <i>Journal of the American Chemical Society</i> , 2015, 137, 7502-7508.	6.6	54

#	ARTICLE	IF	CITATIONS
7695	Extremely strong organic-metal oxide electronic coupling caused by nucleophilic addition reaction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16285-16293.	1.3	16
7696	Binding to gold nanoclusters alters the hydrogen bonding interactions and electronic properties of canonical and size-expanded DNA base pairs. <i>RSC Advances</i> , 2015, 5, 49408-49419.	1.7	9
7697	Microwave-assisted large scale synthesis of lanthanide metal-organic frameworks (Ln-MOFs), having a preferred conformation and photoluminescence properties. <i>Dalton Transactions</i> , 2015, 44, 11954-11962.	1.6	70
7698	Synthesis, luminescence and electrochemical properties of luminescent dinuclear mixed-valence gold complexes with alkynyl bridges. <i>Inorganic Chemistry Frontiers</i> , 2015, 2, 453-466.	3.0	7
7699	Efficient halogen photoelimination from dibromo, dichloro and difluoro tellurophenes. <i>Dalton Transactions</i> , 2015, 44, 2092-2096.	1.6	53
7700	Origin of Fast Catalysis in Allylic Amination Reactions Catalyzed by Pd-Ti Heterobimetallic Complexes. <i>Journal of the American Chemical Society</i> , 2015, 137, 7371-7378.	6.6	49
7701	Aryl-substituted organomolybdenum(ii) complexes as olefin epoxidation catalysts. <i>Catalysis Science and Technology</i> , 2015, 5, 4772-4777.	2.1	9
7702	Molecular dynamic studies of amyloid-beta interactions with curcumin and Cu ²⁺ ions. <i>Chemical Papers</i> , 2015, 69, .	1.0	16
7703	Near IR Emitting Red-Shifting Ratiometric Fluorophores Based on Borondipyrromethene. <i>Organic Letters</i> , 2015, 17, 3022-3025.	2.4	54
7704	Effect of phenylamine moiety on the structure, optical properties, and phosphorescence efficiencies of some red-emitting iridium(III) complexes: A theoretical study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015, 311, 85-94.	2.0	7
7705	On the interaction between gold and silver metal atoms and DNA/RNA nucleobases - a comprehensive computational study of ground state properties. <i>Nanotechnology Reviews</i> , 2015, 4, 173-191.	2.6	23
7706	Utilizing alkoxyphenyl substituents for side-chain engineering of efficient benzo[1,2-b:4,5-b']dithiophene-based small molecule organic solar cells. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17391-17398.	1.3	24
7707	The performance of low-cost commercial cloud computing as an alternative in computational chemistry. <i>Journal of Computational Chemistry</i> , 2015, 36, 926-933.	1.5	18
7708	Fused thiophene and its periphery fluorinated substitution derivatives: a theoretical study for organic semiconductors. <i>Semiconductor Science and Technology</i> , 2015, 30, 065002.	1.0	2
7709	Location and Electronic Nature of Phosphorus in the Si Nanocrystal - SiO ₂ System. <i>Scientific Reports</i> , 2015, 5, 9702.	1.6	61
7710	A theoretical investigation on the metal-metal interaction in a series of pyrazolate bridged platinum(II) complexes. <i>Synthetic Metals</i> , 2015, 205, 222-227.	2.1	12
7711	Hydroxyl and amino functionalized cyclometalated Ir(III) complexes: Synthesis, characterization and cytotoxicity studies. <i>Journal of Organometallic Chemistry</i> , 2015, 791, 175-182.	0.8	18
7712	Effect of water on carbonation of mineral aerosol surface models of kaolinite: a density functional theory study. <i>Environmental Earth Sciences</i> , 2015, 73, 7053-7060.	1.3	12

#	ARTICLE	IF	CITATIONS
7713	Spectroscopic characterization and molecular modeling of novel palladium(II) complexes with carbazates and hydrazides. <i>Journal of Molecular Structure</i> , 2015, 1097, 15-22.	1.8	22
7714	Explorations of the solubilizing effectiveness of CH ₃ OCH ₂ CH ₂ O substituents in the photocyclizations of some 1,2-diarylethylenes to [n]phenacenes. <i>Tetrahedron Letters</i> , 2015, 56, 3342-3345.	0.7	1
7715	Application of the embedding potential method in calculations of the electronic structure and X-ray emission spectra of crystal MgO clusters. <i>Optics and Spectroscopy (English Translation of Optika i Tj ETQq0 0 0 rgBT/Overlap 10 Tf 5</i>	0.2	0
7716	Computational exploration of the gas adsorption on the iron tetracarboxylate metal-organic framework MIL-102. <i>Molecular Simulation</i> , 2015, 41, 1357-1370.	0.9	14
7717	Studies on an on/off-switchable immunosensor for troponin T. <i>Biosensors and Bioelectronics</i> , 2015, 73, 100-107.	5.3	22
7718	Impact of Coordination Geometry, Bite Angle, and Trans Influence on Metal-Ligand Covalency in Phenyl-Substituted Phosphine Complexes of Ni and Pd. <i>Inorganic Chemistry</i> , 2015, 54, 5646-5659.	1.9	31
7719	Activation and Oxidation of Mesitylene C-H Bonds by (Phebox)Iridium(III) Complexes. <i>Organometallics</i> , 2015, 34, 2879-2888.	1.1	18
7720	Converging nuclear magnetic shielding calculations with respect to basis and system size in protein systems. <i>Journal of Biomolecular NMR</i> , 2015, 62, 327-340.	1.6	47
7721	On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C ₆₀) with Organoboron Compounds in the Presence of Water. <i>ChemistryOpen</i> , 2015, 4, 774-778.	0.9	12
7722	Freezing the Bioactive Conformation to Boost Potency: The Identification of BAY8501, a Selective and Potent Inhibitor of Human Neutrophil Elastase for Pulmonary Diseases. <i>ChemMedChem</i> , 2015, 10, 1163-1173.	1.6	56
7723	Synthesis of Ethers via Reaction of Carbanions and Monoperoxyacetals. <i>Journal of Organic Chemistry</i> , 2015, 80, 12100-12114.	1.7	47
7724	Conformational gating of DNA conductance. <i>Nature Communications</i> , 2015, 6, 8870.	5.8	75
7725	Open-Ended Recursive Calculation of Single Residues of Response Functions for Perturbation-Dependent Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4814-4824.	2.3	5
7726	The antiradical activity of some selected flavones and flavonols. Experimental and quantum mechanical study. <i>Journal of Molecular Modeling</i> , 2015, 21, 307.	0.8	56
7727	Fluorescence from an H-aggregated naphthalenediimide based peptide: photophysical and computational investigation of this rare phenomenon. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30398-30403.	1.3	40
7728	Thermal Isomerizations of Diethynyl Cyclobutadienes and Implications for Fullerene Formation. <i>Journal of Organic Chemistry</i> , 2015, 80, 11863-11868.	1.7	5
7729	Energy Alignment of Frontier Orbitals and Suppression of Charge Recombinations in P3HT/SWNT. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26258-26265.	1.5	7
7730	Computational Chemistry Analysis of Hydrodesulfurization Reactions Catalyzed by Molybdenum Disulfide Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2015, 119, 29157-29170.	1.5	21

#	ARTICLE	IF	CITATIONS
7731	Radical-induced, proton-transfer-driven fragmentations in [b ₅ H]E TM ions derived from pentaalanyl tryptophan. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10699-10707.	1.3	4
7732	Phase-Programmed Nanofabrication: Effect of Organophosphite Precursor Reactivity on the Evolution of Nickel and Nickel Phosphide Nanocrystals. <i>Chemistry of Materials</i> , 2015, 27, 8021-8031.	3.2	44
7733	Absence of Stereodirecting Participation by 2-O-Alkoxy carbonylmethyl Ethers in 4,6-O-Benzylidene-Directed Mannosylation. <i>Journal of Organic Chemistry</i> , 2015, 80, 12300-12310.	1.7	14
7734	Upward Shift in Conduction Band of Ta ₂ O ₅ Due to Surface Dipoles Induced by N-Doping. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26925-26936.	1.5	27
7735	How to Optimize the Interface between Photosensitizers and TiO ₂ Nanocrystals with Molecular Engineering to Enhance Performances of Dye-Sensitized Solar Cells?. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 25341-25351.	4.0	28
7736	Theoretical study of the BINOL-zinc complex-catalyzed asymmetric inverse-electron-demand imino Diels-Alder reaction: mechanism and stereochemistry. <i>RSC Advances</i> , 2015, 5, 93318-93330.	1.7	2
7737	Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 13048-13054.	1.1	13
7738	Discovery of low energy pathways to metal-mediated Bi-N bond reduction guided by computation and experiment. <i>Chemical Science</i> , 2015, 6, 7258-7266.	3.7	6
7739	Steroid Derived Mesoionic Gold and Silver Mono- and Polymetallic Carbenes. <i>Inorganic Chemistry</i> , 2015, 54, 11174-11185.	1.9	17
7740	Multi-reference character and Ce 4 f orbital contributions in terminal multiple Ce Z bonds of Cp ₂ CeZ (Z = CH ₂ , CH ⁺ , NH, O, F +) complexes. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 34-44.	1.1	4
7741	Molecular Structures of Free Boron Clusters. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 17-48.	0.6	11
7742	A weight averaged approach for predicting amide vibrational bands of a sphingomyelin bilayer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29113-29123.	1.3	13
7743	The Photoluminescence Properties of the Alkali Metals Functionalized Adamantane Studied by Using Linear-Response Time-Dependent Density Functional Theory (TD-DFT) Calculations. <i>Advanced Materials Research</i> , 2015, 1131, 117-122.	0.3	1
7744	Identification of Serine Conformers by Matrix-Isolation IR Spectroscopy Aided by Near-Infrared Laser-Induced Conformational Change, 2D Correlation Analysis, and Quantum Mechanical Anharmonic Computations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10496-10510.	1.2	38
7745	Investigating Interfacial Electron Transfer in Highly Efficient Porphyrin-Sensitized Solar Cells. <i>ACS Symposium Series</i> , 2015, , 169-188.	0.5	0
7746	Choice of ab initio method for calculations of the key steps for the mechanism of rearrangement of sulfated pyranosides into furanosides. <i>Russian Chemical Bulletin</i> , 2015, 64, 558-561.	0.4	1
7747	Different outcomes in the reactions of WCl ₆ with carboxylic acids. <i>Polyhedron</i> , 2015, 99, 141-146.	1.0	11
7748	Synthesis and reactivity of dinuclear Cp*Ru tert-butylamido and cyclometallated Bis(trimethylsilyl)amido complexes. <i>Journal of Organometallic Chemistry</i> , 2015, 797, 60-66.	0.8	8

#	ARTICLE	IF	CITATIONS
7749	Unusual loss of electron mobility upon furan for thiophene substitution in a molecular semiconductor. <i>Organic Electronics</i> , 2015, 18, 118-125.	1.4	21
7750	Catalyst-Controlled C–C Bond Cleavages in Metal Halide-Catalyzed Cycloisomerization of 3-Acylcyclopropenes via a Formal 1,1-Halometalation Mechanism: Insights from Quantum Chemical Calculations. <i>ACS Catalysis</i> , 2015, 5, 859-868.	5.5	33
7751	Heterolytic Activation of Dihydrogen Molecule by Hydroxo-/Sulfido-Bridged Ruthenium–Germanium Dinuclear Complex. Theoretical Insights. <i>Inorganic Chemistry</i> , 2015, 54, 576-585.	1.9	9
7752	Impact of sulfur heteroatoms on the activity of quaternary ammonium salts as phase transfer catalysts for nucleophilic displacement reactions. <i>Journal of Molecular Catalysis A</i> , 2015, 398, 282-288.	4.8	3
7753	Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzuki–Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers. <i>Organometallics</i> , 2015, 34, 381-394.	1.1	38
7754	Synthesis, characterization and photophysical study of ethynyl pyrene derivatives as promising materials for organic optoelectronics. <i>Journal of Luminescence</i> , 2015, 161, 37-46.	1.5	15
7755	Computational Insights into the Isomerism of Hexacoordinate Metal–Sarcophagine Complexes: The Relationship between Structure and Stability. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 503-511.	1.0	1
7756	Evaluation of nitrogen-rich macrocyclic ligands for the chelation of therapeutic bismuth radioisotopes. <i>Nuclear Medicine and Biology</i> , 2015, 42, 428-438.	0.3	41
7757	A QM/MM study of the initial steps of catalytic mechanism of nitrile hydratase. <i>Chemical Physics Letters</i> , 2015, 623, 8-13.	1.2	8
7758	Effects of the electronic structure of five-membered N-heterocyclic carbenes on insertion of silanes and boranes into the NHC–N bond. <i>Dalton Transactions</i> , 2015, 44, 3318-3325.	1.6	23
7759	Iridium(III) N-heterocyclic carbene complexes: an experimental and theoretical study of structural, spectroscopic, electrochemical and electrogenerated chemiluminescence properties. <i>Dalton Transactions</i> , 2015, 44, 8564-8576.	1.6	47
7760	Mechanism of the N-Hydroxylation of Primary and Secondary Amines by Cytochrome P450. <i>Chemical Research in Toxicology</i> , 2015, 28, 597-603.	1.7	27
7761	Spectroscopic, computational and electrochemical studies on the formation of the copper complex of 1-amino-4-hydroxy-9,10-anthraquinone and effect of it on superoxide formation by NADH dehydrogenase. <i>Dalton Transactions</i> , 2015, 44, 5428-5440.	1.6	32
7762	The effect of leaving radical on the formation of tetrahydroselenophene by S–H ring closure: an experimental and computational study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2310-2316.	1.5	7
7763	Syndioselective ring-opening polymerization and copolymerization of trans-1,4-cyclohexadiene carbonate mediated by achiral metal- and organo-catalysts. <i>Polymer Chemistry</i> , 2015, 6, 1961-1971.	1.9	28
7764	Insight into the Mechanisms of Luminescence of Aminobenzonitrile and Dimethylaminobenzonitrile in Polar Solvents. An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1983-1995.	1.1	26
7765	Possibility of [1,5] Sigmatropic Shifts in Bicyclo[4.2.0]octa-2,4-dienes. <i>Journal of Organic Chemistry</i> , 2015, 80, 2609-2620.	1.7	13
7766	Unravelling the Photodegradation Mechanisms of a Low Bandgap Polymer by Combining Experimental and Modeling Approaches. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2166-2176.	1.5	36

#	ARTICLE	IF	CITATIONS
7767	Vanadyl cationic complexes as catalysts in olefin oxidation. Dalton Transactions, 2015, 44, 5125-5138.	1.6	47
7768	Tris(2,2'-azobispyridine) Complexes of Copper(II): X-ray Structures, Reactivities, and the Radical Nonradical Bis(ligand) Analogues. Inorganic Chemistry, 2015, 54, 1300-1313.	1.9	21
7769	Reactivity of vinylidene complexes of ruthenium with hydrazines and hydroxylamines. Dalton Transactions, 2015, 44, 3439-3446.	1.6	11
7770	Computational studies on the radiative and nonradiative processes of luminescent N-heteroleptic platinum(II) complexes. Organic Electronics, 2015, 19, 7-14.	1.4	7
7771	Theoretical investigation of isotope exchange reaction in tritium-contaminated mineral oil in vacuum pump. Journal of Hazardous Materials, 2015, 287, 42-50.	6.5	4
7772	Density Functional Theory and Hydrogen Bonds: Are We There Yet?. ChemPhysChem, 2015, 16, 978-985.	1.0	129
7773	Spin Component-Scaled Second-Order Møller-Plesset Perturbation Theory for Calculating NMR Shieldings. Journal of Chemical Theory and Computation, 2015, 11, 37-44.	2.3	16
7774	Establishing the Steric Bulk of Main Group Hydrides in Reduction Reactions. Israel Journal of Chemistry, 2015, 55, 226-234.	1.0	8
7775	Time-Resolved Study of 1,8-Naphthalic Anhydride and 1,4,5,8-Naphthalene-tetracarboxylic Dianhydride. Journal of Physical Chemistry A, 2015, 119, 6006-6016.	1.1	9
7776	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	1.1	78
7777	Time-Resolved Photodetachment Anisotropy: Gas-Phase Rotational and Vibrational Dynamics of the Fluorescein Anion. Journal of Physical Chemistry Letters, 2015, 6, 189-194.	2.1	20
7778	Effect of H ₂ Binding on the Nonadiabatic Transition Probability between Singlet and Triplet States of the [NiFe]-Hydrogenase Active Site. Journal of Physical Chemistry A, 2015, 119, 1066-1073.	1.1	21
7779	Rhodium(III)-Catalyzed Hydrazine-Directed C-H Activation for Indole Synthesis: Mechanism and Role of Internal Oxidant Probed by DFT Studies. Organometallics, 2015, 34, 309-318.	1.1	105
7780	Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS-QM/MM) Calculations. 1. Estimation of Polarization Energies. Journal of Physical Chemistry A, 2015, 119, 1511-1523.	1.1	23
7781	Ultrathin Gold Nanowires: Soft-Templating versus Liquid Phase Synthesis, a Quantitative Study. Journal of Physical Chemistry C, 2015, 119, 4422-4430.	1.5	40
7782	[H ₃ Fe _n (CO) ₁₂ (IrCOD)] ⁿ⁺ (n = 1, 2) and [H ₂ Fe ₃ (CO) ₁₀ (IrCOD)] ⁺ Bimetallic Fe-Ir Hydride Carbonyl Clusters. Organometallics, 2015, 34, 189-197.	1.1	2
7783	Axial Coordination Dichotomy in Dirhodium Carbenoid Catalysis: A Curious Case of Cooperative Asymmetric Dual-Catalytic Approach toward Amino Esters. Journal of Organic Chemistry, 2015, 80, 2192-2197.	1.7	26
7784	Mechanistic Study of Ru-NHC-Catalyzed Hydrodefluorination of Fluoropyridines: The Influence of the NHC on the Regioselectivity of C-F Activation and Chemoselectivity of C-F versus C-H Bond Cleavage. ACS Catalysis, 2015, 5, 776-787.	5.5	36

#	ARTICLE	IF	CITATIONS
7785	Computational Mechanistic Studies on Reactions of Transition Metal Complexes with Noninnocent Pincer Ligands: Aromatization vs. Dearomatization or Not. <i>ACS Catalysis</i> , 2015, 5, 1895-1913.	5.5	75
7786	Mechanistic Study and Ligand Design for the Formation of Zinc Formate Complexes from Zinc Hydride Complexes and Carbon Dioxide. <i>Organometallics</i> , 2015, 34, 121-126.	1.1	11
7787	Reactivity of Damaged Pyrimidines: Formation of a Schiff Base Intermediate at the Glycosidic Bond of Saturated Dihydrouridine. <i>Journal of the American Chemical Society</i> , 2015, 137, 3318-3329.	6.6	5
7788	Steady-State and Femtosecond Transient Absorption Spectroscopy of New Two-Photon Absorbing Fluorene-Containing Quinolinium Cation Membrane Probes. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 2833-2846.	4.0	32
7789	Activation of C-H, Si-H, and C-F Bonds with Tp-Rh(PMe ₃) ₃ Complexes: Kinetics, Mechanism, and Selectivity. <i>Journal of the American Chemical Society</i> , 2015, 137, 1258-1272.	6.6	39
7790	Plagioclase Dissolution during CO ₂ -SO ₂ Cosequestration: Effects of Sulfate. <i>Environmental Science & Technology</i> , 2015, 49, 1946-1954.	4.6	23
7791	Embedded Mean-Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 568-580.	2.3	83
7792	Brominated Chemistry for Chemical Vapor Deposition of Electronic Grade SiC. <i>Chemistry of Materials</i> , 2015, 27, 793-801.	3.2	9
7793	Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1102-1109.	2.3	98
7794	Origins of Hydration Differences in Homochiral and Racemic Crystals of Aspartic Acid. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1396-1403.	1.1	7
7795	Density Functional Theory Study on the Formation of Reactive Benzoquinone Imines by Hydrogen Abstraction. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 660-666.	2.5	8
7796	Exploitation and Application of a Highly Sensitive Ru(II) Complex-Based Phosphorescent Chemodosimeter for Hg ²⁺ in Aqueous Solutions and Living Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 4247-4256.	4.0	32
7797	Effect of surface hydroxylation on the catalytic activity of a Cr(II)/SiO ₂ model system of Phillips catalyst. <i>Journal of Catalysis</i> , 2015, 324, 79-87.	3.1	19
7798	Dimerization of Two Alkyne Units: Model Studies, Intermediate Trapping Experiments, and Kinetic Studies. <i>Journal of the American Chemical Society</i> , 2015, 137, 1833-1843.	6.6	41
7799	Highly sensitive detection of low-level water content in organic solvents and cyanide in aqueous media using novel solvatochromic AIEE fluorophores. <i>RSC Advances</i> , 2015, 5, 12191-12201.	1.7	78
7800	Triplet-singlet gap in structurally flexible organic diradicals. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	7
7801	Amido Analogues of Nonbent Lanthanide (II) and Calcium Metallocenes. Heterolytic Cleavage of Î-Bond Ln-Carbazolyl Ligand Promoted by Lewis Base Coordination. <i>Organometallics</i> , 2015, 34, 555-562.	1.1	16
7802	Mechanism of [3+2] Cycloaddition of Alkynes to the [Mo ₃ S ₄ (acac) ₃ (py) ₃][PF ₆] ₃ Cluster. <i>Chemistry - A European Journal</i> , 2015, 21, 2835-2844.	1.7	12

#	ARTICLE	IF	CITATIONS
7803	Stereospecificity in vanadium Schiff base complexes: Formation, crystallization and epimerization processes. <i>Journal of Inorganic Biochemistry</i> , 2015, 147, 65-70.	1.5	9
7804	Synthesis, characterization, antioxidant and selective xanthine oxidase inhibitory studies of transition metal complexes of novel amino acid bearing Schiff base ligand. <i>Inorganica Chimica Acta</i> , 2015, 428, 117-126.	1.2	38
7805	Rhodium-catalyzed C-H functionalization-based approach to eight-membered lactams. <i>Chemical Science</i> , 2015, 6, 2275-2285.	3.7	126
7806	Light and Chemically Driven Molecular Machines Showing a Unidirectional Four-State Switching Cycle. <i>Journal of Organic Chemistry</i> , 2015, 80, 1887-1895.	1.7	20
7807	A comparative computational study on the interactions of N719 and N749 dyes with iodine in dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4379-4387.	1.3	14
7808	Unexpected 1,2-Migration in Metallasilabenzenes: Theoretical Evidence for Reluctance of Silicon to Participate in π Bonding. <i>Chemistry - an Asian Journal</i> , 2015, 10, 405-410.	1.7	19
7809	Spin-State Ordering in Hydroxo-Bridged Diiron(III)bisporphyrin Complexes. <i>Inorganic Chemistry</i> , 2015, 54, 1919-1930.	1.9	49
7810	Natural Abundance ^{15}N -NMR by Dynamic Nuclear Polarization: Fast Analysis of Binding Sites of a Novel Amine-Linked Immobilized Dirhodium Catalyst. <i>Chemistry - A European Journal</i> , 2015, 21, 3798-3805.	1.7	59
7811	Influence of structural and electronic properties of organomolybdenum(ii) complexes of the type $[\text{CpMo}(\text{CO})_3\text{R}]$ and $[\text{CpMo}(\text{O}_2)(\text{O})\text{R}]$ ($\text{R} = \text{Cl}, \text{CH}_3, \text{CF}_3$) on the catalytic olefin epoxidation. <i>Catalysis Science and Technology</i> , 2015, 5, 2282-2289.	2.1	13
7812	Dinuclear Bridging Bidentate Zinc/Stearate Complex in Sulfur Cross-Linking of Rubber. <i>Macromolecules</i> , 2015, 48, 462-475.	2.2	61
7813	The Theoretical Estimation of the Bioluminescent Efficiency of the Firefly via a Nonadiabatic Molecular Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 540-548.	2.1	47
7814	Hydroamination of C=C Multiple Bonds with Hydrazine Catalyzed by N-Heterocyclic Carbene-Gold(I) Complexes: Substrate and Ligand Effects. <i>ACS Catalysis</i> , 2015, 5, 815-829.	5.5	49
7815	Structural Progression in Clusters of Ionized Water, $(\text{H}_2\text{O})_n^+ = 5$. <i>Journal of Physical Chemistry A</i> , 2015, 119, 752-766.	1.1	42
7816	Experimental and theoretical charge density distribution in Pigment Yellow 101. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4677-4686.	1.3	12
7817	Virtual screening of molecular properties of chitosan and derivatives in search for druggable molecules. <i>International Journal of Biological Macromolecules</i> , 2015, 74, 392-396.	3.6	9
7818	Revisitation of the PCl_5 -chlorination reaction of α -amino acids: Spectroscopic and DFT insights, and synthesis of the L-proline-derived 2,5-diketopiperazine. <i>Inorganica Chimica Acta</i> , 2015, 427, 150-154.	1.2	8
7819	An ab initio study of structure, stability, and spectroscopic parameters of 5-atomic $[\text{C}, \text{C}, \text{H}, \text{N}, \text{S}]$ isomers. <i>Journal of Molecular Structure</i> , 2015, 1090, 76-85.	1.8	8
7820	Mechanism of Brønsted Acid-Catalyzed Glucose Dehydration. <i>ChemSusChem</i> , 2015, 8, 1334-1341.	3.6	135

#	ARTICLE	IF	CITATIONS
7821	Zn ²⁺ responsive two-photon fluorescent probes based on branch structure: a computational investigation. <i>Molecular Physics</i> , 2015, 113, 584-607.	0.8	2
7822	Energy Expression of the Chemical Bond Between Atoms in Hydrides and Oxides and Its Application to Materials Design. , 2015, , 183-213.		1
7823	New insights into dissociation of deprotonated 2,4-dinitrotoluene by combined high-resolution mass spectrometry and density functional theory calculations. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 29-34.	0.7	2
7824	Photoinduced Phenomena in Nucleic Acids II. <i>Topics in Current Chemistry</i> , 2015, , .	4.0	15
7825	Photoisomerization of Silyl-Substituted Cyclobutadiene Induced by f ^π ĩ [*] Excitation: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 442-451.	1.1	1
7826	Sterically Controlled Functionalization of Carbon Surfaces with ⁶ C ₆ H ₄ CH ₂ X (X = OSO ₂ Me or N ₃) Groups for Surface Attachment of Redox-Active Molecules. <i>Langmuir</i> , 2015, 31, 1189-1195.	1.6	20
7827	A new phenylimidorhenium(V) compound containing the 2-[(2-hydroxyethylimino)methyl]phenol Schiff-base ligand: experimental and theoretical aspects. <i>Journal of Coordination Chemistry</i> , 2015, 68, 599-615.	0.8	9
7828	The Synthesis and STM/AFM Imaging of ¹⁴ C ¹³ Benzo[<i>a</i>]pyrenes. <i>Chemistry - A European Journal</i> , 2015, 21, 2011-2018.	1.7	39
7829	Inter ^π -Aromatic Distances in <i>Geobacter Sulfurreducens</i> Pili Relevant to Biofilm Charge Transport. <i>Advanced Materials</i> , 2015, 27, 1908-1911.	11.1	41
7830	Incorporation of novel azobenzene dyes bearing oligo(ethylene glycol) spacers into first generation dendrimers. <i>Dyes and Pigments</i> , 2015, 116, 1-12.	2.0	8
7831	Formylated chloro-bridged iridium(III) dimers as OLED materials: opening up new possibilities. <i>Dalton Transactions</i> , 2015, 44, 8419-8432.	1.6	39
7832	Mechanistic Insight into Marine Bioluminescence: Photochemistry of the Chemiexcited <i>Cypridina</i> (Sea Firefly) Lumophore. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 591-599.	2.3	60
7833	Conformational Flexibility of Hoveyda-Type and Grubbs-Type Complexes Bearing Acyclic Carbenes and Its Impact on Their Catalytic Properties. <i>Organometallics</i> , 2015, 34, 563-570.	1.1	23
7834	Magnetic Alignments of Endohedral Metallofullerene Nanorods under Magnetic Fields. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015, 23, 35-39.	1.0	5
7835	Comparative Study of Oxygen Reduction Reaction Mechanism on Nitrogen-, Phosphorus-, and Boron-Doped Graphene Surfaces for Fuel Cell Applications. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2004-2009.	1.5	85
7836	Comparative Study on Pyrido[3,4- <i>b</i>]pyrazine-Based Sensitizers by Tuning Bulky Donors for Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 2760-2771.	4.0	52
7837	Orthometalation of Dibenzo[1,2]quinoxaline with Ruthenium(II/III), Osmium(II/III/IV), and Rhodium(III) Ions and Orthometalated [RuNO] ^{6/7} Derivatives. <i>Inorganic Chemistry</i> , 2015, 54, 1384-1394.	1.9	13
7838	A Mechanistic Investigation of the Kinetic Resolution of Secondary Aromatic Alcohols Using a Ferrocene-Based Planar Chiral 4-(Dimethylamino)pyridine Catalyst. <i>Chemistry - A European Journal</i> , 2015, 21, 5623-5631.	1.7	14

#	ARTICLE	IF	CITATIONS
7839	Co(III) complexes of tetradentate X3L type ligands: Synthesis, electronic structure, and reactivity. <i>Inorganica Chimica Acta</i> , 2015, 430, 30-35.	1.2	11
7841	An Optically and Thermally Switchable Electronic Structure Based on an Anthracene-BODIPY Conjugate. <i>Chemistry - A European Journal</i> , 2015, 21, 4966-4974.	1.7	26
7842	Dianions as Formal Oxidants: Synthesis and Characterization of Aromatic Dilithionickeloles from 1,4-Dithio-1,3-butadienes and [Ni(cod) ₂]. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5999-6002.	7.2	60
7843	Chiral differentiation of the noscapine and hydrastine stereoisomers by electrospray ionization tandem mass spectrometry. <i>Journal of Mass Spectrometry</i> , 2015, 50, 240-246.	0.7	9
7844	Heteroleptic platinum(II) NHC complexes with a C [∞] C* cyclometalated ligand - synthesis, structure and photophysics. <i>Journal of Materials Chemistry C</i> , 2015, 3, 1680-1693.	2.7	55
7845	Modeling the antiferromagnetic MnII/MnII system within the protein phosphatase-5 catalytic site. <i>Journal of Molecular Modeling</i> , 2015, 21, 14.	0.8	5
7846	Computational evidence for structural consequences of kiteplatin damage on DNA. <i>Journal of Biological Inorganic Chemistry</i> , 2015, 20, 35-48.	1.1	12
7847	Quantitative structure-property relationship modeling of ruthenium sensitizers for solar cells applications: novel tools for designing promising candidates. <i>RSC Advances</i> , 2015, 5, 23865-23873.	1.7	14
7848	Coordination Induced Atropisomerism in an NHC-Based Rhodium Macrocycle. <i>Organometallics</i> , 2015, 34, 913-917.	1.1	32
7849	Theories of phosphorescence in organo-transition metal complexes - From relativistic effects to simple models and design principles for organic light-emitting diodes. <i>Coordination Chemistry Reviews</i> , 2015, 295, 46-79.	9.5	93
7850	Computational and spectroscopic characterization of key intermediates of the Selective Catalytic Reduction cycle of NO on zeolite-supported Cu catalyst. <i>Inorganica Chimica Acta</i> , 2015, 430, 132-143.	1.2	16
7852	Highly-selective absorption control in photosynthetic chlorin dyes. <i>Journal of Porphyrins and Phthalocyanines</i> , 2015, 19, 601-609.	0.4	0
7853	Synthesis of One-Dimensional Schiff Base Polymers that Contain an Oligothiophene Building Block on the Graphite Surface. <i>Chemistry - A European Journal</i> , 2015, 21, 6898-6905.	1.7	6
7855	Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20093-20099.	1.3	16
7856	Oxidation of [CpMo(CO)3R] olefin epoxidation precatalysts with tert-butylhydroperoxide. <i>Journal of Catalysis</i> , 2015, 329, 269-285.	3.1	13
7857	Platinum trimethyl bipyridyl thiolates - new, tunable, red- to near IR emitting luminophores for bioimaging applications. <i>Chemical Communications</i> , 2015, 51, 11441-11444.	2.2	13
7858	Stacking in RNA: NMR of Four Tetramers Benchmark Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2729-2742.	2.3	99
7859	Theoretical investigation of the mechanism of tritiated methane dehydrogenation reaction using nickel-based catalysts. <i>Fusion Engineering and Design</i> , 2015, 95, 91-98.	1.0	2

#	ARTICLE	IF	CITATIONS
7860	1,4-Dithiineâ€”Puckered in the Gas Phase but Planar in Crystals: Role of Cooperativity. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15770-15776.	1.5	22
7861	Mechanistic Insights into the Cu(I)- and Cu(II)-Catalyzed Cyclization of <i>o</i> -Alkynylbenzaldehydes: The Solvent DMF and Oxidation State of Copper Affect the Reaction Mechanism. <i>Journal of Organic Chemistry</i> , 2015, 80, 6553-6563.	1.7	21
7862	Stability and spatial arrangement of the 2,4-dichlorophenoxyacetic acid and β -cyclodextrin inclusion compound: A theoretical study. <i>Chemical Physics Letters</i> , 2015, 633, 158-162.	1.2	10
7863	Improving DIIS convergence for metallic systems using Gaussian basis set. <i>Chemical Physics Letters</i> , 2015, 635, 201-204.	1.2	7
7864	Toward a Unified Mechanism for Oxoammonium Salt-Mediated Oxidation Reactions: A Theoretical and Experimental Study Using a Hydride Transfer Model. <i>Journal of Organic Chemistry</i> , 2015, 80, 8150-8167.	1.7	55
7865	Metal-free catalytic C-H bond activation and borylation of heteroarenes. <i>Science</i> , 2015, 349, 513-516.	6.0	379
7866	Static polarization of the supramolecular dyads of fullerene C60 with porphyrin derivatives. <i>Journal of Porphyrins and Phthalocyanines</i> , 2015, 19, 838-844.	0.4	1
7867	Antioxidative Potency and UVâ€”Vis spectra features of the compounds resulting from the chelation of Fe ²⁺ by Caffeic Acid Phenethyl Ester and two of its derivatives. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 135-147.	1.1	18
7868	Stability, Reactivity, Selectivity, Catalysis, and Predictions of 1,3,2,5-Diazadiborinine: Computational Insight into a Boronâ€”Boron Frustrated Lewis Pair. <i>Journal of Organic Chemistry</i> , 2015, 80, 8790-8795.	1.7	24
7869	Factors affecting the solubility of ionic compounds. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 132-137.	1.1	10
7870	Solvent effects to compute UVâ€”vis spectra for ionic metal complexes. <i>Chemical Physics Letters</i> , 2015, 636, 39-45.	1.2	11
7871	Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 Â°C: a theoretical investigation. <i>New Journal of Chemistry</i> , 2015, 39, 7703-7715.	1.4	15
7872	Multiconfiguration Pair-Density Functional Theory Outperforms Kohnâ€”Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3643-3649.	2.3	40
7873	Correlations among experimental and theoretical NMR data to determine the absolute stereochemistry of darcyrine, a pentacyclic indole alkaloid isolated from <i>Rauvolfia grandiflora</i> . <i>Journal of Molecular Structure</i> , 2015, 1098, 76-83.	1.8	2
7874	Incremental evaluation of coupled cluster dipole polarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14284-14296.	1.3	13
7875	ESR study of singlet oxygen generation and its behavior during the photo-oxidation of P3HT in solution. <i>Chemical Physics Letters</i> , 2015, 624, 87-92.	1.2	35
7876	Modeling EPR parameters of nitrogen containing conjugated radical cations. <i>RSC Advances</i> , 2015, 5, 62551-62562.	1.7	10
7877	Chemical and spectroscopic characterizations, ESI-QTOF mass spectrometric measurements and DFT studies of new complexes of palladium(II) with tryptamine and mefenamic acid. <i>Journal of Molecular Structure</i> , 2015, 1100, 6-13.	1.8	15

#	ARTICLE	IF	CITATIONS
7878	Structure-Property Relationships for Exciton and Charge Reorganization Energies of Dipolar Organic Semiconductors: A Combined Valence Bond Self-Consistent Field and Time-Dependent Hartree-Fock and DFT Study of Merocyanine Dyes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17602-17611.	1.5	26
7879	Spectroscopic and Computational Investigation of the H155A Variant of Cysteine Dioxygenase: Geometric and Electronic Consequences of a Third-Sphere Amino Acid Substitution. <i>Biochemistry</i> , 2015, 54, 2874-2884.	1.2	26
7880	A copper(II) complex with a Cu-S bond. Attenuated total reflectance, electron paramagnetic resonance, resonance Raman and atoms-in-molecule calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 96-99.	2.0	7
7881	Improving Rydberg Excitations within Time-Dependent Density Functional Theory with Generalized Gradient Approximations: The Exchange-Enhancement-for-Large-Gradient Scheme. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3123-3130.	2.3	28
7882	Cryogenic Spectroscopy and Quantum Molecular Dynamics Determine the Structure of Cyclic Intermediates Involved in Peptide Sequence Scrambling. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2524-2529.	2.1	4
7883	Theoretical Study on Internal Alkyne/Vinylidene Isomerization in Group 8 Transition-Metal Complexes. <i>Organometallics</i> , 2015, 34, 3934-3943.	1.1	26
7884	Force field parameters for aminoorganosilanes. <i>Journal of Molecular Structure</i> , 2015, 1079, 363-369.	1.8	4
7885	Hydrogen-release mechanisms in LiNH ₂ BH ₃ -NH ₃ BH ₃ : A theoretical study. <i>Journal of Molecular Structure</i> , 2015, 1081, 437-442.	1.8	5
7886	Development of Prediction Models for the Reactivity of Organic Compounds with Ozone in Aqueous Solution by Quantum Chemical Calculations: The Role of Delocalized and Localized Molecular Orbitals. <i>Environmental Science & Technology</i> , 2015, 49, 9925-9935.	4.6	83
7887	Virtual Screening for Transition State Analogue Inhibitors of IRAP Based on Quantum Mechanically Derived Reaction Coordinates. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1984-1993.	2.5	9
7888	Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4283-4293.	2.3	17
7889	Encapsulated Guests in the Smallest Spaces: Shrinking Guests by Compression and Investigations under Solvent-Free Conditions. <i>Journal of Organic Chemistry</i> , 2015, 80, 8065-8072.	1.7	5
7890	Mechanistic Understanding of the Divergent Reactivity of Cyclopropenes in Rh(III)-Catalyzed C-H Activation/Cycloaddition Reactions of <i>N</i> -Phenoxyacetamide and <i>N</i> -Pivaloxybenzamide. <i>Journal of Organic Chemistry</i> , 2015, 80, 8113-8121.	1.7	67
7891	Ground-State Electronic Structure of RC-LH1 and LH2 Pigment Assemblies of Purple Bacteria via the EBF-MO Method. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8934-8943.	1.1	4
7892	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. <i>ACS Catalysis</i> , 2015, 5, 4897-4912.	5.5	19
7893	Triazine-Substituted and Acyl Hydrazones: Experiment and Computation Reveal a Stability Inversion at Low pH. <i>Molecular Pharmaceutics</i> , 2015, 12, 2924-2927.	2.3	19
7894	Experimental and DFT Studies Explain Solvent Control of C-H Activation and Product Selectivity in the Rh(III)-Catalyzed Formation of Neutral and Cationic Heterocycles. <i>Journal of the American Chemical Society</i> , 2015, 137, 9659-9669.	6.6	108
7895	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19306-19314.	1.3	160

#	ARTICLE	IF	CITATIONS
7896	Half-sandwich Ru(η^6 -C ₆ H ₆) complexes with chiral aroylthioureas for enhanced asymmetric transfer hydrogenation of ketones – experimental and theoretical studies. <i>Catalysis Science and Technology</i> , 2015, 5, 4790-4799.	2.1	28
7897	Icosahedral metallocarborane/carborane species derived from 1,1- η^2 -bis(o-carborane). <i>Dalton Transactions</i> , 2015, 44, 5628-5637.	1.6	34
7898	Metallacyclobutanes from Schrock-Type d ⁰ Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis. <i>Organometallics</i> , 2015, 34, 1668-1680.	1.1	55
7899	N-Coordinated Tin(II) Trifluoromethanesulfonates and Their Reactions with Transition Metal Carbonyls. <i>Inorganic Chemistry</i> , 2015, 54, 6792-6800.	1.9	14
7900	Reactivity Pattern of Bromonucleosides Induced by 2-Hydroxypropyl Radicals: Photochemical, Radiation Chemical, and Computational Studies. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6545-6554.	1.2	2
7901	Bio-inspired computational design of iron catalysts for the hydrogenation of carbon dioxide. <i>Chemical Communications</i> , 2015, 51, 13098-13101.	2.2	41
7902	N ₂ Activation by an Iron Complex with a Strong Electron-Donating Iminophosphorane Ligand. <i>Inorganic Chemistry</i> , 2015, 54, 9271-9281.	1.9	40
7903	Accuracy of Protein Embedding Potentials: An Analysis in Terms of Electrostatic Potentials. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1832-1842.	2.3	50
7904	Accurate Electron Densities at Nuclei Using Small Ramp-Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3679-3683.	2.3	6
7905	Electron Injection from Copper Diimine Sensitizers into TiO ₂ : Structural Effects and Their Implications for Solar Energy Conversion Devices. <i>Journal of the American Chemical Society</i> , 2015, 137, 9670-9684.	6.6	60
7906	Highly enantioselective construction of tertiary thioethers and alcohols via phosphine-catalyzed asymmetric β -addition reactions of 5H-thiazol-4-ones and 5H-oxazol-4-ones: scope and mechanistic understandings. <i>Chemical Science</i> , 2015, 6, 4912-4922.	3.7	117
7907	Active space and basis set effects in CASPT_2 models of the 1,3-butadiene-ethene cycloaddition and the 1,3-butadiene dimerization. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 989-1001.	1.0	4
7908	The chlorinating behaviour of WCl ₆ towards α -aminoacids. <i>Dalton Transactions</i> , 2015, 44, 8729-8738.	1.6	14
7909	Modulating Electrical Properties of InAs Nanowires <i>via</i> Molecular Monolayers. <i>ACS Nano</i> , 2015, 9, 7545-7552.	7.3	33
7910	Determining the effect of side reactions on product distributions in RAFT polymerization by MALDI-TOF MS. <i>Polymer Chemistry</i> , 2015, 6, 5437-5450.	1.9	29
7911	Molecular hydrogen binding affinities of metal cation decorated substituted benzene systems: insight from computational exploration. <i>RSC Advances</i> , 2015, 5, 57647-57656.	1.7	8
7912	STM study of oligo(phenylene-ethynylene)s. <i>New Journal of Physics</i> , 2015, 17, 053043.	1.2	7
7913	Conformational preferences for isomeric N,N- η^2 -bis(pyridin- <i>n</i> -ylmethyl)ethanedithiodiamides, <i>n</i> = 2, 3 and 4: a combined crystallographic and DFT study. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2015, 230, 531-541.	0.4	6

#	ARTICLE	IF	CITATIONS
7914	Molecular features contributing to the lower viscosity of phosphonium ionic liquids compared to their ammonium analogues. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20205-20216.	1.3	38
7915	A theoretical investigation of substituent effects on the stability and reactivity of N-heterocyclic olefin carboxylates. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 8533-8544.	1.5	26
7916	Effect of donor strength of extended alkyl auxiliary groups on optoelectronic and charge transport properties of novel naphtha[2,1-b:6,5-ba [€] ²]difuran derivatives: simple yet effective strategy. <i>Journal of Molecular Modeling</i> , 2015, 21, 199.	0.8	13
7917	Gas-phase structure and conformations of copper(II) 2,9,16,23-tetra-tert-butyl phthalocyanine. <i>Structural Chemistry</i> , 2015, 26, 1531-1541.	1.0	3
7918	Design and development of molecularly imprinted polymers for the selective extraction of deltamethrin in olive oil: An integrated computational-assisted approach. <i>Journal of Chromatography A</i> , 2015, 1409, 1-10.	1.8	32
7919	Tuning the Emission of Cationic Iridium (III) Complexes Towards the Red Through Methoxy Substitution of the Cyclometalating Ligand. <i>Scientific Reports</i> , 2015, 5, 12325.	1.6	81
7920	A computational mechanistic investigation of hydrogen production in water using the [RhIII(dmbpy)2Cl2]+/[RuII(bpy)3]2+/ascorbic acid photocatalytic system. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10497-10509.	1.3	19
7921	Influence of pH and type of counterion on the formation of bismuth(III) complexes with tropolonato and 5-methyltropolonato ligands: Synthesis, structure, spectroscopic characterization and calculation studies. <i>Inorganica Chimica Acta</i> , 2015, 436, 57-68.	1.2	8
7922	Handling Magnetic Coupling in Trinuclear Cu(II) Complexes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3650-3660.	2.3	13
7923	Azide addition to Sc2@C66: favorable activity on unsaturated linear triquinanes and dramatic reactivity difference compared with the free C66 cage. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20485-20489.	1.3	4
7924	Synthesis, characterization, photophysical properties, and catalytic activity of an SCS bis(N-heterocyclic thione) (SCS-NHT) Pd pincer complex. <i>Dalton Transactions</i> , 2015, 44, 14475-14482.	1.6	41
7925	Synthesis of Biologically Active Piperidine Metabolites of Clopidogrel: Determination of Structure and Analyte Development. <i>Journal of Organic Chemistry</i> , 2015, 80, 7019-7032.	1.7	19
7926	Synthesis and Characterization of Nanobuilding Blocks [<i>σ</i> -RStyrPhSiO _{1.5}] _{10,12} (R = Me, MeO, NBoc, and CN). Unexpected Photophysical Properties Arising from Apparent Asymmetric Cage Functionalization as Supported by Modeling Studies. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15846-15858.	1.5	10
7927	Probing keto [€] enol tautomerism using photoelectron spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19991-19996.	1.3	5
7928	5-Thiocyanato-2 [€] -deoxyuridine as a possible radiosensitizer: electron-induced formation of uracil-C5-thiyl radical and its dimerization. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16907-16916.	1.3	29
7929	Synthesis and structural analysis of Co-doped BaTiO3. <i>Journal of Molecular Structure</i> , 2015, 1099, 502-509.	1.8	32
7930	Revealing the parameters to design the habit modifiers for rock-salt crystals: empirical to rational approach. <i>Canadian Journal of Chemistry</i> , 2015, 93, 1219-1225.	0.6	3
7931	DFT/TDDFT investigation on the electronic structures and photophysical properties of phosphorescent platinum(II) complexes with triarylboron/triaryl nitrogen-functionalized N-heterocyclic carbene chelate ligands. <i>Chemical Physics Letters</i> , 2015, 635, 217-223.	1.2	8

#	ARTICLE	IF	CITATIONS
7932	Thermal Cis-to-Trans Isomerization of Azobenzene-Containing Molecules Enhanced by Gold Nanoparticles: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 17369-17377.	1.5	52
7933	The electronic states of a double carbon vacancy defect in pyrene: a model study for graphene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12778-12785.	1.3	17
7934	Electronic stress tensor analysis of molecules in gas phase of CVD process for gesbte alloy. <i>Journal of Computational Chemistry</i> , 2015, 36, 1240-1251.	1.5	10
7935	The effect of density functional dispersion correction (DFT-D3) on lignans. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 60-63.	1.1	6
7936	A DFT study on structures, frontier molecular orbitals and UV-vis spectra of [M(L)(N ₃)(C ₇ H ₅ N)(PPh ₃)] (M= Ru and Fe; L= Tp and Cp). <i>Journal of Organometallic Chemistry</i> , 2015, 791, 72-81.	0.8	15
7937	Synthesis of poly(thiophene-alt-pyrrole) from a difunctionalized thienylpyrrole by Kumada polycondensation. <i>Tetrahedron</i> , 2015, 71, 5399-5406.	1.0	7
7938	Mechanistic Understanding of the Aryl-Dependent Ring Formations in Rh(III)-Catalyzed C-H Activation/Cycloaddition of Benzamides and Methylene cyclopropanes by DFT Calculations. <i>Organometallics</i> , 2015, 34, 3012-3020.	1.1	68
7939	How Can We Understand Au ₈ Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au ₂₄ (ER) ₂₀ and Au ₂₀ (ER) ₁₆ (E = Se, S; R = Ph, Me)? A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 8593-8602.	6.6	25
7940	Site-selective formation of an iron(IV) oxo species at the more electron-rich iron atom of heteroleptic 1/4-nitrido diiron phthalocyanines. <i>Chemical Science</i> , 2015, 6, 5063-5075.	3.7	70
7941	Contrasting the optical properties of the different isomers of oligophenylene. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 17854-17863.	1.3	25
7942	Phosphorescent, Cyclometalated Cinchophen-Derived Platinum Complexes: Syntheses, Structures, and Electronic Properties. <i>Inorganic Chemistry</i> , 2015, 54, 6528-6536.	1.9	23
7943	4-N,N-Dimethylaminophenyl azide photooxidation: effect of conditions on the reaction pathway. Ring contraction of benzene to cyclopentadiene due to a strongly electron-donating substituent. <i>Tetrahedron Letters</i> , 2015, 56, 4661-4665.	0.7	10
7944	Synthesis and Reactivity of Oxorhenium(V) Methyl, Benzyl, and Phenyl Complexes with CO: Implications for a Unique Mechanism for Migratory Insertion. <i>Organometallics</i> , 2015, 34, 3152-3158.	1.1	15
7945	Mechanistic insights into the synergistic catalysis by Au(I), Ga(III), and counterions in the Nakamura reaction. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 7412-7420.	1.5	28
7946	Design and application of a water-soluble phosphorescent Ru(II) complex as turn-on sensing material for Hg ²⁺ . <i>Journal of Materials Chemistry B</i> , 2015, 3, 6205-6212.	2.9	18
7947	Generalized vibrational perturbation theory for rovibrational energies of linear, symmetric and asymmetric tops: Theory, approximations, and automated approaches to deal with medium-large molecular systems. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 948-982.	1.0	95
7948	Mechanism of palladium(II)-catalyzed reaction between styrene and carbazole. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 47-51.	1.1	3
7949	Synthesis of Carboxylate Cp*Zr(IV) Species: Toward the Formation of Novel Metallocavitands. <i>Inorganic Chemistry</i> , 2015, 54, 5547-5555.	1.9	7

#	ARTICLE	IF	CITATIONS
7950	Powerful Bis-facially Pyrazolate-Bridged Dinuclear Ruthenium Epoxidation Catalyst. <i>Inorganic Chemistry</i> , 2015, 54, 6782-6791.	1.9	11
7951	Anharmonic simulations of the vibrational spectrum of sulfated compounds: application to the glycosaminoglycan fragment glucosamine 6-sulfate. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25705-25713.	1.3	33
7952	Photophysical, electrochemical, and spectroelectrochemical investigation of electronic σ -push π -pull benzothiadiazole fluorophores. <i>Pure and Applied Chemistry</i> , 2015, 87, 649-661.	0.9	19
7953	Theoretical Studies on the Redox-Stimulated Isomerization in Electrochromic Osmium Sulfoxide Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4244-4251.	1.1	6
7954	Controlling Factors in the Rates of Oxidation of Anilines and Phenols by Triplet Methylene Blue in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3233-3243.	1.1	48
7955	Stoichiometric and Catalytic Solid \rightarrow Gas Reactivity of Rhodium Bis-phosphine Complexes. <i>Organometallics</i> , 2015, 34, 1487-1497.	1.1	24
7956	Oxidative Addition of Chlorohydrocarbons to a Rhodium Tris(pyrazolyl)borate Complex. <i>Organometallics</i> , 2015, 34, 1552-1566.	1.1	21
7957	Rational Synthesis and Characterization of Dimolybdenum(II) Compounds Bearing Ferrocenyl-Containing Ligands toward Modulation of Electronic Coupling. <i>Inorganic Chemistry</i> , 2015, 54, 3272-3280.	1.9	4
7958	Catalytic Activity of Molybdenum(II) Complexes in Homogeneous and Heterogeneous Conditions. <i>Organometallics</i> , 2015, 34, 1465-1478.	1.1	21
7959	Synthesis and some properties of 2 H-benzimidazole 1,3-dioxides. <i>Tetrahedron</i> , 2015, 71, 7233-7244.	1.0	14
7960	Synthesis and structure of rhodium(σ) silyl carbonyl complexes: photochemical C \rightarrow F and C \rightarrow H bond activation of fluorinated aromatic compounds. <i>Dalton Transactions</i> , 2015, 44, 9450-9469.	1.6	19
7961	Ruthenium \rightarrow Catalyzed Oxidative Coupling of Primary Amines with Internal Alkynes through C \rightarrow H Bond Activation: Scope and Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2015, 21, 8626-8636.	1.7	38
7962	Preference for sulfoxide S- or O-bonding to 3d transition metals \rightarrow DFT insights. <i>Journal of Organometallic Chemistry</i> , 2015, 792, 167-176.	0.8	9
7963	Asymmetric binuclear Ni(II) and Cu(II) Schiff base metallopolymers. <i>RSC Advances</i> , 2015, 5, 39495-39504.	1.7	4
7964	Theoretical investigation of the hydrogen shift reactions in peroxy radicals derived from the atmospheric decomposition of 3-methyl-3-buten-1-ol (MBO331). <i>Chemical Physics Letters</i> , 2015, 619, 236-240.	1.2	19
7965	The first diperoxidovanadium complex with a monodentate amine ligand: Synthesis, characterization and crystal structure of methylbenzylammonium oxido-diperoxido-methylbenzylaminevanadate monohydrate. <i>Inorganic Chemistry Communication</i> , 2015, 56, 105-107.	1.8	9
7966	Theoretical analysis of the S \rightarrow P bond in a family of compounds that involve a P2S2 ring: role of the PBE0-1/5 exchange \rightarrow correlation functional. <i>Computational and Theoretical Chemistry</i> , 2015, 1062, 36-43.	1.1	5
7967	Synthesis and Photophysics of a 2,7-Disubstituted Donor \rightarrow Acceptor Pyrene Derivative: An Example of the Application of Sequential Ir-Catalyzed C \rightarrow H Borylation and Substitution Chemistry. <i>Journal of Organic Chemistry</i> , 2015, 80, 5658-5665.	1.7	64

#	ARTICLE	IF	CITATIONS
7968	Palladium catalysed sequential imine arylation/Suzuki-Miyaura coupling: synthesis of β -(biaryl)benzylamines. <i>Tetrahedron</i> , 2015, 71, 3314-3324.	1.0	6
7969	On copper-copper bond in hydrated cupric acetate. <i>Computational and Theoretical Chemistry</i> , 2015, 1061, 1-5.	1.1	14
7970	Mechanism of trifluoromethylation reactions with well-defined NHC copper trifluoromethyl complexes and iodobenzene: A computational exploration. <i>Chinese Chemical Letters</i> , 2015, 26, 564-566.	4.8	9
7971	Comparing spectroscopic and electrochemical properties of complexes of type $Cp^*M(\eta^3-C_3H_5)(CO)_2$ ($Cp^* = Ni, Pd, Pt$): A complementary experimental and DFT study. <i>Journal of Organometallic Chemistry</i> , 2015, 792, 154-166.	0.8	8
7972	Inclusion process of tetracycline in β and γ -cyclodextrins: A theoretical investigation. <i>Chemical Physics Letters</i> , 2015, 626, 80-84.	1.2	20
7973	The Stabilizing Role of the Intramolecular C-H...O Hydrogen Bond in Cyclic Amides Derived From β -Methylbenzylamine. <i>Journal of Organic Chemistry</i> , 2015, 80, 4481-4490.	1.7	27
7974	Boyd Group Electronegativity Influence on the Parr Global Electrophilicity of Vilsmeier Reagent-Derived Imidates: New Insights toward Improving Mitsunobu Chemistry. <i>Helvetica Chimica Acta</i> , 2015, 98, 582-588.	1.0	0
7975	Designing hydrophobic sheet protected Eu(III)-tetracycline complex using long chain unsaturated fatty acid: Efficient antenna effect in aqueous medium. <i>Journal of Luminescence</i> , 2015, 160, 262-270.	1.5	6
7976	Competitive formation of the methylene and methylene ether bridges in the urea-formaldehyde reaction in alkaline solution: a combined experimental and theoretical study. <i>Wood Science and Technology</i> , 2015, 49, 475-493.	1.4	30
7977	Oxygen Activation by N-doped Graphitic Carbon Nanostructures. <i>Materials Research Society Symposia Proceedings</i> , 2015, 1725, 12.	0.1	0
7978	Applicability of Mulliken's formula for photoinduced and intramolecular charge-transfer energies. <i>Chemical Physics Letters</i> , 2015, 625, 98-103.	1.2	7
7979	Photodynamic behavior of electronic coupling in a N-methylformamide dimer. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12356-12364.	1.3	0
7980	Electronic Circular Dichroism of Highly Conjugated π -Systems: Breakdown of the Tamm-Dancoff/Configuration Interaction Singles Approximation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3653-3662.	1.1	23
7981	Characterizing the Intermediates Compound I and II in the Cytochrome P450 Catalytic Cycle with Nonlinear X-ray Spectroscopy: A Simulation Study. <i>ChemPhysChem</i> , 2015, 16, 2006-2014.	1.0	5
7982	Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Synthesis, Characterization, and Application in OLEDs. <i>Chemistry - A European Journal</i> , 2015, 21, 9133-9149.	1.7	47
7983	Investigation of Fragmentation of Tryptophan Nitrogen Radical Cation. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1388-1393.	1.2	8
7984	Excitation of the 4 lowest electronic transitions in methanol by low-energy electrons. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 115208.	0.6	17
7985	Unconventional bond functions for quantum chemical calculations. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	7

#	ARTICLE	IF	CITATIONS
7986	Model Studies on the Dimerization of 1,3-Diacetylenes. <i>Journal of Organic Chemistry</i> , 2015, 80, 5077-5083.	1.7	11
7987	Free-radical copolymerisation of acrylamides, acrylates, and $\hat{1}\pm$ -olefins. <i>Molecular Physics</i> , 2015, 113, 1809-1822.	0.8	2
7988	Solution structural characterization of an array of nanoscale aqueous inorganic Ga ₁₃ âˆ™xIn _x (0 â‰ˆ% x â‰ˆ%) Tj ETQq0,0,0 rgBT /Overlock 1	3.7	12
7989	Linker dependence of interfacial electron transfer rates in Fe(II)-polypyridine sensitized solar cells. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 134205.	0.7	19
7990	Explicit solvent simulations of the aqueous oxidation potential and reorganization energy for neutral molecules: gas phase, linear solvent response, and non-linear response contributions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14811-14826.	1.3	19
7991	Electronically excited states of PANH anions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14761-14772.	1.3	23
7992	Fe(III) salEen derived Schiff base complexes as potential contrast agents. <i>Inorganica Chimica Acta</i> , 2015, 432, 258-266.	1.2	10
7993	Comparison of 2-Arylnaphtho[2,3- <i>b</i>]phospholes and 2-Arylbenzo[<i>b</i>]phospholes: Effects of 2-Aryl Groups and Fused Arene Moieties on Their Optical and Photophysical Properties. <i>Journal of Organic Chemistry</i>, 2015, 80, 5944-5950.</i></i>	1.7	46
7994	Ratiometric Iridium(III) Complex-Based Phosphorescent Chemodosimeter for Hg ²⁺ Applicable in Time-Resolved Luminescence Assay and Live Cell Imaging. <i>Analytical Chemistry</i> , 2015, 87, 3255-3262.	3.2	37
7995	Preparation of pyranilidene complexes of ruthenium. <i>Dalton Transactions</i> , 2015, 44, 7411-7418.	1.6	4
7996	Absolute configuration of remisporines A & B. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 4169-4173.	1.5	9
7997	Insights into the coordination chemistry of alkanes to metal carbonyls from quantum chemical calculations. <i>Journal of Organometallic Chemistry</i> , 2015, 793, 241-247.	0.8	3
7998	Mass Spectrometry and Theoretical Studies on Nâ€™C Bond Cleavages in the <i>b</i>N-<i>b</i>Sulfonylamidino Thymine Derivatives. <i>Journal of the American Society for Mass Spectrometry</i>, 2015, 26, 833-842.</i></i>	1.2	2
7999	Novel, axially chiral analogues of nickelocene with nickeladibenzofluorenyl ligand. <i>Journal of Organometallic Chemistry</i> , 2015, 785, 26-31.	0.8	2
8000	Reduction of hydroxy-functionalised carbaboranyl carboxylic acids and ketones by organolithium reagents. <i>Dalton Transactions</i> , 2015, 44, 6638-6644.	1.6	6
8001	Synthesis of jiadifenin using Mizorokiâ€™Heck and Tsujiâ€™Trost reactions. <i>Tetrahedron</i> , 2015, 71, 2199-2209.	1.0	15
8002	Atropurpuranâ€™missing biosynthetic link leading to the hetidine and arcutine C 20 -diterpenoid alkaloids or an oxidative degradation product?. <i>Tetrahedron Letters</i> , 2015, 56, 3600-3603.	0.7	25
8003	Improved open-circuit voltage of benzodithiophene based polymer solar cells using bulky terthiophene side group. <i>Solar Energy Materials and Solar Cells</i> , 2015, 138, 26-34.	3.0	23

#	ARTICLE	IF	CITATIONS
8004	<i>Ab Initio</i> Molecular Dynamics of High-Temperature Unimolecular Dissociation of Gas-Phase RDX and Its Dissociation Products. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2747-2759.	1.1	47
8005	Design of a Versatile and Improved Precatalyst Scaffold for Palladium-Catalyzed Cross-Coupling: (η^3 -1- tBu-indenyl) $_{2}$ ($\eta^4\text{-Cl}$) $_{2}$ Pd $_{2}$. <i>ACS Catalysis</i> , 2015, 5, 3680-3688.	5.5	133
8006	Complexes of fluconazole with sodium p-sulfonatocalix[n]arenes: characterization, solubility and antifungal activity. <i>RSC Advances</i> , 2015, 5, 44317-44325.	1.7	24
8007	Molecular Modeling and Optimization. , 2015, , 11-38.		0
8008	Effect of Sulfuric and Triflic Acids on the Hydration of Vanadium Cations: An <i>Ab Initio</i> Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5749-5761.	1.1	29
8009	Divalent metals can reside on bonds in fullerenes. <i>Dalton Transactions</i> , 2015, 44, 9561-9568.	1.6	9
8010	Characterization of compounds derived from copper-oxamate and imidazolium by X-ray absorption and vibrational spectroscopies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 142, 303-310.	2.0	9
8011	Computational Study of Monosubstituted Azo(tetrazolepentazolium)-Based Ionic Dimers. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5826-5841.	1.1	5
8012	Mechanistic study on the Cp*iridium-catalyzed N-alkylation of amines with alcohols. <i>RSC Advances</i> , 2015, 5, 22996-23008.	1.7	18
8013	Stereoselective Syntheses of (+)-2- <i>epi</i> -Deoxoprosopinine, ($\hat{\alpha}$)-Deoxoprosophylline, (+)- <i>cis</i> -195A, and 2,5-Di- <i>epi</i> - <i>cis</i> -195A from a Common Chiral Nonracemic Building Block. <i>Journal of Organic Chemistry</i> , 2015, 80, 5236-5251.	1.7	13
8014	Trimethylamine sorption into thin layers of fluoroalkoxy and alkyloxy substituted phthalocyanines: Optical detection and DFT calculations. <i>Sensors and Actuators B: Chemical</i> , 2015, 216, 204-211.	4.0	17
8015	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. <i>Chemistry - A European Journal</i> , 2015, 21, 9083-9092.	1.7	116
8016	Unusual crystallographic existence of a hydrated zinc(ii) bisulphate complex: experimental and theoretical observations. <i>RSC Advances</i> , 2015, 5, 42681-42688.	1.7	5
8017	Structural Control of Nonadiabatic Bond Formation: The Photochemical Formation and Stability of Substituted 4a,4b-Dihydrotriphenylenes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3972-3985.	1.1	14
8018	Phonon Modes of Organic Electro-Optic Molecular Crystals for Terahertz Photonics. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10031-10039.	1.5	20
8019	Directional Control of π -Conjugation Enabled by Distortion of the Donor Plane in Diarylaminoanthracenes: A Photophysical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4898-4906.	1.1	69
8020	Synthesis of $\hat{\pm}$ -Amino Acidato Derivatives of Niobium and Tantalum Pentahalides and Their Conversion into Iminium Salts. <i>Inorganic Chemistry</i> , 2015, 54, 4047-4055.	1.9	18
8021	Silane-Functionalized $\langle i \rangle N \langle /i \rangle$ -Heterocyclic Carbene $\hat{\text{C}}$ Cobalt Complexes Containing a Five-Coordinate Silicon with a Covalent Co $\hat{\text{C}}$ Si Bond. <i>Organometallics</i> , 2015, 34, 1546-1551.	1.1	34

#	ARTICLE	IF	CITATIONS
8022	Reversible Substrate Activation and Catalysis at an Intact Metal–Metal Bond Using a Redox-Active Supporting Ligand. <i>Journal of the American Chemical Society</i> , 2015, 137, 6104-6110.	6.6	146
8023	The Reaction Mechanism with Free Energy Barriers for Electrochemical Dihydrogen Evolution on MoS ₂ . <i>Journal of the American Chemical Society</i> , 2015, 137, 6692-6698.	6.6	173
8024	Azole Assisted C–H Bond Activation Promoted by an Osmium-Polyhydride: Discerning between N and NH. <i>Organometallics</i> , 2015, 34, 1898-1910.	1.1	29
8025	Theoretical investigation of different functional groups effect on the photophysical performance of tricarbonylrhenium(I) complexes with tetrathiafulvalene derivative as dyes in dye-sensitized solar cell. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	3
8026	C [∞] C* cyclometalated platinum(II) N-heterocyclic carbene complexes with a sterically demanding 1 ² -diketonato ligand synthesis, characterization and photophysical properties. <i>Dalton Transactions</i> , 2015, 44, 8444-8455.	1.6	24
8027	Synthesis of Polyurethanes Using Organocatalysis: A Perspective. <i>Macromolecules</i> , 2015, 48, 3153-3165.	2.2	237
8028	Establishing the Hydride Donor Abilities of Main Group Hydrides. <i>Organometallics</i> , 2015, 34, 1818-1827.	1.1	155
8029	Insights into Laccase Engineering from Molecular Simulations: Toward a Binding-Focused Strategy. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1447-1453.	2.1	55
8030	A Strategy to Stabilize Kesterite CZTS for High-Performance Solar Cells. <i>Chemistry of Materials</i> , 2015, 27, 2920-2927.	3.2	63
8031	The Synthesis and Structural Characterization of Polycyclic Derivatives of Cobalt Bis(dicarbollide)(1 ⁺). <i>Inorganic Chemistry</i> , 2015, 54, 3148-3158.	1.9	12
8032	Synthesis of hexabenzocoronene-layered compounds. <i>Tetrahedron Letters</i> , 2015, 56, 2086-2090.	0.7	6
8033	One-Step Synthesis of a [20]Silafullerane with an Endohedral Chloride Ion. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 5429-5433.	7.2	79
8034	Nickel complexes of 1,2,4-triazole derived amido-functionalized N-heterocyclic carbene ligands: Synthesis, theoretical studies and catalytic application. <i>Journal of Organometallic Chemistry</i> , 2015, 786, 63-70.	0.8	22
8035	Mononuclear zinc(II), cadmium(II), cobalt(III) and di-nuclear nickel(II) complexes of a 14π electron diimine ligand: Syntheses, structures, photoluminescence and DFT investigations. <i>Inorganica Chimica Acta</i> , 2015, 430, 199-207.	1.2	7
8036	Regioselective synthesis and ab initio calculations of fused heterocycles thermally and under microwave irradiation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 148, 175-183.	2.0	6
8037	Conformational landscape and low lying excited states of imatinib. <i>Journal of Molecular Modeling</i> , 2015, 21, 84.	0.8	5
8038	A Study on the Effect of Dianionic Tridentate Ligands on the Radiative and Nonradiative Processes for Gold(III) Alkynyl Systems by a Computational Approach. <i>Inorganic Chemistry</i> , 2015, 54, 3624-3630.	1.9	36
8039	To the limit of gas-phase electron diffraction: Molecular structure of magnesium octa(m-trifluoromethylphenyl)porphyrzine. <i>Journal of Molecular Structure</i> , 2015, 1092, 104-112.	1.8	14

#	ARTICLE	IF	CITATIONS
8040	Linear Photophysics, Stimulated Emission, and Ultrafast Spectroscopy of New Two-Photon Absorbing Diketopyrrolopyrrole Derivatives. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8864-8875.	1.5	16
8041	Diffusion of Benzene in the Breathing Metal-Organic Framework MIL-53(Cr): A Joint Experimental-Computational Investigation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 8217-8225.	1.5	38
8042	Influence of substituents on cation-anion contacts in imidazolium perchlorates. <i>Dalton Transactions</i> , 2015, 44, 8669-8677.	1.6	9
8043	Density Functional Theory Study of Rh(III)-Catalyzed C-H Activations and Intermolecular Annulations between Benzamide Derivatives and Allenes. <i>Inorganic Chemistry</i> , 2015, 54, 3958-3969.	1.9	25
8044	Redox processes of 2,6-dichlorophenolindophenolate in different solvents. A combined electrochemical, spectroelectrochemical, photochemical, and theoretical study. <i>Journal of Solid State Electrochemistry</i> , 2015, 19, 2633-2642.	1.2	8
8045	Isatin-phenylhydrazone dyes and boron complexes with large Stokes shifts: synthesis and solid-state fluorescence characteristics. <i>Tetrahedron</i> , 2015, 71, 3802-3809.	1.0	10
8046	C-H and H-H bond activation via ligand dearomatization/rearomatization of a PN ₃ -P-rhodium complex. <i>Dalton Transactions</i> , 2015, 44, 15111-15115.	1.6	33
8047	Swivel-Cruciform Stilbenes Based on Bithiophene. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2394-2404.	1.2	2
8048	Large impact of reorganization energy on photovoltaic conversion due to interfacial charge-transfer transitions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12228-12237.	1.3	43
8049	Electronic structure and spectroscopic properties of 6-aminophenanthridine and its derivatives: Insights from density functional theory. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 846-852.	1.0	0
8050	Modeling, kinetic, and equilibrium characterization of paraquat adsorption onto polyurethane foam using the ion-pairing technique. <i>Journal of Environmental Management</i> , 2015, 156, 200-208.	3.8	23
8051	DFT investigations on the ring-opening polymerization of substituted cyclic carbonates catalyzed by zinc-diketiminato complexes. <i>Polymer Chemistry</i> , 2015, 6, 3336-3352.	1.9	23
8052	Computational Molecular Simulation of the Oxidative Adsorption of Ferrous Iron at the Hematite (001)-Water Interface. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9242-9252.	1.5	30
8053	Second-order Møller-Plesset perturbation (MP2) theory at finite temperature: relation with Surjain's density matrix MP2 and its application to linear-scaling divide-and-conquer method. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	9
8054	Computational design of faster rotating second-generation light-driven molecular motors by control of steric effects. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21740-21751.	1.3	24
8055	Quantum chemical protocols for modeling reactions and spectra in astrophysical ice analogs: the challenging case of the C ⁺ + H ₂ O reaction in icy grain mantles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28705-28718.	1.3	8
8056	Facet shapes and thermo-stabilities of H ₂ SO ₄ -HNO ₃ hydrates involved in polar stratospheric clouds. <i>Journal of Molecular Modeling</i> , 2015, 21, 238.	0.8	2
8057	P(OH) to P=OH Tautomerism: A Theoretical and Experimental Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 10025-10032.	1.7	114

#	ARTICLE	IF	CITATIONS
8058	Bis(pyrrolidene) Schiff Base Aluminum Complexes as Isoselective-Biased Initiators for the Controlled Ring-Opening Polymerization of <i>rac</i> -Lactide: Experimental and Theoretical Studies. <i>Macromolecules</i> , 2015, 48, 6846-6861.	2.2	57
8059	Use of 5-formylfuranboronic acid in the formation of bicyclic boronates with photophysical properties. <i>Inorganica Chimica Acta</i> , 2015, 438, 23-30.	1.2	3
8060	Generalized Reaction Mechanism for the Selective Aerobic Oxidation of Aryl and Alkyl Alcohols over Nitrogen-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26438-26450.	1.5	26
8061	Photophysical characterization of the 9,10-disubstituted anthracene chromophore and its applications in triplet-triplet annihilation photon upconversion. <i>Journal of Materials Chemistry C</i> , 2015, 3, 11111-11121.	2.7	119
8062	Intermolecular Sulfur-Oxygen Interactions: Theoretical and Statistical Investigations. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2138-2153.	2.5	91
8063	Interplay of Molecular Orientation, Film Formation, and Optoelectronic Properties on Isoindigo- and Thienoisindigo-Based Copolymers for Organic Field Effect Transistor and Organic Photovoltaic Applications. <i>Chemistry of Materials</i> , 2015, 27, 6837-6847.	3.2	60
8064	Electronic Structure and Absorption Properties of Strongly Coupled Porphyrin-Perylene Arrays. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9879-9888.	1.1	19
8065	DFT and Kinetic Monte Carlo Study of TMS-Substituted Ruthenium Vinyl Carbenes: Key Intermediates for Stereoselective Cyclizations. <i>ACS Catalysis</i> , 2015, 5, 6255-6262.	5.5	10
8066	Geometric and electronic structures of potassium-adsorbed rubrene complexes. <i>Journal of Chemical Physics</i> , 2015, 142, 244702.	1.2	3
8067	Bingel-Hirsch Reaction on Sc ₂ @C ₆₆ : A Highly Regioselective Bond Neighboring to Unsaturated Linear Triquinanes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26196-26201.	1.5	8
8068	A QM/MM program using frozen localized orbitals and the Huzinaga equation. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	6
8069	Stable Germanolates and Germanes with Exocyclic Structures. <i>Organometallics</i> , 2015, 34, 5291-5297.	1.1	24
8070	Effects of an acidic-alkaline environment on the reactivity of 5-carboxycytosine with hydroxyl radicals. <i>RSC Advances</i> , 2015, 5, 87364-87376.	1.7	2
8071	^{99m} Tc labeled macrocyclic aza-oxa and aza-thia probes: synthesis, characterization and in vitro & in vivo biological studies. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2015, 83, 299-307.	0.9	0
8072	Carbocation Stability in H-ZSM5 at High Temperature. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11397-11405.	1.1	14
8073	Toward an Accurate Modeling of Ionic Liquid-TiO ₂ Interfaces. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25260-25267.	1.5	25
8074	DFT Mechanistic Study of Functionalizations of β -Ene-Cyclopropanes and Alkylidenecyclopropanes via Allylic C-H and C-C Bond Cleavage Facilitated by a Zirconocene Complex. <i>Organometallics</i> , 2015, 34, 5233-5244.	1.1	9
8075	A family of mixed-ligand oxidovanadium(<i>v</i>) complexes with aroylhydrazone ligands: a combined experimental and computational study on the electronic effects of para substituents of hydrazone ligands on the electronic properties, DNA binding and nuclease activities. <i>RSC Advances</i> , 2015, 5, 92456-92472.	1.7	21

#	ARTICLE	IF	CITATIONS
8076	Iridium-Catalyzed Asymmetric Hydrogenation with Simple Cyclohexane-Based P/S Ligands: <i>In Situ</i> HP-NMR and DFT Calculations for the Characterization of Reaction Intermediates. <i>Organometallics</i> , 2015, 34, 5321-5334.	1.1	30
8077	How Bonding in Manganous Phosphates Affects their Mn(II) ^{31}P Hyperfine Interactions. <i>Inorganic Chemistry</i> , 2015, 54, 10422-10428.	1.9	7
8078	Trimerization of Alkynes in the Presence of a Hydrotris(pyrazolyl)borate Iridium Catalyst and the Effect of Substituent Groups on the Reaction Mechanism: A Computational Study. <i>Organometallics</i> , 2015, 34, 4965-4974.	1.1	18
8079	Platinum-catalyzed reduction of amides with hydrosilanes bearing dual Si-H groups: a theoretical study of the reaction mechanism. <i>Dalton Transactions</i> , 2015, 44, 19344-19356.	1.6	22
8080	A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E6101-10.	3.3	42
8081	Key factors in determining the arrangement of π -conjugated oligomers inside carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22668-22677.	1.3	12
8082	CASSCF and MRMP2 investigation of the interaction of arsenic adatoms with carbon dimers on the diamond (100)-2 Å^{-1} surface. <i>Surface Science</i> , 2015, 641, 159-165.	0.8	5
8083	Anisotropic elliptical dichroism and influence of imperfection of circular polarization upon anisotropic circular dichroism. <i>Journal of Chemical Physics</i> , 2015, 142, 154102.	1.2	3
8084	The Mechanism of Iron(II)-Catalyzed Asymmetric Mukaiyama Aldol Reaction in Aqueous Media: Density Functional Theory and Artificial Force-Induced Reaction Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 11085-11094.	6.6	41
8085	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	1.2	605
8086	A comparison of neutral and charged species of one- and two-dimensional models of graphene nanoribbons using multireference theory. <i>Journal of Chemical Physics</i> , 2015, 142, 054302.	1.2	15
8087	Gas phase measurements of mono-fluoro-benzoic acids and the dimer of 3-fluoro-benzoic acid. <i>Journal of Chemical Physics</i> , 2015, 142, 144303.	1.2	10
8088	Analysis and comparison of CVS-ADC approaches up to third order for the calculation of core-excited states. <i>Journal of Chemical Physics</i> , 2015, 142, 214104.	1.2	93
8089	The origin for highly enantioselective induction of 1-naphthol to isatin-derived N-Boc ketimines catalyzed by quinine thiourea catalyst: an experimental and computational study. <i>RSC Advances</i> , 2015, 5, 69493-69501.	1.7	41
8090	Rigid Coumarins: a Complete DFT, TD-DFT and Non Linear Optical Property Study. <i>Journal of Fluorescence</i> , 2015, 25, 1469-1480.	1.3	34
8091	Genetic determinants of antithyroid drug-induced agranulocytosis by human leukocyte antigen genotyping and genome-wide association study. <i>Nature Communications</i> , 2015, 6, 7633.	5.8	93
8092	Conformational and structural studies of N-methylacetohydroxamic acid and of its mono- and bis-chelated uranium(VI) complexes. <i>Journal of Inorganic Biochemistry</i> , 2015, 151, 164-175.	1.5	8
8093	Computational insight into the mechanism of the Pd(0)-Brønsted acid cooperatively catalysed head-to-tail dimerization of terminal alkynes. <i>RSC Advances</i> , 2015, 5, 84636-84642.	1.7	6

#	ARTICLE	IF	CITATIONS
8094	Chromophore-Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4825-4839.	2.3	65
8095	The addition of CO ₂ to four superbase ionic liquids: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28674-28682.	1.3	20
8096	The nature of bathochromic shift in the solvated chloranilic acid: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2015, 211, 187-191.	2.3	1
8097	Excited State Absorption from Real-Time Time-Dependent Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4294-4303.	2.3	70
8098	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5197-5208.	2.3	35
8099	Nucleobases tagged to gold nanoclusters cause a mechanistic crossover in the oxidation of CO. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24275-24281.	1.3	7
8100	Molecular iodine adsorption within Hofmann-type structures M(L)[M(CN) ₄] (M = Ni, Co; M Tj F1Qq 0 0 rgBT /Ove	1.6	27
8101	Controlling the Fluorescence Response of PET Sensors via the Metal-Ion π -Contacting Ability of the Fluorophore: Coumarin, a Weaker π Contacter. <i>Inorganic Chemistry</i> , 2015, 54, 9976-9988.	1.9	15
8102	Theoretical examination of competitive $\hat{1}^2$ -radical-induced cleavages of N $\hat{1}$ C $\hat{1}$ and C $\hat{1}$ C $\hat{1}$ bonds of peptides. <i>Canadian Journal of Chemistry</i> , 2015, 93, 1355-1362.	0.6	3
8103	DFT study of molecular hydrogen interaction with photoexcited TiO ₂ surface: Nanocluster model. <i>Chemical Physics Letters</i> , 2015, 639, 225-229.	1.2	6
8104	Exploring the influence of steric hindrance and electronic nature of substituents in the supramolecular arrangements of 5-(substituted phenyl)-2-formylpyrroles. <i>CrystEngComm</i> , 2015, 17, 6406-6419.	1.3	13
8105	Interfacial charge-transfer transitions in a TiO ₂ -benzenedithiol complex with Ti-S-C linkages. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29867-29873.	1.3	34
8106	Characterization of O $\hat{1}$ -Centers on Single Crystalline MgO(001)-Films. <i>Topics in Catalysis</i> , 2015, 58, 811-823.	1.3	5
8107	DFT Study on the Homogeneous Palladium-Catalyzed N-Alkylation of Amines with Alcohols. <i>ACS Catalysis</i> , 2015, 5, 5728-5740.	5.5	26
8108	Correlations between metal spin states and vibrational spectra of $\hat{1}$ trinuclear Fe(II) complex exhibiting spin crossover. <i>Journal of Molecular Structure</i> , 2015, 1101, 8-13.	1.8	2
8109	Synthesis and electronic properties of π -extended flavins. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 10198-10204.	1.5	7
8110	Development of highly accurate approximate scheme for computing the charge transfer integral. <i>Journal of Chemical Physics</i> , 2015, 143, 074109.	1.2	4
8111	Partition, orientation and mobility of ubiquinones in a lipid bilayer. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 1560-1573.	0.5	59

#	ARTICLE	IF	CITATIONS
8112	Reactions of Azine Anions with Nitrogen and Oxygen Atoms: Implications for Titan's Upper Atmosphere and Interstellar Chemistry. <i>Journal of the American Chemical Society</i> , 2015, 137, 10700-10709.	6.6	23
8113	Infrared Spectroscopy of Mobility-Selected H ⁺ -Gly-Pro-Gly-Gly (GPGG). <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1444-1454.	1.2	65
8114	Possibility of Copper-Ion-Exchanged MFI-Type Zeolite as C-H Bond Activation Material for Propane and the Driving Force for Activation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21483-21496.	1.5	12
8115	Inclusion complex thermodynamics: The β -cyclodextrin and sertraline complex example. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 11-17.	1.3	29
8116	Gold-Catalyzed Proto- and Deuterodeboronation. <i>Journal of Organic Chemistry</i> , 2015, 80, 9807-9816.	1.7	28
8117	Role of the Chemically Non-Innocent Ligand in the Catalytic Formation of Hydrogen and Carbon Dioxide from Methanol and Water with the Metal as the Spectator. <i>Journal of the American Chemical Society</i> , 2015, 137, 12330-12342.	6.6	67
8118	Microwave-assisted synthesis, characterisation and mesomorphic investigations of novel disubstituted aroylhydrazones. <i>Liquid Crystals</i> , 2015, 42, 1179-1190.	0.9	8
8119	Understanding Precatalyst Activation in Cross-Coupling Reactions: Alcohol Facilitated Reduction from Pd(II) to Pd(0) in Precatalysts of the Type (i-3-allyl)Pd(L)(Cl) and (i-3-indenyl)Pd(L)(Cl). <i>ACS Catalysis</i> , 2015, 5, 5596-5606.	5.5	89
8120	In silico studies on the origin of selective uptake of carbon dioxide with cucurbit[7]uril amorphous material. <i>RSC Advances</i> , 2015, 5, 72469-72475.	1.7	6
8121	Interstellar Anions: The Role of Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9941-9953.	1.1	47
8122	U@C ₂₈ : the electronic structure induced by the 32-electron principle. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23308-23311.	1.3	40
8123	Calculations of hyperfine coupling constant of copper(II) in aqueous environment. Finite temperature molecular dynamics and relativistic effects. <i>Journal of Molecular Modeling</i> , 2015, 21, 237.	0.8	4
8124	A theoretical study of substituted indeno[1,2-b]fluorene compounds and their possible applications in solar cells. <i>Chemical Physics Letters</i> , 2015, 636, 31-34.	1.2	11
8125	Photochromic Diarylethenes with Heterocyclic Aromatic Rings: Correlation between Thermal Bistability and Geometrical Characters of Transition States. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9140-9147.	1.1	14
8126	In vitro model reaction of sulfur containing bio-relevant ligands with Pt(II) complex: kinetics, mechanism, bioactivity and computational studies. <i>RSC Advances</i> , 2015, 5, 76987-76999.	1.7	17
8127	Reactions of Imines, Nitriles, and Isocyanides with Pentaphenylborole: Coordination, Ring Expansion, C-H Bond Activation, and Hydrogen Migration Reactions. <i>Inorganic Chemistry</i> , 2015, 54, 8957-8968.	1.9	50
8128	Two-photon absorption of fluorescent protein chromophores incorporating non-canonical amino acids: TD-DFT screening and classical dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25563-25571.	1.3	21
8129	Carbon-Nitrogen Bond Construction and Carbon-Oxygen Double Bond Cleavage on a Molecular Titanium Oxonitride: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2015, 54, 9401-9412.	1.9	12

#	ARTICLE	IF	CITATIONS
8130	Synthesis of Azepines via a [6 + 1] Annulation of Ynenitriles with Reformatsky Reagents. <i>Journal of Organic Chemistry</i> , 2015, 80, 9480-9494.	1.7	22
8131	Systematic Investigations on the Roles of the Electron Acceptor and Neighboring Ethynylene Moiety in Porphyrins for Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 21956-21965.	4.0	76
8132	Synthesis and energetic properties of high-nitrogen substituted bishomocubanes. <i>Journal of Materials Chemistry A</i> , 2015, 3, 22118-22128.	5.2	29
8133	Structural characterization of $\hat{\pm}$ -amino acid complexes of molybdates: a spectroscopic and DFT study. <i>RSC Advances</i> , 2015, 5, 9010-9018.	1.7	8
8134	Constrained formation of 2-(1-(arylimino)ethyl)-7-arylimino-6,6-dimethylcyclopentapyridines and their cobalt(Co^{II}) chloride complexes: synthesis, characterization and ethylene polymerization. <i>RSC Advances</i> , 2015, 5, 32720-32729.	1.7	61
8135	Aggregation behavior of dodecylsulfonate-based surface active ionic liquids in water. <i>Journal of Molecular Liquids</i> , 2015, 212, 23-29.	2.3	23
8136	$\text{C}^{\text{sup}}\hat{\text{S}}^{\text{C}^*}$ Cyclometalated Platinum(II) Complexes with Dibenzofuranyl-1,2,4-triazol-5-ylidene Ligands: Synthesis, Characterization, and Photoluminescent Properties. <i>Organometallics</i> , 2015, 34, 4433-4440.	1.1	20
8137	Computational prediction of cyclometalated Ir(III), Rh(III) and Co(III) amido complexes to capture up to three CO ₂ molecules. <i>Dalton Transactions</i> , 2015, 44, 16847-16853.	1.6	2
8138	Application of Koopmans's theorem for density functional theory to full valence-band photoemission spectroscopy modeling. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 149, 434-440.	2.0	10
8139	Fluoride-free Hiyama coupling by palladium abnormal N-heterocyclic carbene complexes. <i>Dalton Transactions</i> , 2015, 44, 17617-17628.	1.6	44
8140	Mechanistic study for the formation of polyoxymethylene dimethyl ethers promoted by sulfonic acid-functionalized ionic liquids. <i>Journal of Molecular Catalysis A</i> , 2015, 408, 228-236.	4.8	53
8141	Charge-transfer complex versus $\hat{\text{f}}$ -complex formed between TiO ₂ and bis(dicyanomethylene) electron acceptors. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27343-27356.	1.3	21
8142	Oximes in the Isoxazolone, Pyrazolone, and 1,2,3-Triazolone Series: Experimental and Computational Investigation of Energies and Structures of E/Z Isomers of $\hat{\pm}$ -Oxo-Oximes in the Gas Phase and in Solution. <i>Australian Journal of Chemistry</i> , 2015, 68, 1329.	0.5	5
8143	Benchmarking the completely renormalised equation-of-motion coupled-cluster approaches for vertical excitation energies. <i>Molecular Physics</i> , 2015, 113, 3085-3127.	0.8	43
8144	Dipyrrin-based complexes for solution-processed organic solar cells. <i>Chemical Research in Chinese Universities</i> , 2015, 31, 801-808.	1.3	7
8145	Correlating geometry of multidimensional carbon allotropes molecules and stability. <i>Organic Electronics</i> , 2015, 26, 395-399.	1.4	11
8146	Energy-Efficient Computational Chemistry: Comparison of x86 and ARM Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5055-5061.	2.3	17
8147	Two-dimensional carbon-based conductive materials with dynamically controlled asymmetric Dirac cones. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31902-31910.	1.3	5

#	ARTICLE	IF	CITATIONS
8148	Toxicity Originating from Thiophene Containing Drugs: Exploring the Mechanism using Quantum Chemical Methods. <i>Chemical Research in Toxicology</i> , 2015, 28, 2364-2376.	1.7	35
8149	<i>anti</i> -Diradical Formation in 1,3-Dipolar Cycloadditions of Nitrile Oxides to Acetylenes. <i>Journal of Organic Chemistry</i> , 2015, 80, 12321-12332.	1.7	29
8150	Novel phosphorescent iridium(III) complexes containing 2-thienyl quinazoline ligands: synthesis, photophysical properties and theoretical calculations. <i>RSC Advances</i> , 2015, 5, 97841-97848.	1.7	12
8151	Porphyrins Containing a Triphenylamine Donor and up to Eight Alkoxy Chains for Dye-Sensitized Solar Cells: A High Efficiency of 10.9%. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 27976-27985.	4.0	137
8152	A Computational Re-examination of the Criegee Intermediate's Sulfur Dioxide Reaction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10316-10335.	1.1	60
8153	Molecular structures of Pr@C ₇₂ and Pr@C ₇₂ (C ₆ H ₃ Cl ₂): a combined experimental-theoretical investigation. <i>RSC Advances</i> , 2015, 5, 97568-97578.	1.7	6
8154	A Suite of Tetraphenylethylene-Based Discrete Organoplatinum(II) Metallacycles: Controllable Structure and Stoichiometry, Aggregation-Induced Emission, and Nitroaromatics Sensing. <i>Journal of the American Chemical Society</i> , 2015, 137, 15276-15286.	6.6	260
8155	A catalytic route to dibenzodiazepines involving Buchwald-Hartwig coupling: reaction scope and mechanistic consideration. <i>RSC Advances</i> , 2015, 5, 99990-99999.	1.7	12
8156	Metal- and Ligand-Assisted CO ₂ Insertion into Ru-C, Ru-N, and Ru-O Bonds of Ruthenium(II) Phosphine Complexes: A Density Functional Theory Study. <i>Inorganic Chemistry</i> , 2015, 54, 502-512.	1.9	9
8157	Computational studies of the effects of ortho- and para- ring activation on the kinetics of S _N Ar reactions of 1-chloro-2-nitrobenzene and 1-phenoxy-2-nitrobenzene with aniline. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 57-67.	0.9	10
8158	Cyclometalated Fe(II) Complexes as Sensitizers in Dye-Sensitized Solar Cells. <i>Inorganic Chemistry</i> , 2015, 54, 560-569.	1.9	78
8159	Molecular insight into the interaction mechanisms of amino-2-H-imidazole derivatives with BACE1 protease: A QM/MM and QAIM study. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 389-397.	1.0	20
8160	Experimental and Computational Study of the Catalytic Asymmetric 4-Electrocyclization of N-Heterocycles. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2762-2765.	7.2	50
8161	Structure and catalytic activities of ferrous centers confined on the interface between carbon nanotubes and humic acid. <i>Nanoscale</i> , 2015, 7, 2651-2658.	2.8	7
8162	Quantum Chemical Approach to Estimating the Thermodynamics of Metabolic Reactions. <i>Scientific Reports</i> , 2014, 4, 7022.	1.6	34
8164	Structural insights into the interactions of <i>apt</i> riboswitch with novel guanine analogues: a molecular dynamics simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 234-243.	2.0	3
8165	Finding the Reactive Electron in Paramagnetic Systems: A Critical Evaluation of Accuracies for EPR Spectroscopy and Density Functional Theory Using 1,3,5-Triphenyl Verdazyl Radical as a Testcase. <i>Applied Magnetic Resonance</i> , 2015, 46, 117-139.	0.6	8
8166	Composite Method for Implicit Representation of Solvent in Dimethyl Sulfoxide and Acetonitrile. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5173-5180.	1.1	22

#	ARTICLE	IF	CITATIONS
8167	Efficient light-to-current conversion by organic-inorganic interfacial charge-transfer transitions in TiO ₂ chemically adsorbed with 2-anthraic acid. <i>Chemical Physics Letters</i> , 2015, 619, 180-184.	1.2	51
8168	Analysis of computational models for an accurate study of electronic excitations in GFP. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2582-2588.	1.3	47
8169	A Combined Experimental and Computational Investigation on the Unusual Molecular Mechanism of the Lossen Rearrangement Reaction Activated by Carcinogenic Halogenated Quinones. <i>Journal of Organic Chemistry</i> , 2015, 80, 180-189.	1.7	24
8170	Synthesis and Characterization of Nitrogen-Rich Macrocyclic Ligands and an Investigation of Their Coordination Chemistry with Lanthanum(III). <i>Inorganic Chemistry</i> , 2015, 54, 97-109.	1.9	14
8171	Rhodamine-based fluorescent probe for highly selective detection of glutathione over cysteine and homocysteine. <i>Sensors and Actuators B: Chemical</i> , 2015, 209, 838-845.	4.0	56
8173	Are Solvent and Dispersion Effects Crucial in Olefin Polymerization DFT Calculations? Some Insights from Propylene Coordination and Insertion Reactions with Group 3 and 4 Metallocenes. <i>ACS Catalysis</i> , 2015, 5, 416-425.	5.5	61
8174	Metalloporphyrins with all the pyrrole nitrogens replaced with phosphorus atoms, MP(P) ₄ (M = Sc, Ti). <i>Journal of Inorganic Biochemistry</i> , 2015, 143, 20-33.	0.9	12
8175	Ring closing metathesis by Hoveyda-Grubbs catalysts: A theoretical approach of some aspects of the initiation mechanism and the influence of solvent. <i>Inorganica Chimica Acta</i> , 2015, 426, 20-28.	1.2	8
8176	Structural and theoretical studies on rhodium and iridium complexes with 5-nitrosopyrimidines. Effects on the proteolytic regulatory enzymes of the renin-angiotensin system in human tumoral brain cells. <i>Journal of Inorganic Biochemistry</i> , 2015, 143, 20-33.	1.5	12
8177	On the origins of regioselectivity in the orthoester Claisen rearrangement of bisallylic alcohols. <i>Tetrahedron Letters</i> , 2015, 56, 1297-1301.	0.7	1
8178	Dihydrogen Catalysis of the Reversible Formation and Cleavage of C-H and Ni-H Bonds of Aminopyridinate Ligands Bound to (i- ⁵ - ⁵ -Me ⁵)Ir ^{III} . <i>Chemistry - A European Journal</i> , 2015, 21, 2576-2587.	1.7	13
8179	Anion binding by biotin[6]uril in water. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 369-373.	1.5	76
8180	Theoretical Insights into the Impact of Ru Catalyst Anchors on the Efficiency of Photocatalytic CO ₂ Reduction on Ta ₂ O ₅ . <i>Journal of Physical Chemistry B</i> , 2015, 119, 7186-7197.	1.2	20
8181	Segmented Contracted Basis Sets Optimized for Nuclear Magnetic Shielding. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 132-138.	2.3	235
8182	A contribution to the rational design of Ru(CO) ₃ Cl ₂ L complexes for in vivo delivery of CO. <i>Dalton Transactions</i> , 2015, 44, 5058-5075.	1.6	67
8183	Oxidative halogenation of cisplatin and carboplatin: synthesis, spectroscopy, and crystal and molecular structures of Pt(^{iv}) prodrugs. <i>Dalton Transactions</i> , 2015, 44, 119-129.	1.6	49
8184	Mind the correct basis set: A case study for predicting gas phase acidities of small compounds using calculations from first principles. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 42-49.	1.0	2
8185	Transformation of Zwitterionic Pyridine Derivatives to a Spiro-Fused Ring System: Azoniabenzo[<i>de</i>]fluorine. <i>Synthesis and Mechanistic Rationalization</i> . <i>Journal of Organic Chemistry</i> , 2015, 80, 174-179.	1.7	2

#	ARTICLE	IF	CITATIONS
8186	Rhodium Bis(quinolinyl)benzene Complexes for Methane Activation and Functionalization. <i>Chemistry - A European Journal</i> , 2015, 21, 1286-1293.	1.7	24
8187	Neutral benzoquinolate cyclometalated platinum(II) complexes as precursors in the preparation of luminescent Pt ^{II} -Ag complexes. <i>Inorganica Chimica Acta</i> , 2015, 424, 136-149.	1.2	23
8188	Initiation stage of alkene metathesis: Insights from natural bond orbital and charge decomposition analyses. <i>Chemical Physics Letters</i> , 2015, 618, 174-181.	1.2	6
8189	Differences and Comparisons of the Properties and Reactivities of Iron(III)-hydroperoxo Complexes with Saturated Coordination Sphere. <i>Chemistry - A European Journal</i> , 2015, 21, 1221-1236.	1.7	67
8190	(C ¹ S ²)-cyclometalated platinum(II) imidazo[1,5-a]pyridine NHC complexes – Synthesis and characterization. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 155-163.	0.8	18
8191	An insight into a base-free Michael addition reaction as catalyzed by a bifunctional nickel N-heterocyclic carbene complex using density functional theory studies. <i>Journal of Organometallic Chemistry</i> , 2015, 775, 109-116.	0.8	23
8192	Computationally motivated synthesis and enzyme kinetic evaluation of N-(2-d-glucopyranosyl)-1,2,4-triazolecarboxamides as glycogen phosphorylase inhibitors. <i>MedChemComm</i> , 2015, 6, 80-89.	3.5	10
8193	Infrared and Raman bands of cyclopentadienyl ligands as indicators of electronic configuration of metal centers in metallocenes. <i>Journal of Organometallic Chemistry</i> , 2015, 776, 30-34.	0.8	15
8194	A new D-π-A type organic sensitizer based on substituted dihydroindolo [2,3-b] carbazole and DPP unit with a bulky branched alkyl chain for highly efficient DSCs. <i>Journal of Materials Chemistry A</i> , 2015, 3, 3777-3784.	5.2	25
8195	Analytic gradients, geometry optimization and excited state potential energy surfaces from the particle-particle random phase approximation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1025-1038.	1.3	21
8196	1,2-migration in N-phosphano functionalized N-heterocyclic carbenes. <i>Journal of Computational Chemistry</i> , 2015, 36, 42-48.	1.5	3
8197	Design of UV-Vis-NIR panchromatic crown-phthalocyanines with controllable aggregation. <i>Dalton Transactions</i> , 2015, 44, 1366-1378.	1.6	18
8198	4-aryloxy-5-bis(arylethynyl)aryl-1,2,4-triazoles: Multitasking Skeleton as a Self-Assembling Unit. <i>Chemistry - A European Journal</i> , 2015, 21, 1795-1802.	1.7	24
8199	Reactions of heteroallenes with cyclam-based Zr(IV) complexes. <i>Dalton Transactions</i> , 2015, 44, 1441-1455.	1.6	12
8200	Effect of COOH group on the performance of rhenium (I) tricarbonyl complexes with tetrathiafulvalene-fused phenanthroline ligands as dyes in DSSC: DFT/TD-DFT theoretical investigations. <i>Structural Chemistry</i> , 2015, 26, 421-430.	1.0	9
8201	Theoretical evidence of metal-induced structural distortions in a series of bipyrimidine-based ligands. <i>Dalton Transactions</i> , 2015, 44, 506-510.	1.6	6
8202	Synthesis and the absolute configuration of both enantiomers of 4,5-dihydroxy-3-(formyl)cyclopent-2-enone acetonide as a new chiral building block for prostanoid synthesis. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 807-816.	1.5	7
8203	Molecular Structure of 1,2-Bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane in the Gas, Liquid, and Solid Phases: Unusual Conformational Changes between Phases. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1600-1608.	1.1	3

#	ARTICLE	IF	CITATIONS
8204	Calculations of pK_a 's and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5134-5144.	1.1	111
8205	Computing pK_a values of hexa-aqua transition metal complexes. <i>Journal of Computational Chemistry</i> , 2015, 36, 69-78.	1.5	26
8206	Synthesis, physical properties and OLED performance of azatetracenes. <i>Dyes and Pigments</i> , 2015, 112, 93-98.	2.0	38
8207	Design and synthesis of star-burst triphenylamine-based π -conjugated molecules. <i>Dyes and Pigments</i> , 2015, 113, 1-7.	2.0	35
8208	The qualitative and quantitative accuracy of DFT methods in computing $1J(C-F)$, $1J(C-N)$ and $nJ(F-F)$ spin-spin coupling of fluorobenzene and fluoropyridine molecules. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2015, 151, 18-25.	1.1	2
8209	Near-Infrared Laser-Induced Structural Changes of Glycine-Water Complexes in an Ar Matrix. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2429-2437.	1.1	9
8210	Acylation of dipyrromethanes at the β and β^2 positions and further development of fluorescent Zn^{2+} probes. <i>Sensors and Actuators B: Chemical</i> , 2015, 206, 291-302.	4.0	24
8211	Dual emission behavior of phenyleneethynylene gold(I) complexes dictated by intersystem crossing: A theoretical perspective. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 259-266.	2.0	3
8212	Synthesis of highly reactive polyisobutylene with $FeCl_3$ /ether complexes in hexane; kinetic and mechanistic studies. <i>Polymer Chemistry</i> , 2015, 6, 322-329.	1.9	30
8213	One-pot synthesis of (R)-2-acetoxy-1-indanone from 1,2-indanedione combining metal catalyzed hydrogenation and chemoenzymatic dynamic kinetic resolution. <i>Catalysis Science and Technology</i> , 2015, 5, 150-160.	2.1	18
8214	Light-Induced Reaction of Benzene with Carbonates. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 319-324.	0.6	0
8215	Methylpalladium complexes with pyrimidine-functionalized N-heterocyclic carbene ligands. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 1557-1565.	1.3	3
8216	Ab initio and first principles theoretical investigations of triplet-triplet fluorescence in trimethylenemethane biradicals. <i>RSC Advances</i> , 2016, 6, 83668-83672.	1.7	3
8217	Structural Analysis and Reactivity of Tetramethylcopper(III) Complex towards Nitrogen Donor Ligands by Density Functional Theory. <i>Advances in Chemistry</i> , 2016, 2016, 1-8.	1.1	0
8219	Self-consistent Field Molecular Orbital Theory. , 2016, , 63-125.		1
8220	Intermolecular interactions in multi-component crystals of acridinone/thioacridinone derivatives: Structural and energetics investigations. <i>Journal of Molecular Structure</i> , 2016, 1125, 36-46.	1.8	3
8221	Nickel Catalysts for the Dehydrative Decarbonylation of Carboxylic Acids to Alkenes. <i>Organometallics</i> , 2016, 35, 2391-2400.	1.1	47
8222	A single Ti O C linkage induces interfacial charge-transfer transitions between TiO_2 and a π -conjugated molecule. <i>Chemical Physics Letters</i> , 2016, 657, 172-176.	1.2	50

#	ARTICLE	IF	CITATIONS
8223	General Force-Field Parametrization Scheme for Molecular Dynamics Simulations of Conjugated Materials in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3813-3824.	2.3	35
8224	Electronic Absorption Spectra of Tetrapyrrole-Based Pigments via TD-DFT: A Reduced Orbital Space Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5816-5825.	1.1	3
8225	Lithium-Ion Model Behavior in an Ethylene Carbonate Electrolyte Using Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2016, 120, 16322-16332.	1.5	83
8226	Theoretical study of lithium ionic conductors by electronic stress tensor density and electronic kinetic energy density. <i>Journal of Computational Chemistry</i> , 2016, 37, 1924-1934.	1.5	7
8227	Efficient determination of accurate atomic polarizabilities for polarizable embedding calculations. <i>Journal of Computational Chemistry</i> , 2016, 37, 2052-2059.	1.5	8
8228	Tuning of the electronic properties of H-passivated armchair graphene nanoribbons by mild border oxidation: Theoretical study on periodic models. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1281-1284.	1.0	1
8229	Mechanistic Insight into the Copper-Catalyzed Regiodivergent Silacarboxylation of Allenes with CO ₂ . <i>Chemistry - an Asian Journal</i> , 2016, 11, 2201-2209.	1.7	12
8230	Formation and High Reactivity of the <i>anti</i> -Dioxo Form of High-Spin Oxodioxoiron(IV) as the Active Species That Cleaves Strong C-H Bonds. <i>Chemistry - A European Journal</i> , 2016, 22, 5924-5936.	1.7	21
8231	Spectroscopic, Electrochemical and Computational Characterisation of Ru Species Involved in Catalytic Water Oxidation: Evidence for a $[\text{Ru}^{\text{V}}(\text{O})(\text{Py})_2(\text{Me})\text{tacn}]$ Intermediate. <i>Chemistry - A European Journal</i> , 2016, 22, 10111-10126.	1.7	21
8232	Saddle-Shaped Cyclic Indole Tetramers: 3D Electroactive Molecules. <i>Chemistry - A European Journal</i> , 2016, 22, 10651-10660.	1.7	7
8233	Attractive Dispersion Interactions Versus Steric Repulsion of <i>tert</i> -Butyl groups in the Crystal Packing of a $\text{D}_{3\text{h}}$ -Symmetric Tris(quinoxalinophenanthrophenazine). <i>Chemistry - A European Journal</i> , 2016, 22, 646-655.	1.7	43
8234	The Origin of Anti-Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by $[\text{Rh}(\text{DPEphos})]^+$. <i>Chemistry - A European Journal</i> , 2016, 22, 9311-9320.	1.7	28
8235	DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 7545-7553.	1.7	32
8236	Influence of a polarizable surrounding on the electronically excited states of aggregated perylene materials. <i>Journal of Computational Chemistry</i> , 2016, 37, 1601-1610.	1.5	14
8237	Theoretical study of aromatic-antiaromatic pairs as material in organic solar cells of double light harvesting. <i>Chemical Physics Letters</i> , 2016, 659, 31-35.	1.2	3
8238	An arylene-vinylene based donor-acceptor-donor small molecule for the donor compound in high-voltage organic solar cells. <i>Solar Energy Materials and Solar Cells</i> , 2016, 155, 348-355.	3.0	14
8239	Synthetic methodology to prepare polysubstituted 2-aminopyrans. Synthesis of the C32-C38 subunit of immunosuppressant sanglifephrin A. <i>Tetrahedron</i> , 2016, 72, 4798-4812.	1.0	7
8240	Systematic study of transition-metal (Fe, Co, Ni, Cu) phthalocyanines as electrocatalysts for oxygen reduction and their evaluation by DFT. <i>RSC Advances</i> , 2016, 6, 67049-67056.	1.7	86

#	ARTICLE	IF	CITATIONS
8241	Triarylboryl-Functionalized Oxadiazole as a Host Material with Electron Transporting Property for Green PhOLEDs. Bulletin of the Korean Chemical Society, 2016, 37, 864-870.	1.0	2
8242	Silver(I)-Catalyzed Addition of Phenols to Alkyne Cobalt Cluster Stabilized Carbocations. Chemistry - A European Journal, 2016, 22, 9015-9023.	1.7	8
8243	Excitation spectra of Bi/Si(001) interfaces. Materialwissenschaft Und Werkstofftechnik, 2016, 47, 120-127.	0.5	4
8244	Structural and electronic characteristics of intercalated monopotassium-rubrene: Simulation on a commodity computing cluster. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650035.	1.8	1
8245	The Effect of Pyridyl Nitrogen Atom Position in Pyrido[3,4-b]pyrazines in Donor-Acceptor-Acceptor Dyes on Absorption, Energy Levels, and Photovoltaic Performances of Dye-Sensitized Solar Cells. Asian Journal of Organic Chemistry, 2016, 5, 293-300.	1.3	6
8246	Synthesis of Five-Porphyrin Nanorings by Using Ferrocene and Corannulene Templates. Angewandte Chemie, 2016, 128, 8498-8502.	1.6	20
8247	Termination Mechanism of the Radical Polymerization of Acrylates. Macromolecular Rapid Communications, 2016, 37, 506-513.	2.0	39
8248	Twisted olefinic building blocks for low bandgap polymers in solar cells and ambipolar field-effect transistors. Journal of Polymer Science Part A, 2016, 54, 889-899.	2.5	7
8249	Baeckeins J and K, Two Novel Methylated Biflavonoids from the Roots of <i>Baeckea frutescens</i> and Their Cytoprotective Activities. Helvetica Chimica Acta, 2016, 99, 499-505.	1.0	3
8250	Cysteine Radical/Metal Ion Adducts: A Gas-Phase Structural Elucidation and Reactivity Study. ChemPlusChem, 2016, 81, 444-452.	1.3	8
8251	Mixed-Valence o-Iminobenzoquinone and o-Iminobenzosemiquinonate Anion Radical Complexes of Cobalt: Valence Tautomerism. European Journal of Inorganic Chemistry, 2016, 2016, 3680-3690.	1.0	18
8252	o-Iminobenzoquinone and o-Iminobenzosemiquinonate Anion Radical Complexes of Rhodium and Ruthenium. European Journal of Inorganic Chemistry, 2016, 2016, 3691-3697.	1.0	12
8253	Structure, Electronic and Nonlinear Optical Properties of Furyloxazoles and Thienyloxazoles. Journal of Physics: Conference Series, 2016, 707, 012002.	0.3	0
8254	Calcium Vapor Adsorption on the Metal-Organic Framework NU-1000: Structure and Energetics. Journal of Physical Chemistry C, 2016, 120, 16850-16862.	1.5	16
8255	Non-covalent S-H...O interactions control conformation in a scaffold that disrupts islet amyloid polypeptide fibrillation. Chemical Science, 2016, 7, 6435-6439.	3.7	22
8256	Computational Characterization of the Origin of Selectivity in Cycloaddition Reactions Catalyzed by Phosphoric Acid Derivatives. Chemistry - an Asian Journal, 2016, 11, 411-416.	1.7	25
8257	Unprecedented Spectroscopic and Computational Evidence for Allenyl and Propargyl Titanocene(IV) Complexes: Electrophilic Quenching of Their Metallotropic Equilibrium. Chemistry - A European Journal, 2016, 22, 2427-2439.	1.7	14
8258	Diastereoselective Synthesis of and Mechanistic Understanding for the Formation of 2-Piperidinones from Imines and Cyano-Substituted Anhydrides. Chemistry - A European Journal, 2016, 22, 4794-4801.	1.7	19

#	ARTICLE	IF	CITATIONS
8259	Insights into the Cascade Reaction of CO and Heteroallenes Mediated by Dinitrogen Hafnocene Complexes: The Indirect Effect of Nitride's Nucleophilicity. <i>Chemistry - A European Journal</i> , 2016, 22, 4743-4747.	1.7	1
8260	Electronic Structures and Chiroptical Properties of Post-functionalized Helicene Quinones. <i>Chemistry - A European Journal</i> , 2016, 22, 7152-7157.	1.7	8
8261	The Antiferromagnetic Spin Coupling in Non-Kekulé Acenes: Impressive Polyradical Character Revealed by High-Level Multireference Methods. <i>ChemPhysChem</i> , 2016, 17, 2013-2021.	1.0	4
8262	Janus all-cis-1,2,3,4,5,6-Hexafluorocyclohexane: A Molecular Motif for Aggregation-Induced Enhanced Polarization. <i>ChemPhysChem</i> , 2016, 17, 2373-2381.	1.0	29
8263	A computational study on the electronic and nonlinear optical properties of graphyne subunit. <i>AIP Conference Proceedings</i> , 2016, . .	0.3	1
8264	Phosphorescent Thiazol-2-ylidene Platinum(II) Complexes with \hat{I}^2 -Ketoiminates: Single Isomer Formation by Ligand Architecture. <i>Organometallics</i> , 2016, 35, 4050-4059.	1.1	11
8265	Experimental and theoretical evaluation of structures of Pr_2C_2 and its functionalized adduct with adamantylidene carbene. <i>RSC Advances</i> , 2016, 6, 115113-115119.	1.7	6
8266	Numerical Estimation of the Pseudo-Jahn-Teller Effect Using Nonadiabatic Coupling Integrals in Monocyclic and Bicyclic Conjugated Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10207-10215.	1.1	3
8267	Cost-Effective Implementation of Multiconformer Transition State Theory for Peroxy Radical Hydrogen Shift Reactions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10072-10087.	1.1	91
8268	Osmium(II) Complexes Containing a Dianionic CCCC-Donor Tetradentate Ligand. <i>Organometallics</i> , 2016, 35, 3981-3995.	1.1	31
8269	Enantioselection mechanism in Rh-catalyzed asymmetric hydrogenation. <i>Russian Chemical Bulletin</i> , 2016, 65, 1514-1534.	0.4	16
8270	Properties of iron sulfide, hydrosulfide, and mixed sulfide/hydrosulfide cluster anions through photoelectron spectroscopy and density functional theory calculations. <i>Journal of Chemical Physics</i> , 2016, 145, 154302.	1.2	13
8271	Probing the electronic structure and Au-C chemical bonding in AuCn^+ and AuCnH^+ ($n = 2, 4, \text{ and } 6$) using high-resolution photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2016, 145, 064304.	1.2	18
8272	Spectroscopy and quantum-chemical calculations of nitro-bis-bipyridyl complexes of ruthenium(II) with 4-substituted pyridine ligands. <i>Optics and Spectroscopy (English Translation of Optika I)</i> Tj ETQq1 1 0.784314xgBT /Overlock 10		
8273	The rovibrational nature of cis- and trans-HNNS: A possible nitrogen molecule progenitor. <i>Journal of Chemical Physics</i> , 2016, 145, 204302.	1.2	6
8274	Theoretical study on electronic structures, spectra, and charge transporting properties of two Pt(II) complexes with triazenido ligands. <i>Russian Journal of General Chemistry</i> , 2016, 86, 2817-2826.	0.3	1
8275	Nuclei-selected atomic-orbital response-theory formulation for the calculation of NMR shielding tensors using density-fitting. <i>Journal of Chemical Physics</i> , 2016, 145, 234108.	1.2	7
8276	Signatures of Size-Dependent Structural Patterns in Hydrated Copper(I) Clusters, $\text{Cu}^+(\text{H}_2\text{O})_n$. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10252-10263.	1.1	7

#	ARTICLE	IF	CITATIONS
8295	Local electric fields and molecular properties in heterogeneous environments through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10070-10080.	1.3	60
8296	Excited-State Absorption from Real-Time Time-Dependent Density Functional Theory: Optical Limiting in Zinc Phthalocyanine. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1387-1391.	2.1	31
8297	Overcoming artificial broadening in Gd ³⁺ distance distributions arising from dipolar pseudo-secular terms in DEER experiments. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12847-12859.	1.3	28
8298	Radical non-radical states of the [Ru(PIQ)] core in complexes (PIQ = 9,10-phenanthreneiminoquinone). <i>Dalton Transactions</i> , 2016, 45, 8236-8247.	1.6	5
8299	Cyanide-bridged iron complexes as biomimetics of tri-iron arrangements in maturases of the H cluster of the di-iron hydrogenase. <i>Chemical Science</i> , 2016, 7, 3710-3719.	3.7	20
8300	Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented \hat{I}^2 -Oxygen Transfer Mechanism. <i>Inorganic Chemistry</i> , 2016, 55, 6080-6084.	1.9	40
8301	Inclusion of ¹³ C and D in protonated acetylene. <i>Chemical Physics Letters</i> , 2016, 650, 126-129.	1.2	13
8302	Excess Electron Attachment to the Nucleoside Pair 2-Deoxyadenosine (dA)-2-Deoxythymidine (dT). <i>Journal of Physical Chemistry B</i> , 2016, 120, 4955-4962.	1.2	4
8303	Fragmentation of Protonated <i>N</i> -(3-Aminophenyl)Benzamide and Its Derivatives in Gas Phase. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 917-926.	1.2	6
8304	Bistriazine-based streptocyanines. Preparation, structural determination and optoelectronic properties. <i>Dyes and Pigments</i> , 2016, 131, 307-319.	2.0	6
8305	Controlling Coordination Geometries: Ru Carbene Complexes with Tetra-NHC Ligands. <i>Inorganic Chemistry</i> , 2016, 55, 6010-6017.	1.9	19
8306	The Interplay between Homogeneous and Heterogeneous Phases of PdAu Catalysts for the Oxidation of Alcohols. <i>ACS Catalysis</i> , 2016, 6, 4135-4143.	5.5	30
8307	N≡N pnictogen bonds in Boc-DOPA-OMe. <i>Chemical Physics Letters</i> , 2016, 653, 117-121.	1.2	6
8308	Experimental and Computational Studies of the Mechanisms of Hydroamination/Cyclisation of Unactivated α,β -Amino-alkenes with CCC-NHC Pincer Zr Complexes. <i>Australian Journal of Chemistry</i> , 2016, 69, 573.	0.5	10
8309	Structural, Hirshfeld surface and theoretical analysis of two conformational polymorphs of <i>N,N'</i> -bis(pyridin-3-ylmethyl)oxalamide. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2016, 231, 415-425.	0.4	10
8310	Computational Methods to Predict the Regioselectivity of Electrophilic Aromatic Substitution Reactions of Heteroaromatic Systems. <i>Journal of Organic Chemistry</i> , 2016, 81, 5128-5134.	1.7	25
8311	Modern ab initio valence bond theory calculations reveal charge shift bonding in protic ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15783-15790.	1.3	8
8312	Synthesis and Photovoltaic Properties of Powerful Electron-Donating Indeno[1,2- <i>bc</i>]thiophene-Based Green Dye-Sensitizers for Dye-Sensitized Solar Cells. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 3518-3525.	3.2	35

#	ARTICLE	IF	CITATIONS
8313	Bismuth(III) complexes with 2-acetylpyridine- and 2-benzoylpyridine-derived hydrazones: Antimicrobial and cytotoxic activities and effects on the clonogenic survival of human solid tumor cells. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 2988-2998.	1.4	39
8314	Longer-Wavelength-Absorbing, Extended Chalcogenorhodamine Dyes. <i>Organometallics</i> , 2016, 35, 1944-1955.	1.1	18
8315	Ligand K-edge XAS, DFT, and TDDFT analysis of pincer linker variations in Rh(<i>κ</i> -PNP) complexes: reactivity insights from electronic structure. <i>Dalton Transactions</i> , 2016, 45, 9774-9785.	1.6	26
8316	Proton-hydride tautomerism in hydrogen evolution catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 6409-6414.	3.3	114
8317	An EPR and DFT study on the primary radical formed in hydroxylation reactions of 2,6-dimethoxy-1,4-benzoquinone. <i>Molecular Physics</i> , 2016, 114, 1856-1866.	0.8	1
8318	Kinetic studies of fluorinated aryl molybdenum(<i>κ</i> -tricarboxyl) precursors in epoxidation catalysis. <i>Catalysis Science and Technology</i> , 2016, 6, 4970-4977.	2.1	11
8319	The radical mechanism of biological methane synthesis by methyl-coenzyme M reductase. <i>Science</i> , 2016, 352, 953-958.	6.0	129
8320	Insights into Bulk Electrolyte Effects on the Operative Voltage of Electrochemical Double-Layer Capacitors. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12325-12336.	1.5	15
8321	Metal-ligand cooperative activation of element-hydrogen bonds (element = C, N, O, Cl, B) on a dinuclear ruthenium bridging imido complex. <i>Journal of Organometallic Chemistry</i> , 2016, 812, 158-166.	0.8	6
8322	Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics "Monte Carlo Canonical Propagation Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1449-1458.	2.3	9
8323	Development of a True Transition State Force Field from Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1833-1844.	2.3	27
8324	Dynamic Reaction Mechanisms of ClO ⁻ with CH ₃ Cl: Comparison Between Direct Dynamics Trajectory Simulations and Experiment. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1813-1818.	1.1	2
8325	Enhanced Photoluminescence Quantum Yields through Excimer Formation of Cyclometalated Platinum(II) N-Heterocyclic Carbene Complexes. <i>Organometallics</i> , 2016, 35, 673-680.	1.1	62
8326	Ab initio study of the enantio-selective magnetic-field-induced second harmonic generation in chiral molecules. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1846-1858.	1.3	3
8327	Energetic pathways and influence of the metallacyclobutane intermediates formed during isobutene/2-butene cross-metathesis over WH ₃ /Al ₂ O ₃ supported catalyst. <i>Catalysis Science and Technology</i> , 2016, 6, 3386-3393.	2.1	4
8328	Puzzles in Bonding and Spectroscopy: The Case of Dicarbon ⁺ . <i>Science Progress</i> , 2016, 99, 1-58.	1.0	13
8329	Synthesis, characterization, and mesomorphic investigations of diester-substituted salicylaldehydes and their copper (II) complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2016, 624, 77-90.	0.4	6
8330	Experimental and theoretical evaluation of the inhibition properties of ketoprofen for the corrosion of a copper surface in hydrochloric acid. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2016, 52, 356-371.	0.3	13

#	ARTICLE	IF	CITATIONS
8331	Enantioselective Oxidative Rearrangements with Chiral Hypervalent Iodine Reagents. <i>Chemistry - A European Journal</i> , 2016, 22, 4030-4035.	1.7	78
8332	Control of a photoswitching chelator by metal ions: <sc>DFT</sc>, <sc>NBO</sc>, and <sc>QTAIM</sc> analysis. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 27-34.	1.0	24
8333	Emergence of Function in P450-Proteins: A Combined Quantum Mechanical/Molecular Mechanical and Molecular Dynamics Study of the Reactive Species in the H ₂ O ₂ -Dependent Cytochrome P450 _{SP1±} and Its Regio- and Enantioselective Hydroxylation of Fatty Acids. <i>Journal of the American Chemical Society</i> , 2016, 138, 6786-6797.	6.6	54
8334	Ligand-Binding Affinity Estimates Supported by Quantum-Mechanical Methods. <i>Chemical Reviews</i> , 2016, 116, 5520-5566.	23.0	216
8335	Mechanism of Pd-Catalyzed Decarbonylation of Biomass-Derived Hydrocinnamic Acid to Styrene following Activation as an Anhydride. <i>Inorganic Chemistry</i> , 2016, 55, 4124-4131.	1.9	29
8336	Interplay of Nitrogen-Atom Inversion and Conformational Inversion in Enantiomerization of 1 <i>H</i> -1-Benzazepines. <i>Journal of Organic Chemistry</i> , 2016, 81, 3313-3320.	1.7	9
8337	Impact of chirality on the photoinduced charge transfer in linked systems containing naproxen enantiomers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12733-12741.	1.3	14
8338	Synthesis of Functionalized 1,3,2-Benzodiazaborole Cores Using Bench-Stable Components. <i>Journal of Organic Chemistry</i> , 2016, 81, 3771-3779.	1.7	21
8339	Kinetic Isotope Effects in Multipath VTST: Application to a Hydrogen Abstraction Reaction. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1911-1918.	1.2	11
8340	Coordination Compounds of Niobium(IV) Oxide Dihalides Including the Synthesis and the Crystallographic Characterization of NHC Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 4173-4182.	1.9	17
8341	Conceptual design of tetraazaporphyrin- and subtetraazaporphyrin-based functional nanocarbon materials: electronic structures, topologies, optical properties, and methane storage capacities. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13503-13518.	1.3	3
8342	Transition Metal Substitution Effects on Metal-to-Polyoxometalate Charge Transfer. <i>Inorganic Chemistry</i> , 2016, 55, 4308-4319.	1.9	24
8343	Noninnocent Proton-Responsive Ligand Facilitates Reductive Deprotonation and Hinders CO ₂ Reduction Catalysis in [Ru(tpy)(6DHBP)(NCCH ₃) ²⁺ (6DHBP =) Tj ETQp 0 0 rg 87 /Overlo	1.1	0
8344	Gas-Phase Structures of Ketene and Acetic Acid from Acetic Anhydride Using Very-High-Temperature Gas Electron Diffraction. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2041-2048.	1.1	13
8345	<i>Pr</i> ₂ Nâ€‘Pâ€‘Fe(CO) ₄ in Olefinic Solvents: A Reservoir of a Transient Phosphinidene Complex Capable of Substrate Hopping. <i>Organometallics</i> , 2016, 35, 1170-1176.	1.1	30
8346	A reduced dimensionality model of torsional vibrations in star molecules. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 77, 131-137.	1.3	0
8347	Construction of Stereogenic 1,1-Disubstituted Cycloalkanones via 1° Amine Thiourea Dual Catalysis: Experimental Scope and Computational Analyses. <i>Journal of Organic Chemistry</i> , 2016, 81, 3629-3637.	1.7	22
8348	Nucleoside-2â€²,3â€²-bis(thio)phosphate antioxidants are also capable of disassembly of amyloid beta ₄₂ -Zn(II)/Cu(II) aggregates via Zn(II)/Cu(II)-chelation. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 4640-4653.	1.5	9

#	ARTICLE	IF	CITATIONS
8349	Self-Assembled Core-Satellite Gold Nanoparticle Networks for Ultrasensitive Detection of Chiral Molecules by Recognition Tunneling Current. <i>ACS Nano</i> , 2016, 10, 5096-5103.	7.3	47
8350	Proton Transfer Mechanism of Organocatalyzed Isomerization of Alkynoates into Allenones: Enantioselectivity and Reversibility. A DFT Study. <i>ACS Catalysis</i> , 2016, 6, 2988-2996.	5.5	16
8351	Substituent effects and chemoselectivity of the intramolecular Buchner reaction of diazoacetamide derivatives catalyzed by the di-Rh-complex. <i>Dalton Transactions</i> , 2016, 45, 8506-8512.	1.6	25
8352	Tuning the photochemical properties of the fulvalene-tetracarbonyl-diruthenium system. <i>Dalton Transactions</i> , 2016, 45, 8740-8744.	1.6	37
8353	Systematic Introduction of Aromatic Rings to Diphosphine Ligands for Emission Color Tuning of Dinuclear Copper(I) Iodide Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 5227-5236.	1.9	63
8354	The fragment molecular orbital method combined with density-functional tight-binding and the polarizable continuum model. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22047-22061.	1.3	59
8355	Dimeric binding of plant alkaloid ellipticine to human serum proteins. <i>RSC Advances</i> , 2016, 6, 44096-44105.	1.7	6
8356	Mechanism for Ag(I)-catalyzed decarboxylative chlorination: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
8357	Amine Molecular Cages as Supramolecular Fluorescent Explosive Sensors: A Computational Perspective. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5063-5072.	1.2	28
8358	Theoretical study on the isomerization of propargyl derivative to conjugated diene under Au(I)-catalyzed reaction: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2016, 1083, 38-45.	1.1	7
8359	The Optical Signature of Charges in Conjugated Polymers. <i>ACS Central Science</i> , 2016, 2, 309-315.	5.3	77
8360	Experimental and theoretical studies of molecular complexes of theophylline with some phenylboronic acids. <i>RSC Advances</i> , 2016, 6, 43060-43068.	1.7	11
8361	Analysis of a bicyclic, triple disulphide molecular nanopropeller. <i>RSC Advances</i> , 2016, 6, 43509-43517.	1.7	3
8362	Electronic structures of TiO ₂ -TCNE, -TCNQ, and -2,6-TCNAQ surface complexes studied by ionization potential measurements and DFT calculations: Mechanism of the shift of interfacial charge-transfer bands. <i>Chemical Physics Letters</i> , 2016, 653, 11-16.	1.2	14
8363	Metal-Free Synthesis of 3-Arylquinolin-2-ones from Acrylic Amides via a Highly Regioselective 1,2-Aryl Migration: An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 4058-4065.	1.7	35
8364	Unsymmetrical PNP-Pincer Type Phosphaalkene Ligands Protected by a Fused-Ring Bulky Eind Group: Synthesis and Applications to Rh(I) and Ir(I) Complexes. <i>Organometallics</i> , 2016, 35, 1526-1533.	1.1	22
8365	Isolation of [Ru(IPr) ₂ (CO)H] (IPr = 1,3-Bis(2,6-diisopropylphenoxy)isopropan-2-ylidene) Organometallics, 2016, 35, 1301-1312.	1.1	19
8366	Distributions, profiles and formation mechanisms of polychlorinated naphthalenes in cement kilns co-processing municipal waste incinerator fly ash. <i>Chemosphere</i> , 2016, 155, 348-357.	4.2	51

#	ARTICLE	IF	CITATIONS
8367	Radical and Non-Radical States of the [Os(PIQ)] Core (PIQ = 9,10-Phenanthreneiminoquinone): Iminosemiquinone to Iminoquinone Conversion Promoted o-Metalation Reaction. <i>Inorganic Chemistry</i> , 2016, 55, 4746-4756.	1.9	13
8368	A Direct Mechanism of Ultrafast Intramolecular Singlet Fission in Pentacene Dimers. <i>ACS Central Science</i> , 2016, 2, 316-324.	5.3	176
8369	Aqueous phase hydration and hydrate acidity of perfluoroalkyl and n:2 fluorotelomer aldehydes. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2016, 51, 579-582.	0.9	3
8370	A DFT investigation on the host/guest inclusion process of prilocaine into β -cyclodextrin. <i>Chemical Physics Letters</i> , 2016, 652, 123-129.	1.2	25
8371	Mechanism, catalysis and predictions of 1,3,2-diazaphospholenes: theoretical insight into highly polarized P-H bonds. <i>Organic Chemistry Frontiers</i> , 2016, 3, 423-433.	2.3	19
8372	Ethylene C-H Bond Activation by Neutral Mn ₂ O ₅ Clusters under Visible Light Irradiation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1709-1716.	2.1	13
8373	Theoretical characterization of the surface composition of ruthenium nanoparticles in equilibrium with syngas. <i>Nanoscale</i> , 2016, 8, 10974-10992.	2.8	43
8374	Distinguishing binding modes of a new phosphonium dye with DNA by surface-enhanced Raman spectroscopy. <i>RSC Advances</i> , 2016, 6, 41927-41936.	1.7	4
8375	Two pathways of proton transfer reaction to (triphos)Cu(I)-BH ₄ via a dihydrogen bond [triphos = 1,1,1-tris(diphenylphosphinomethyl)ethane]. <i>Dalton Transactions</i> , 2016, 45, 9127-9135.	1.6	14
8376	1-Pyrenyl- and 3-Perylenyl-antimony(V) Derivatives for the Fluorescence Turn-On Sensing of Fluoride Ions in Water at Sub-ppm Concentrations. <i>Organometallics</i> , 2016, 35, 1854-1860.	1.1	65
8377	Computational Exploration of Rh ^{III} /Rh ^V and Rh ^{III} /Rh ^I Catalysis in Rhodium(III)-Catalyzed C-H Activation Reactions of <i>N</i> -Phenoxyacetamides with Alkynes. <i>Journal of the American Chemical Society</i> , 2016, 138, 6861-6868.	6.6	116
8378	Reactions C ₂ H ₂ + OH and C ₂ + H ₂ O: Ab initio study of the potential energy surfaces. <i>Russian Journal of Physical Chemistry B</i> , 2016, 10, 143-152.	0.2	2
8379	Direct simulation of electron transfer in the cobalt hexammine($\text{Co}(\text{NH}_3)_6^{3+}$) self-exchange reaction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26117-26124.	1.3	13
8380	Excited State Trends in Bidirectionally Expanded Closed-Shell PAH and PANH Anions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7327-7334.	1.1	8
8381	Triazolobenzothiadiazole-Based Copolymers for Polymer Light-Emitting Diodes: Pure Near-Infrared Emission via Optimized Energy and Charge Transfer. <i>Advanced Optical Materials</i> , 2016, 4, 2068-2076.	3.6	48
8382	Paramagnetic NMR of Phenolic Oxime Copper Complexes: A Joint Experimental and Density Functional Study. <i>Chemistry - A European Journal</i> , 2016, 22, 15328-15339.	1.7	22
8383	Accelerating ab initio molecular dynamics simulations by linear prediction methods. <i>Chemical Physics Letters</i> , 2016, 661, 42-47.	1.2	7
8384	Synthesis of a highly reactive form of WO ₂ Cl ₂ , its conversion into nanocrystalline mono-hydrated WO ₃ and coordination compounds with tetramethylurea. <i>Dalton Transactions</i> , 2016, 45, 15342-15349.	1.6	8

#	ARTICLE	IF	CITATIONS
8385	Influence of ethynyl position on benzothiadiazole based Dâ€“Aâ€“iâ€“A dye-sensitized solar cells: spectral response and photovoltage performance. <i>Journal of Materials Chemistry C</i> , 2016, 4, 9203-9211.	2.7	34
8386	Lanthanide selective adsorption by ion-imprinted polymer with chelidonic acid monoamide groups. <i>Separation Science and Technology</i> , 2016, 51, 2887-2895.	1.3	2
8387	A Frustrated Lewis Pair Catalyzed Asymmetric Transfer Hydrogenation of Imines Using Ammonia Borane. <i>Journal of the American Chemical Society</i> , 2016, 138, 12956-12962.	6.6	147
8388	The divide-and-conquer second-order proton propagator method based on nuclear orbital plus molecular orbital theory for the efficient computation of proton binding energies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27422-27431.	1.3	11
8389	The influence of different substituents on the geometrical changes in the heterocyclic moiety of 1,2-diphospholes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 1646-1649.	0.8	10
8390	The origin of 1560 cm ⁻¹ band in experimental IR spectra of water adsorbed on TiO ₂ surface: Ab initio assessment. <i>Chemical Physics Letters</i> , 2016, 662, 97-101.	1.2	12
8391	Dopant induced modulation in the structure and electronic properties of Au ₁₀ cluster. <i>RSC Advances</i> , 2016, 6, 87115-87123.	1.7	3
8392	Cytotoxic, DNA binding and drug reservoir property of Pt(II)â€“sulfur complexes: In-vitro kinetics, mechanism with bio-relevant molecules in aqueous medium and a theoretical approach. <i>Polyhedron</i> , 2016, 119, 84-97.	1.0	13
8393	A precedent of van-der-Waals interactions outmatching Coulomb explosion. <i>Carbon</i> , 2016, 109, 843-850.	5.4	16
8394	Proton-coupled electron transfer in [pyridineâ€“(H ₂ O)] ⁿ⁺ , n = 3, 4, clusters. <i>Chemical Physics Letters</i> , 2016, 661, 196-199.	1.2	1
8395	A Model for the pH-Dependent Selectivity of the Oxygen Reduction Reaction Electrocatalyzed by N-Doped Graphitic Carbon. <i>Journal of the American Chemical Society</i> , 2016, 138, 13923-13929.	6.6	88
8396	Exploring Redox States, Doping and Ordering of Electroactive Starâ€“Shaped Oligo(aniline)s. <i>Chemistry - A European Journal</i> , 2016, 22, 16950-16956.	1.7	15
8397	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Lowâ€“Pressure Mass Spectrometry and Computational Study. <i>Chemistry - A European Journal</i> , 2016, 22, 18608-18619.	1.7	74
8398	Structural effects on the electronic characteristics of intramolecularly intercalated alkali-rubrene complexes. <i>Materials Chemistry and Physics</i> , 2016, 183, 44-55.	2.0	2
8399	Cationic Î€-Stacking Columns of Coronene Molecules with Fully Charged and Charge-Disproportionated States. <i>Crystal Growth and Design</i> , 2016, 16, 5994-6000.	1.4	8
8400	Mobility versus Alignment of a Semiconducting Î€-Extended Discotic Liquid-Crystalline Triindole. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 26964-26971.	4.0	34
8401	Novel Stannatranes N(CH ₂ CMe ₂ O) ₂ (CMe ₂ CH ₂ O)SnO- <i>tert</i> -Bu and Related Oligonuclear Tin(IV) Oxoclusters. Two Isomers in One Crystal. <i>Inorganic Chemistry</i> , 2016, 55, 10218-10228.	1.9	24
8402	Millimeter-Wave Spectroscopy, X-ray Crystal Structure, and Quantum Chemical Studies of Diketene: Resolving Ambiguities Concerning the Structure of the Ketene Dimer. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7753-7763.	1.1	6

#	ARTICLE	IF	CITATIONS
8403	Different Conformations of 2-Deoxycytidine in the Gas and Solid Phases: Competition between Intra- and Intermolecular Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8199-8210.	1.1	12
8404	New insights in the mechanism of the microwave-assisted Pauson-Khand reaction. <i>Tetrahedron</i> , 2016, 72, 7443-7448.	1.0	8
8405	High-Valent Manganese Oxo Valence Tautomers and the Influence of Lewis/Brønsted Acids on C-H Bond Cleavage. <i>Inorganic Chemistry</i> , 2016, 55, 10800-10809.	1.9	43
8406	Pure- $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi} \rangle \text{N} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -representability conditions of two-fermion reduced density matrices. <i>Physical Review A</i> , 2016, 94, .	1.0	47
8407	Protonation and electronic structure of 2,6-dichlorophenolindophenolate during reduction. A theoretical study including explicit solvent. <i>Journal of Molecular Modeling</i> , 2016, 22, 251.	0.8	3
8408	Clay Organic Hybrid Films Exhibiting Reversible Fluorescent Color Switching Induced by Swelling and Drying of a Clay Mineral. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23813-23822.	1.5	15
8409	A comparative study of the photophysics of phenyl, thienyl, and chalcogen substituted rhodamine dyes. <i>Photochemical and Photobiological Sciences</i> , 2016, 15, 1417-1432.	1.6	17
8410	Regioselective Atomic Layer Deposition in Metal Organic Frameworks Directed by Dispersion Interactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 13513-13516.	6.6	78
8411	Modulation of the exfoliated graphene work function through cycloaddition of nitrile imines. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29582-29590.	1.3	16
8412	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28339-28352.	1.3	23
8413	Air water partition coefficients for a suite of polycyclic aromatic and other C_{10} through C_{20} unsaturated hydrocarbons. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2016, 51, 938-953.	0.9	2
8414	Investigating the Structural Features and Spectroscopic Properties of Bis(tetrazolato)-Based Coordination Polymers. <i>Crystal Growth and Design</i> , 2016, 16, 6390-6404.	1.4	10
8415	The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores. <i>Journal of Organic Chemistry</i> , 2016, 81, 10955-10963.	1.7	17
8416	Mechanistic Investigation into Olefin Epoxidation with H_2O_2 Catalyzed by Aqua-Coordinated Sandwich-Type Polyoxometalates: Role of the Noble Metal and Active Oxygen Position. <i>ChemistryOpen</i> , 2016, 5, 470-476.	0.9	6
8417	Coloration of tyrosine by organic-semiconductor interfacial charge-transfer transitions. <i>Chemical Physics Letters</i> , 2016, 664, 178-183.	1.2	25
8418	Rotationally Hindered Biphenyls and Terphenyls: Synthesis, Molecular Dynamics, and Configurational Assignment. <i>Journal of Organic Chemistry</i> , 2016, 81, 10721-10732.	1.7	12
8419	Theoretical studies on characterization of heterofullerene $C_{58}B_2$ isomers by X-ray spectroscopy. <i>RSC Advances</i> , 2016, 6, 96752-96761.	1.7	12
8420	Influence of Ligand Architecture in Tuning Reaction Bifurcation Pathways for Chlorite Oxidation by Non-Heme Iron Complexes. <i>Inorganic Chemistry</i> , 2016, 55, 10170-10181.	1.9	17

#	ARTICLE	IF	CITATIONS
8421	Terahertz Phonon Modes of Highly Efficient Electro-optic Phenyltriene OH1 Crystals. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24360-24369.	1.5	12
8422	Platinum(0)-mediated C–O bond activation of ethers via an SN2 mechanism. <i>Dalton Transactions</i> , 2016, 45, 18842-18850.	1.6	4
8423	Hydrolysis mechanism of anticancer drug lobaplatin in aqueous medium under neutral and acidic conditions: A DFT study. <i>Chemical Physics Letters</i> , 2016, 663, 115-122.	1.2	16
8424	Theoretical Study of the Catalytic Hydrogenation of Alkenes by a Disilaferracyclic Complex: Can the Fe–Si σ -Bond-Assisted Activation of H–H Bonds Allow Development of a Catalysis of Iron?. <i>Journal of Organic Chemistry</i> , 2016, 81, 10900-10911.	1.7	18
8425	The effects of Lewis acid complexation on type I radical photoinitiators and implications for pulsed laser polymerization. <i>Polymer Chemistry</i> , 2016, 7, 6400-6412.	1.9	23
8426	Calculations of BODIPY dyes in the ground and excited states using the M06-2X and PBE0 functionals. <i>Journal of Molecular Modeling</i> , 2016, 22, 260.	0.8	21
8427	Radical-induced dissociation leading to the loss of CO ₂ from the oxazolone ring of [b ⁵ H] E TM + ions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18119-18127.	1.3	2
8428	Effect of the Ancillary Ligand on the Mechanism for CO Migratory Insertion in High-Valent Oxorhenium Complexes. <i>Organometallics</i> , 2016, 35, 3530-3537.	1.1	8
8429	Kinetics Aspects of the Reversible Assembly of Copper in Heterometallic Mo ₃ CuS ₄ Clusters with 4,4'-Di- <i>tert</i> -butyl-2,2'-bipyridine. <i>Inorganic Chemistry</i> , 2016, 55, 9912-9922.	1.9	13
8430	Extended Intermolecular Interactions Governing Photocurrent–Voltage Relations in Ternary Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3936-3944.	2.1	11
8431	Asymmetric Catalyzed Allylic Substitution Using a Pd/P ^S Catalyst Library with Exceptional High Substrate and Nucleophile Versatility: DFT and Pd-allyl Key Intermediates Studies. <i>Organometallics</i> , 2016, 35, 3323-3335.	1.1	21
8432	Stereoisomers of an azine-linked donor–acceptor conjugated polymer: the impact of molecular conformation on electrical performance. <i>RSC Advances</i> , 2016, 6, 44272-44278.	1.7	8
8433	Design of Assembled Systems Based on Conjugated Polyphenylene Derivatives and Carbon Nanohorns. <i>Chemistry - A European Journal</i> , 2016, 22, 11643-11651.	1.7	4
8434	Quantum Dynamics Simulations of Excited State Energy Transfer in a Zinc–Free-Base Porphyrin Dyad. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8075-8084.	1.1	11
8435	Extending Hexaazatriphenylene with Mono-/Bithiophenes in Acceptor–Donor Diads and Acceptor–Donor–Acceptor Triads. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23276-23285.	1.5	5
8436	A mechanistic study on guanidine-catalyzed chemical fixation of CO ₂ with 2-aminobenzonitrile to quinazoline-2,4(1H,3H)-dione. <i>Organic Chemistry Frontiers</i> , 2016, 3, 823-835.	2.3	29
8437	Designing intrinsically photostable low band gap polymers: a smart tool combining EPR spectroscopy and DFT calculations. <i>Journal of Materials Chemistry A</i> , 2016, 4, 15647-15654.	5.2	9
8438	Arene C(sp ²)-H Metalation at Ni ^{II} Modeled with a Reactive PONC _{Ph} Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 8041-8047.	1.9	32

#	ARTICLE	IF	CITATIONS
8439	Equation of Motion Theory for Excited States in Variational Monte Carlo and the Jastrow Antisymmetric Geminal Power in Hilbert Space. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3719-3726.	2.3	15
8440	Computational Mechanistic Study of Thionation of Carbonyl Compounds with Lawesson's Reagent. <i>Journal of Organic Chemistry</i> , 2016, 81, 7733-7740.	1.7	40
8441	Bisanthra-thianthrene: synthesis, structure and oxidation properties. <i>RSC Advances</i> , 2016, 6, 70700-70703.	1.7	11
8442	Mechanistically Inspired Route toward Hexahydro-2 <i>H</i> -chromenes via Consecutive [4 + 2] Cycloadditions. <i>Organic Letters</i> , 2016, 18, 3976-3979.	2.4	11
8443	The Effect of Core Correlation on the MP2 Hydration Free Energies of Li ⁺ , Na ⁺ , and K ⁺ . <i>Journal of Physical Chemistry B</i> , 2016, 120, 9088-9096.	1.2	4
8444	Why are <i>sec</i> -alkylperoxyl bimolecular self-reactions orders of magnitude faster than the analogous reactions of <i>tert</i> -alkylperoxyls? The unanticipated role of CH hydrogen bond donation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23673-23679.	1.3	56
8445	Structural and electronic determinants of flavonoid binding to human serum albumin: an extensive ligand-based study. <i>RSC Advances</i> , 2016, 6, 75014-75022.	1.7	15
8446	Computational Study of the Radical Mediated Mechanism of the Formation of C8, C5, and C4 Guanine:Lysine Adducts in the Presence of the Benzophenone Photosensitizer. <i>Chemical Research in Toxicology</i> , 2016, 29, 1396-1409.	1.7	16
8447	Directly probing spin dynamics in a molecular magnet with femtosecond time-resolution. <i>Chemical Science</i> , 2016, 7, 7061-7067.	3.7	38
8448	Water exchange rates and mechanisms in tetrahedral [Be(H ₂ O) ₄] ²⁺ and [Li(H ₂ O) ₄] ⁺ complexes using DFT methods and cluster-continuum models. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1388-1396.	1.0	5
8449	Determining the Impact of Ligand and Alkene Substituents on Bonding in Gold(I)-Alkene Complexes Supported by N-Heterocyclic Carbenes: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6064-6075.	1.1	10
8450	Unusual site selection of NCS ⁻ in trinuclear complexes of Cu(II) and Ni(II) with a reduced N ₂ O ₂ donor Schiff base: Structural, theoretical and magnetic studies. <i>Polyhedron</i> , 2016, 118, 70-80.	1.0	21
8451	High-Efficiency Microiterative Optimization in QM/MM Simulations of Large Flexible Systems. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4632-4643.	2.3	8
8452	Dehydration of Methanediol in Aqueous Solution: An ONIOM(QM/MM) Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6670-6676.	1.1	13
8453	Diketopyrrolopyrrole-based novel ratiometric fluorescent chemodosimeter for Hg ²⁺ detection in aqueous solution and in living cells. <i>Dyes and Pigments</i> , 2016, 134, 586-592.	2.0	15
8454	Benzimidazole based Pt(II) complexes with better normal cell viability than cisplatin: synthesis, substitution behavior, cytotoxicity, DNA binding and DFT study. <i>RSC Advances</i> , 2016, 6, 76600-76613.	1.7	65
8455	Prediction of two-photon absorption enhancement in red fluorescent protein chromophores made from non-canonical amino acids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24408-24416.	1.3	16
8456	Water molecules inside protein structure affect binding of monosaccharides with HIV-1 antibody 2G12. <i>Journal of Computational Chemistry</i> , 2016, 37, 2341-2348.	1.5	3

#	ARTICLE	IF	CITATIONS
8457	Preparation of Capped Octahedral OsHC ₆ Complexes by Sequential Carbon-Directed C-H Bond Activation Reactions. <i>Organometallics</i> , 2016, 35, 2532-2542.	1.1	9
8458	Mechanistic insights from theory on the reduction of CO ₂ , N ₂ O, and SO ₂ molecules using tripodal diimine-enolate substituted magnesium(σ - σ) dimers. <i>Dalton Transactions</i> , 2016, 45, 14789-14800.	1.6	7
8459	3D Macroscopic Graphene Assemblies. , 2016, , 281-294.		0
8460	Small Atomic Orbital Basis Set First-Principles Quantum Chemical Methods for Large Molecular and Periodic Systems: A Critical Analysis of Error Sources. <i>ChemistryOpen</i> , 2016, 5, 94-109.	0.9	57
8461	Ligand modification effects on the electrochromic character of ruthenium sulfoxide complexes: a theoretical perspective. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	0
8462	A comparative examination of density functional performance against the ISOL24/11 isomerization energy benchmark. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 147-152.	1.1	23
8463	Brønsted acidity of protic ionic liquids: a modern ab initio valence bond theory perspective. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26020-26025.	1.3	8
8464	Synthesis, structural characterization, and chemical properties of pentacoordinate model complexes for the active site of [Fe]-hydrogenase. <i>RSC Advances</i> , 2016, 6, 84139-84148.	1.7	7
8465	Rhodium-Catalyzed Enantioselective Intramolecular Hydroacylation of Trisubstituted Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 15619-15623.	1.7	30
8466	Effect of Curvature on Carbon Chemical Shielding in Extended Carbon Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7011-7019.	1.1	10
8467	Mechanism for the Reaction of CO with Oxorhenium Hydrides: Migratory Insertion of CO into Rhenium Hydride and Formyl Bonds leads to Migration from Rhenium to the Oxo Ligand. <i>Organometallics</i> , 2016, 35, 3060-3068.	1.1	13
8468	Mechanistic Insights into the Iridium-Catalyzed Hydrogenations of α,β -Unsaturated Ketones. <i>ChemCatChem</i> , 2016, 8, 3099-3106.	1.8	14
8469	Theoretical Study of the Charge-Transfer State Separation within Marcus Theory: The C ₆₀ -Anthracene Case Study. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 24722-24736.	4.0	19
8470	A mechanistic study and computational prediction of iron, cobalt and manganese cyclopentadienone complexes for hydrogenation of carbon dioxide. <i>Chemical Communications</i> , 2016, 52, 12422-12425.	2.2	28
8471	Rigorous Ab Initio Quantum Embedding for Quantum Chemistry Using Green's Function Theory: Screened Interaction, Nonlocal Self-Energy Relaxation, Orbital Basis, and Chemical Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4856-4870.	2.3	44
8472	Computational Approach for Studying Optical Properties of DNA Systems in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5050-5057.	2.3	26
8473	Indole-Based NLOphoric Donor-Acceptor Styryl Dyes: Synthesis, Spectral Properties and Computational Studies. <i>Journal of Fluorescence</i> , 2016, 26, 2063-2077.	1.3	11
8474	Role of Alkaline Earth Metal Cations in Improving the Hydrogen-Storage Capacity of Polyhydroxy Adamantane: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19932-19941.	1.5	13

#	ARTICLE	IF	CITATIONS
8475	Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3591-3596.	2.1	42
8476	A theoretical study on the spectroscopy, structure, and stability of C ₂ H ₃ NS molecules. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	5
8477	Fragment Molecular Orbital Nonadiabatic Molecular Dynamics for Condensed Phase Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7205-7212.	1.1	20
8478	Selectivity for HCO ₂ [−] over H ₂ in the Electrochemical Catalytic Reduction of CO ₂ by (POCOP)IrH ₂ . <i>ACS Catalysis</i> , 2016, 6, 6362-6371.	5.5	33
8479	Mechanistic insights into ozone-initiated oxidative degradation of saturated hydrocarbons and polymers. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24663-24671.	1.3	25
8480	The role of sodium ions in the solubility of peptides. <i>Structural Chemistry</i> , 2016, 27, 1855-1862.	1.0	2
8481	Singlet versus Triplet Reactivity in an Mn(V) Oxo Species: Testing Theoretical Predictions Against Experimental Evidence. <i>Journal of the American Chemical Society</i> , 2016, 138, 12375-12386.	6.6	88
8482	Regio- and Stereoselective Synthesis of Acetallic Tetrahydropyrans as Building Blocks for Natural Products Preparation, via a Tandem [4+3] Cycloaddition/Ozonolysis Process. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 4674-4695.	1.2	6
8483	Role of Gold Atoms in Oxidation and Reduction of Cationic Rhodium-Gold Oxide Clusters, Rh _n Au _m O _k ⁺ , Studied by Thermal Desorption Spectrometry and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19280-19285.	1.5	3
8484	Core Ionization Initiates Subfemtosecond Charge Migration in the Valence Shell of Molecules. <i>Physical Review Letters</i> , 2016, 117, 093002.	2.9	72
8485	Ab Initio Molecular Dynamics Simulation of Infrared Absorption Spectra of H ₃ O ⁺ and H ₅ O ₂ ⁺ in Nonaqueous Solutions of Trifluoromethanesulfonic Acid Hydrates. <i>Journal of Solution Chemistry</i> , 2016, 45, 1548-1559.	0.6	1
8486	Effects of the Grafting of Lanthanum Complexes on a Silica Surface on the Reactivity: Influence on Ethylene, Propylene, and 1,3-Butadiene Homopolymerization. <i>Inorganic Chemistry</i> , 2016, 55, 10024-10033.	1.9	5
8487	A Triad of Highly Reduced, Linear Iron Nitrosyl Complexes: {FeNO} ^{8−10} . <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11995-11998.	7.2	31
8488	Characterization of berkelium(III) dipicolinate and borate compounds in solution and the solid state. <i>Science</i> , 2016, 353, .	6.0	86
8489	A Triad of Highly Reduced, Linear Iron Nitrosyl Complexes: {FeNO} ^{8−10} . <i>Angewandte Chemie</i> , 2016, 128, 12174-12177.	1.6	5
8490	Arene C-H Bond Coordination versus C-H Bond Cleavage in Low-Valent Group 6 Carbonyl Pincer Complexes. <i>Organometallics</i> , 2016, 35, 3032-3039.	1.1	13
8491	Boron complexes of aromatic ring fused iminopyrrolyl ligands: synthesis, structure, and luminescence properties. <i>Dalton Transactions</i> , 2016, 45, 15603-15620.	1.6	36
8492	The influence hydrogen atom addition has on charge switching during motion of the metal atom in endohedral Ca@C ₆₀ H ₄ isomers. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2016, 374, 20150319.	1.6	3

#	ARTICLE	IF	CITATIONS
8493	Computational investigation on the host-guest inclusion process of norfloxacin into β -cyclodextrin. <i>Journal of Molecular Modeling</i> , 2016, 22, 220.	0.8	12
8494	Synthesis, Aggregation Induced Emission and Mechanochromic Luminescence of New β -Diketone Derivatives Bearing Tetraphenylene Moieties. <i>Journal of Fluorescence</i> , 2016, 26, 2005-2013.	1.3	6
8495	Spectroscopic and Theoretical Identification of Two Thermal Isomerization Pathways for Bistable Chiral Overcrowded Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 13478-13487.	1.7	30
8496	Photoreduction Mechanism of CO ₂ to CO Catalyzed by a Rhenium(I)-Polyoxometalate Hybrid Compound. <i>ACS Catalysis</i> , 2016, 6, 6422-6428.	5.5	58
8497	Methyldiyne-replaced boron nitride fullerenes and nanotubes: a wave function study. <i>New Journal of Chemistry</i> , 2016, 40, 8149-8157.	1.4	7
8498	Extreme π -Loading as a Design Element for Accessing Imido Ligand Reactivity. A CCC-NHC Pincer Tantalum Bis(imido) Complex: Synthesis, Characterization, and Catalytic Oxidative Amination of Alkenes. <i>Organometallics</i> , 2016, 35, 3452-3460.	1.1	31
8499	Solid State Investigation and Characterization of a Nepadutant Precursor: Polymorphic and Pseudopolymorphic Forms of MEN11282. <i>Crystal Growth and Design</i> , 2016, 16, 5294-5304.	1.4	13
8500	Ion-Radical Pair Separation in Larger Oxidized Water Clusters, (H ₂ O) ⁺ _n = 6-21. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7225-7239.	1.1	21
8501	Reductive Carbonylation of Oxorhenium Hydrides Induced by Lewis Acids. <i>Organometallics</i> , 2016, 35, 2822-2829.	1.1	9
8503	Polarizable Embedding Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4242-4253.	2.3	24
8504	Gas-Phase Interaction of Anions with Polyisobutylenes: Collision-Induced Dissociation Study and Quantum Chemical Modeling. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9195-9203.	1.2	0
8505	An adaptive distance-based group contribution method for thermodynamic property prediction. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23822-23830.	1.3	16
8506	Explicitly correlated frequency-independent second-order green's function for accurate ionization energies. <i>Journal of Computational Chemistry</i> , 2016, 37, 2447-2453.	1.5	16
8507	Effect of vanadium valence state on the solution chemistry and the stability of vanadium substituted polyoxometalates. <i>RSC Advances</i> , 2016, 6, 110922-110927.	1.7	2
8508	Computational Design of Cobalt Catalysts for Hydrogenation of Carbon Dioxide and Dehydrogenation of Formic Acid. <i>Inorganic Chemistry</i> , 2016, 55, 12179-12184.	1.9	39
8509	$D_{2d}(23)$ -C ₈₄ versus Sc ₂ C ₂ @ $D_{2d}(23)$ -C ₈₄ : Impact of Endohedral Sc ₂ C ₂ Doping on Chemical Reactivity in the Photolysis of Diazirine. <i>Journal of the American Chemical Society</i> , 2016, 138, 16523-16532.	6.6	24
8510	Synthesis, Spectroscopic Properties and DFT Calculation of Novel Pyrrolo[1,5-a]-1,8-naphthyridine Derivatives through a Facile One-pot Process. <i>Journal of Chemical Sciences</i> , 2016, 128, 1813-1821.	0.7	0
8511	Anharmonic Vibrational Analyses of Pentapeptide Conformations Explored with Enhanced Sampling Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10199-10213.	1.2	11

#	ARTICLE	IF	CITATIONS
8512	Computational Study of the Interactions between Benzene and Crystalline Ice I _h : Ground and Excited States. <i>ChemPhysChem</i> , 2016, 17, 4079-4089.	1.0	5
8513	PyCPR – a python-based implementation of the Conjugate Peak Refinement (CPR) algorithm for finding transition state structures. <i>Journal of Molecular Modeling</i> , 2016, 22, 242.	0.8	10
8514	Quantum molecular motion in the mixed ion-radical complex, [(H ₂ O)(H ₂ S)] ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27450-27459.	1.3	5
8515	Divide-and-Conquer Hartree-Fock-Bogoliubov Method and Its Application to Conjugated Diradical Systems. <i>Chemistry Letters</i> , 2016, 45, 1268-1270.	0.7	6
8516	Radical Stability as a Guideline in C-H Amination Reactions. <i>Advanced Synthesis and Catalysis</i> , 2016, 358, 3983-3991.	2.1	65
8517	Multicolor Photoluminescence Including White-Light Emission by a Single Host-Guest Complex. <i>Journal of the American Chemical Society</i> , 2016, 138, 13541-13550.	6.6	233
8518	Ionic Liquid Solvation versus Catalysis: Computational Insight from a Multisubstituted Imidazole Synthesis in [Et ₂ NH ₂][HSO ₄]. <i>ChemistryOpen</i> , 2016, 5, 460-469.	0.9	18
8519	The molecular shape and the field similarities as criteria to interpret SAR studies for fragment-based design of platinum(IV) anticancer agents. Correlation of physicochemical properties with cytotoxicity. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 69, 39-60.	1.3	7
8520	New methodology for the synthesis of tetrahydrofuro[3,2-b]furan-2(3H)-one derivatives, synthons of natural products with biological interest. <i>Tetrahedron</i> , 2016, 72, 6794-6806.	1.0	3
8521	Evaluation of Generalized Born Models for Large Scale Affinity Prediction of Cyclodextrin Host-Guest Complexes. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2080-2092.	2.5	32
8522	Nucleophilic substitution by amide nitrogen in the aromatic rings of [zn ^{II} H]E ^{TM+} ions; the structures of the [b ₂ â ⁺ H ⁺ 17]E ^{TM+} and [c ₁ â ⁺ 17] ⁺ ions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11168-11175.	1.3	1
8523	Characterization and charge transfer properties of organic BODIPY dyes integrated in TiO ₂ nanotube based dye-sensitized solar cells. <i>RSC Advances</i> , 2016, 6, 91529-91540.	1.7	17
8524	Trimerization of Acetylene Catalyzed by Ir(PH ₂ CH ₂ CH ₂ PH ₂)Cl(cod): A Computational Study. <i>Bulletin of the Chemical Society of Japan</i> , 2016, 89, 584-594.	2.0	1
8525	Hydrogen bonding and delocalization in the ELF analysis approach. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27442-27449.	1.3	27
8526	Regulating ancillary ligands of Ru(II) complexes with square-planar quadridentate ligands for more efficient sensitizers in dye-sensitized solar cells: insights from theoretical investigations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29591-29599.	1.3	9
8527	The Decarboxylation of Î±,Î²-Unsaturated Acid Catalyzed by Prenylated FMN-Dependent Ferulic Acid Decarboxylase and the Enzyme Inhibition. <i>Journal of Organic Chemistry</i> , 2016, 81, 9289-9295.	1.7	25
8528	Electronic Effects on Narcissistic Self-Sorting in Multicomponent Self-Assembly of Fe-Iminopyridine <i>meso</i> -Helicates. <i>Inorganic Chemistry</i> , 2016, 55, 9805-9815.	1.9	28
8529	Mechanism of the Glutathione Persulfide Oxidation Process Catalyzed by Ethylmalonic Encephalopathy Protein 1. <i>ACS Catalysis</i> , 2016, 6, 7010-7020.	5.5	11

#	ARTICLE	IF	CITATIONS
8530	Source function and plane waves: Toward complete bader analysis. <i>Journal of Computational Chemistry</i> , 2016, 37, 2133-2139.	1.5	8
8531	The effect of stacking arrangement on the conjugation in azochromophores revealed by combination of Raman spectroscopy and DFT calculations. <i>Chemical Physics Letters</i> , 2016, 659, 242-246.	1.2	5
8532	Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22712-22718.	1.3	28
8533	Multicomponent Petasis-Boron Mannich Preparation of Alkylaminophenols and Antimicrobial Activity Studies. <i>ChemMedChem</i> , 2016, 11, 2015-2023.	1.6	31
8534	Factors Controlling the Chemoselectivity in the Oxidation of Olefins by Nonheme Manganese(IV)-Oxo Complexes. <i>Journal of the American Chemical Society</i> , 2016, 138, 10654-10663.	6.6	52
8535	Molecular and electronic structures of copper-cuprizone and analogues. <i>Inorganica Chimica Acta</i> , 2016, 451, 23-30.	1.2	7
8536	First principles model calculations of the biosynthetic pathway in selinadiene synthase. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4867-4870.	1.4	11
8537	Theoretical investigations towards the [4+2] cycloaddition of ketenes with 1-azadienes catalyzed by N-heterocyclic carbenes: mechanism and stereoselectivity. <i>Tetrahedron</i> , 2016, 72, 5295-5300.	1.0	16
8538	Nondirected C-H Activation of Arenes with Cp*Ir(III) Acetate Complexes: An Experimental and Computational Study. <i>Organometallics</i> , 2016, 35, 2435-2445.	1.1	13
8539	Axially Chiral Dimeric Naphthalene and Naphthoquinone Metabolites, from Root Cultures of the West African Liana <i>Triphyophyllum peltatum</i> . <i>Journal of Natural Products</i> , 2016, 79, 2094-2103.	1.5	11
8540	Enhanced Photocurrent Density by Spin-Coated NiO Photocathodes for N-Annulated Perylene-Based p-Type Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 19393-19401.	4.0	24
8541	Benchmark fragment-based ¹ H, ¹³ C, ¹⁵ N and ¹⁷ O chemical shift predictions in molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21686-21709.	1.3	94
8542	Mechanistic examination of aerobic Pt oxidation: insertion of molecular oxygen into Pt-H bonds through a radical chain mechanism. <i>Dalton Transactions</i> , 2016, 45, 11650-11656.	1.6	5
8543	Structural diversity of halocarbonyl molybdenum and tungsten PNP pincer complexes through ligand modifications. <i>Dalton Transactions</i> , 2016, 45, 13834-13845.	1.6	11
8544	Generalization of the Kohn-Sham system that can represent arbitrary one-electron density matrices. <i>Physical Review A</i> , 2016, 93, .	1.0	1
8545	Tuning of the Electronic Levels of Oligothiophene-Naphthalimide Assemblies by Chemical Modification. <i>Chemistry - A European Journal</i> , 2016, 22, 13643-13652.	1.7	12
8546	Solvation structure and thermodynamics for Pr(III), Nd(III) and Dy(III) complexes in ionic liquids evaluated by Raman spectroscopy and DFT calculation. <i>Journal of Molecular Structure</i> , 2016, 1125, 186-192.	1.8	9
8547	Interfacial charge-transfer transitions and reorganization energies in sulfur-bridged TiO ₂ -x-benzenedithiol complexes (x: o, m, p). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22286-22292.	1.3	28

#	ARTICLE	IF	CITATIONS
8548	A strategy to minimize the energy offset in carrier injection from excited dyes to inorganic semiconductors for efficient dye-sensitized solar energy conversion. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22244-22253.	1.3	13
8549	Crystal structure and cytotoxic activities of a bis(pyrrolyl-imine) gold(III) complex. <i>Journal of Coordination Chemistry</i> , 2016, 69, 2707-2722.	0.8	2
8550	A generalized operational formula based on total electronic densities to obtain 3D pictures of the dual descriptor to reveal nucleophilic and electrophilic sites accurately on closed-shell molecules. <i>Journal of Computational Chemistry</i> , 2016, 37, 2279-2303.	1.5	16
8551	Reduced graphene oxide enhancing the photoelectrochemical properties of poly(3-hexylthiophene). <i>Carbon</i> , 2016, 109, 57-64.	5.4	6
8552	Anion Complexes with Tetrazine-Based Ligands: Formation of Strong Anion-π Interactions in Solution and in the Solid State. <i>Inorganic Chemistry</i> , 2016, 55, 8013-8024.	1.9	47
8553	Why Replacing Different Oxygens of Thymine with Sulfur Causes Distinct Absorption and Intersystem Crossing. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6342-6350.	1.1	44
8554	Group 14 Dithienometallope-Linked Ethynylene-Conjugated Porphyrin Dimers. <i>Inorganic Chemistry</i> , 2016, 55, 7432-7441.	1.9	20
8555	Proton-Conducting Phenolate-Based Zr Metal-Organic Framework: A Joint Experimental-Modeling Investigation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24503-24510.	1.5	28
8556	Excited states in large molecular systems through polarizable embedding. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20234-20250.	1.3	78
8557	Computational investigation on MB n (M = Li-Cs, Be-Ba, Sc-La and Ti; n = 28 and 38). <i>Journal of Molecular Modeling</i> , 2016, 22, 184.	0.8	12
8558	Nonequimolar Mixture of Organic Acids and Bases: An Exception to the Rule of Thumb for Salt or Cocystal. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7606-7613.	1.2	25
8559	Non-bonding 1,5-H ₂ O interactions govern chemo- and enantioselectivity in isothioureacatalyzed annulations of benzazoles. <i>Chemical Science</i> , 2016, 7, 6919-6927.	3.7	125
8560	Synthesis of a labile sulfur-centred ligand, [S(H)C(PPh ₂ S) ₂] ⁺ : structural diversity in lithium(i), zinc(ii) and nickel(ii) complexes. <i>Dalton Transactions</i> , 2016, 45, 12691-12701.	1.6	3
8561	Relativistic frozen core potential scheme with relaxation of core electrons. <i>Chemical Physics Letters</i> , 2016, 663, 97-103.	1.2	4
8562	Gold(I) Complexes of Ferrocenyl Polyphosphines: Aurophilic Gold Chloride Formation and Phosphine-Concerted Shuttling of a Dinuclear [ClAu-AuCl] Fragment. <i>Inorganic Chemistry</i> , 2016, 55, 10907-10921.	1.9	25
8563	Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8691-8698.	1.1	7
8564	Computational Study of First-Row Transition Metals Supported on MOF NU-1000 for Catalytic Acceptorless Alcohol Dehydrogenation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24697-24705.	1.5	40
8565	Preparation of diazoalkane complexes of iron(ii). <i>RSC Advances</i> , 2016, 6, 97650-97658.	1.7	9

#	ARTICLE	IF	CITATIONS
8566	Size and Site Dependence of the Catalytic Activity of Iridium Clusters toward Ethane Dehydrogenation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9500-9508.	1.1	6
8567	Quinone 1 e ⁻ and 2 e ⁻ /2 H ⁺ Reduction Potentials: Identification and Analysis of Deviations from Systematic Scaling Relationships. <i>Journal of the American Chemical Society</i> , 2016, 138, 15903-15910.	6.6	211
8568	Unconventional exo selectivity in thermal normal-electron-demand Diels-Alder reactions. <i>Scientific Reports</i> , 2016, 6, 35147.	1.6	20
8569	Hydrogen adsorption on Pt-decorated closed-end armchair (3,3), (4,4) and (5,5) single-walled carbon nanotubes. <i>Molecular Physics</i> , 2016, 114, 3508-3517.	0.8	7
8570	Amplitude Determinant Coupled Cluster with Pairwise Doubles. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5841-5850.	2.3	12
8571	Hemibonding between Water Cation and Water. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9618-9624.	1.1	13
8572	A Surface Nanocavity Structure of Bisphenol P on TiO ₂ Showing Interfacial Charge-Transfer Absorption. <i>ChemistrySelect</i> , 2016, 1, 5590-5593.	0.7	19
8573	Density functional theory basis set convergence of sulfuric acid-containing molecular clusters. <i>Computational and Theoretical Chemistry</i> , 2016, 1098, 1-12.	1.1	53
8574	First-Principle Calculations of the Band Shapes of Singlet-Triplet Transitions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24605-24614.	1.5	8
8575	An Exceptionally Stable Metal-Organic Framework Supported Molybdenum(VI) Oxide Catalyst for Cyclohexene Epoxidation. <i>Journal of the American Chemical Society</i> , 2016, 138, 14720-14726.	6.6	211
8576	Enhanced spin-orbit coupling driven by state mixing in organic molecules for OLED applications. <i>Organic Electronics</i> , 2016, 39, 311-317.	1.4	11
8577	Computational modelling of panchromatic porphyrins with strong NIR absorptions for solar energy capture. <i>Chemical Physics Letters</i> , 2016, 665, 40-46.	1.2	4
8578	Mechanisms of Bond Cleavage during Manganese Oxide and UV Degradation of Glyphosate: Results from Phosphate Oxygen Isotopes and Molecular Simulations. <i>Journal of Agricultural and Food Chemistry</i> , 2016, 64, 8474-8482.	2.4	46
8579	Symmetry-Adapted Perturbation Theory Energy Analysis of Alkyl Fluorine-Aromatic Interactions in Torsion Balance Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9292-9298.	1.1	10
8580	Geometrical Structures of Partially Oxidized Rhodium Cluster Cations, Rh ₆ O _m (m = 4, 5, 6), Revealed by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8599-8605.	1.1	11
8581	An operationally flexible fuel cell based on quaternary ammonium-biphosphate ion pairs. <i>Nature Energy</i> , 2016, 1, .	19.8	206
8582	Computational design of ZnP(P) ₄ stacks: Three modes of binding. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650043.	1.8	8
8583	Blue rhenium tricarbonyl DPPZ complexes - low energy charge-transfer absorption at tissue-penetrating wavelengths. <i>Chemical Communications</i> , 2016, 52, 12498-12501.	2.2	10

#	ARTICLE	IF	CITATIONS
8584	Modification of silica-supported tungsten neosilyl oxo precatalysts: impact of substituted phenol on activity and stability in olefin metathesis. <i>Catalysis Science and Technology</i> , 2016, 6, 8532-8539.	2.1	11
8585	Arylamino radical complexes of ruthenium and osmium: dual radical counter in a molecule. <i>Dalton Transactions</i> , 2016, 45, 19428-19440.	1.6	8
8586	Indenyl Compounds with Constrained Hapticity: The Effect of Strong Intramolecular Coordination. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 5250-5264.	1.0	8
8587	Theoretical Calculation of pK_a 's of Selenols in Aqueous Solution Using an Implicit Solvation Model and Explicit Water Molecules. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8916-8922.	1.1	38
8588	The mechanism of Claisen rearrangement of allyl phenyl ether from the perspective of topological analysis of the ELF. <i>New Journal of Chemistry</i> , 2016, 40, 8717-8726.	1.4	18
8589	Building better lithium-sulfur batteries: from LiNO ₃ to solid oxide catalyst. <i>Scientific Reports</i> , 2016, 6, 33154.	1.6	77
8590	Coordination of o-benzosemiquinonate, o-aminobenzosemiquinonate, 4,4'-di-tert-butyl-2,2'-bipyridine and 1,10-phenanthroline anion radicals to oxidovanadium(IV). <i>New Journal of Chemistry</i> , 2016, 40, 10305-10315.	1.4	6
8591	Stille coupling via C–N bond cleavage. <i>Nature Communications</i> , 2016, 7, 12937.	5.8	87
8592	Molecular Dynamics Simulations Reveal that Water Diffusion between Graphene Oxide Layers is Slow. <i>Scientific Reports</i> , 2016, 6, 29484.	1.6	124
8593	A comparative computational study of N-heterocyclic olefin and N-heterocyclic carbene mediated carboxylative cyclization of propargyl alcohols with CO ₂ . <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10875-10885.	1.5	19
8594	How does ammonia bind to the oxygen-evolving complex in the S ₂ state of photosynthetic water oxidation? Theoretical support and implications for the W1 substitution mechanism. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31551-31565.	1.3	15
8595	Structure and Reaction Chemistry of Magnesium Organocuprates Derived from Magnesiacyclopentadienes and Copper(I) Salts. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14762-14765.	7.2	9
8596	Theoretical Study on the Mechanism of the Thermal Retro-Cycloaddition of Isoxazolinofullerenes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 8830-8842.	1.1	6
8597	Structure and Reaction Chemistry of Magnesium Organocuprates Derived from Magnesiacyclopentadienes and Copper(I) Salts. <i>Angewandte Chemie</i> , 2016, 128, 14982-14985.	1.6	2
8598	Syntheses of [Pt ₆ (CO) ₈ (SnCl ₂) ₂ (SnCl ₃) ₃] ⁴⁺ and [Pt ₆ (CO) ₈ (SnCl ₂) ₂ (SnCl ₃) ₃] ₂ (PPh ₃) ₂] ¹⁴⁺ Platinum Carbonyl Clusters Decorated by Sn ^{II} Fragments. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 3939-3949.	1.0	14
8599	Theoretical and experimental study of donor-bridge-acceptor system: model 2-[5-(9H-fluoren-9-ylidene)methyl]thiophen-2-yl]-1,3,4-oxadiazole derivatives. <i>Monatshefte für Chemie</i> , 2016, 147, 2103-2112.	0.9	2
8600	Computational and Experimental Studies of Regioselective S _N Ar Halide Exchange (Halex) Reactions of Pentachloropyridine. <i>Journal of Organic Chemistry</i> , 2016, 81, 10672-10682.	1.7	17
8601	Toward Molecular Magnets of Organic Origin via Anion-π Interaction Involving <i>m</i> -Aminyl Diradical: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9117-9130.	1.1	12

#	ARTICLE	IF	CITATIONS
8602	Formation of Potential Interstellar Noble Gas Molecules in Gas and Adsorbed Phases. ACS Omega, 2016, 1, 765-772.	1.6	14
8603	The Interaction between Graphene and Oxygen Atom. Open Physics, 2016, 14, 690-694.	0.8	4
8605	Gaussian polarizable-ion tight binding. Journal of Chemical Physics, 2016, 145, 144103.	1.2	11
8606	Peptide Reactivity of Isothiocyanates – Implications for Skin Allergy. Scientific Reports, 2016, 6, 21203.	1.6	22
8607	Probing the Origin of Challenge of Realizing Metallaphosphabenzene: Unfavorable 1,2-Migration in Metallapyridines Becomes Feasible in Metallaphosphabenzene. Scientific Reports, 2016, 6, 28543.	1.6	8
8608	A first principle study on the interaction between acetylcholinesterase and acetylcholine, and also rivastigmine in alzheimer's disease case. Journal of Physics: Conference Series, 2016, 739, 012136.	0.3	4
8609	An experimental and theoretical study on the preparation of 4,4'-methylene-bis(N,N-dimethylaniline) in ionic liquid. Journal of Physical Organic Chemistry, 2016, 29, 276-280.	0.9	2
8610	Synthesis of Five-Porphyrin Nanorings by Using Ferrocene and Corannulene Templates. Angewandte Chemie - International Edition, 2016, 55, 8358-8362.	7.2	54
8611	Thermal decomposition of diethyl ketone triperoxide in methyl methacrylate: Theoretical and experimental study of the initial solvation state and its influence on the polymerization process. Journal of Applied Polymer Science, 2016, 133, .	1.3	0
8612	Metal-Free Dehydrogenation of Amine-Boranes by Tunable N-Heterocyclic Iminoboranes. Chemistry - A European Journal, 2016, 22, 2134-2145.	1.7	49
8613	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenic Dicationic Rings. Chemistry - A European Journal, 2016, 22, 2793-2800.	1.7	30
8614	Highly Active and Robust Metalloporphyrin Catalysts for the Synthesis of Cyclic Carbonates from a Broad Range of Epoxides and Carbon Dioxide. Chemistry - A European Journal, 2016, 22, 6556-6563.	1.7	176
8615	Computational Design of Iron Diphosphine Complexes with Pendant Amines for Hydrogenation of CO ₂ to Methanol: A Mimic of [NiFe] Hydrogenase. Chemistry - A European Journal, 2016, 22, 8897-8902.	1.7	14
8616	Electrophilic 5-Substituted Uracils as Potential Radiosensitizers: A Density Functional Theory Study. ChemPhysChem, 2016, 17, 2572-2578.	1.0	20
8617	Oxidovanadium Complexes of 2,2'-Bipyridine, 1,10-Phenanthroline, and p-Nitro-o-aminophenol - Radical versus Nonradical States. European Journal of Inorganic Chemistry, 2016, 2016, 330-338.	1.0	6
8618	Computational Insights into the Mechanisms of H ₂ Activation and H ₂ /D ₂ Isotope Exchange by Dimolybdenum Tetrasulfide Complexes. European Journal of Inorganic Chemistry, 2016, 2016, 1886-1894.	1.0	6
8619	NIR-Raman spectrum and DFT calculations of okadaic acid DSP marine biotoxin microprobe. Journal of Raman Spectroscopy, 2016, 47, 636-642.	1.2	7
8620	Phenanthro[4,5-fgh]quinoxaline-Fused Subphthalocyanines: Synthesis, Structure, and Spectroscopic Characterization. Chemistry - A European Journal, 2016, 22, 9488-9492.	1.7	7

#	ARTICLE	IF	CITATIONS
8621	Computational Insights into the Central Role of Nonbonding Interactions in Modern Covalent Organocatalysis. <i>Accounts of Chemical Research</i> , 2016, 49, 1279-1291.	7.6	56
8622	Theoretical Insights into the Catalytic Mechanism of <i>N</i> -Heterocyclic Olefins in Carboxylative Cyclization of Propargyl Alcohol with CO ₂ . <i>Journal of Organic Chemistry</i> , 2016, 81, 5303-5313.	1.7	44
8623	Heterodinuclear Ni(<i>κ</i>) and Cu(<i>κ</i>) Schiff base complexes and their activity in oxygen reduction. <i>Dalton Transactions</i> , 2016, 45, 14725-14733.	1.6	12
8624	Mitochondria-targeted aggregation induced emission theranostics: crucial importance of in situ activation. <i>Chemical Science</i> , 2016, 7, 6050-6059.	3.7	83
8625	Fullerenes and their derivatives as inhibitors of tumor necrosis factor- α with highly promoted affinities. <i>Journal of Molecular Modeling</i> , 2016, 22, 161.	0.8	11
8626	Phosphorane lifetime and stereo-electronic effects along the alkaline hydrolysis of phosphate esters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18255-18267.	1.3	16
8627	Palladium-catalyzed regioselective and stereo-invertive ring-opening borylation of 2-arylaziridines with bis(pinacolato)diboron: experimental and computational studies. <i>Chemical Science</i> , 2016, 7, 6141-6152.	3.7	69
8628	Tetraphenylethene end-capped diketopyrrolopyrrole fluorogens with AIE and large two-photon absorption cross-sections features and application in bioimaging. <i>Dyes and Pigments</i> , 2016, 133, 201-213.	2.0	33
8629	A New Method To Evaluate Excited States Lifetimes Based on Greenâ€™s Function: Application to Dye-Sensitized Solar Cells. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3074-3086.	2.3	7
8630	Manipulation of electrical characteristics of non-volatile transistor-type memory devices through the acceptor strength of donor-acceptor conjugated copolymers. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5702-5708.	2.7	17
8631	Petascale Simulations of the Morphology and the Molecular Interface of Bulk Heterojunctions. <i>ACS Nano</i> , 2016, 10, 7008-7022.	7.3	25
8632	Tuning Up an Electronic Structure of the Subphthalocyanine Derivatives toward Electron-Transfer Process in Noncovalent Complexes with C ₆₀ and C ₇₀ Fullerenes: Experimental and Theoretical Studies. <i>Inorganic Chemistry</i> , 2016, 55, 9549-9563.	1.9	36
8633	Mechanism of H ₂ Production by Models for the [NiFe]-Hydrogenases: Role of Reduced Hydrides. <i>Journal of the American Chemical Society</i> , 2016, 138, 9234-9245.	6.6	56
8634	Density Functional Exploration of C ₄ H ₃ N Isomers. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5928-5938.	1.1	6
8635	Density Functional Theory Calculation of p <i>K</i> _a â€™s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5726-5735.	1.1	146
8636	Silica-Supported Tungsten Neosilyl Oxo Precatalysts: Impact of the Podality on Activity and Stability in Olefin Metathesis. <i>Organometallics</i> , 2016, 35, 2188-2196.	1.1	31
8637	Computation Sheds Insight into Iron Porphyrin Carbenesâ€™ Electronic Structure, Formation, and Nâ€™H Insertion Reactivity. <i>Journal of the American Chemical Society</i> , 2016, 138, 9597-9610.	6.6	99
8638	Aplicyanins â€™ brominated natural marine products with superbasic character. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2016, 71, 883-889.	0.3	7

#	ARTICLE	IF	CITATIONS
8639	Molecular self-healing mechanisms between C ₆₀ -fullerene and anthracene unveiled by Raman and two-dimensional correlation spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17973-17982.	1.3	14
8640	Divergent ynamide reactivity in the presence of azides – an experimental and computational study. <i>Chemical Science</i> , 2016, 7, 6032-6040.	3.7	32
8641	Homodesmotic method of determining the O–H bond dissociation energies in phenols. <i>Kinetics and Catalysis</i> , 2016, 57, 159-169.	0.3	5
8642	Chromophore-labelled, luminescent platinum complexes: syntheses, structures, and spectroscopic properties. <i>Dalton Transactions</i> , 2016, 45, 10297-10307.	1.6	11
8643	Electrochemical Electron Transfer and Proton-Coupled Electron Transfer: Effects of Double Layer and Ionic Environment on Solvent Reorganization Energies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2917-2925.	2.3	31
8644	Impact of the Kohn–Sham Delocalization Error on the 4f Shell Localization and Population in Lanthanide Complexes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3109-3121.	2.3	49
8645	Selective and reversible self-assembly of C ₆₀ -fullerene on a 9,10-bis(S-acetylthiomethyl)anthracene modified gold surface. <i>RSC Advances</i> , 2016, 6, 53101-53106.	1.7	4
8646	Factors Affecting the Production of Aromatic Immonium Ions in MALDI 157 nm Photodissociation Studies. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 834-846.	1.2	7
8647	Ab initio study of electronic interaction energies and desolvation energies for dopaminergic ligands in the catechol-O-methyltransferase active site. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 146-162.	1.1	10
8648	Experimental and theoretical investigation of structures and relative reactivity of Pr@C ₇₄ and Pr@C ₇₄ (C ₆ H ₃ Cl ₂). <i>Diamond and Related Materials</i> , 2016, 64, 110-118.	1.8	8
8649	Investigation of the energy barrier to the rotation of amide C–N bonds in ACE inhibitors by NMR, dynamic HPLC and DFT. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2016, 128, 416-425.	1.4	4
8650	The structural and photophysical properties of multibranched derivatives with curved conjugated aromatic cores. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6054-6062.	2.7	9
8651	Synthesis and reactivity of a terminal uranium(IV) sulfide supported by siloxide ligands. <i>Chemical Science</i> , 2016, 7, 5846-5856.	3.7	23
8652	A theoretical investigation on hydrolysis mechanism of biologically relevant Pt(II)/Pd(II) complexes with π -donor and σ -acceptor carrier ligand. <i>Chemical Physics Letters</i> , 2016, 657, 148-155.	1.2	4
8653	Absolute configuration of the synthetic cannabinoid MDMB-CHMICA with its chemical characteristics in illegal products. <i>Forensic Toxicology</i> , 2016, 34, 344-352.	1.4	18
8654	How half sandwich ruthenium compounds interact with DNA while not being hydrolyzed; a comparative study. <i>Journal of Inorganic Biochemistry</i> , 2016, 160, 12-23.	1.5	9
8655	Theoretical analysis of complex formation of p-carboxybenzeneboronic acid with a monosaccharide. <i>Journal of Molecular Liquids</i> , 2016, 217, 93-98.	2.3	9
8656	Adsorption and decomposition of monopropellant molecule HAN on Pd(100) and Ir(100) surfaces: A DFT study. <i>Surface Science</i> , 2016, 653, 1-10.	0.8	10

#	ARTICLE	IF	CITATIONS
8657	Theoretical Studies on the Mechanism of Thioesterase-Catalyzed Macrocyclization in Erythromycin Biosynthesis. <i>ACS Catalysis</i> , 2016, 6, 4369-4378.	5.5	32
8658	Structure, formation, thermodynamics and interactions in 9-carboxy-10-methylacridinium-based molecular systems. <i>New Journal of Chemistry</i> , 2016, 40, 7359-7372.	1.4	1
8659	Synthesis, spectroscopic characterization and DFT study of dinuclear ruthenium sawhorse-type complexes derived from the reaction of trinuclear aggregates and (Z)-5-arylidenerhodanines. <i>Journal of Coordination Chemistry</i> , 2016, 69, 2291-2307.	0.8	0
8660	A Fluorescent Polymer Probe with High Selectivity toward Vascular Endothelial Cells for and beyond Noninvasive Two-Photon Intravital Imaging of Brain Vasculature. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 17047-17059.	4.0	20
8661	Nitrogen Molecule Adsorption on Cationic Tantalum Clusters and Rhodium Clusters and Desorption from Their Nitride Clusters Studied by Thermal Desorption Spectrometry. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4089-4095.	1.1	50
8662	Comparing the strength of covalent bonds, intermolecular hydrogen bonds and other intermolecular interactions for organic molecules: X-ray diffraction data and quantum chemical calculations. <i>New Journal of Chemistry</i> , 2016, 40, 6848-6853.	1.4	41
8663	Biophysical Characterization of Fluorotyrosine Probes Site-Specifically Incorporated into Enzymes: <i>E. coli</i> Ribonucleotide Reductase As an Example. <i>Journal of the American Chemical Society</i> , 2016, 138, 7951-7964.	6.6	43
8664	The influence of the DFT approach on the structure and relative stability of models for cellulose I allomorphs. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
8665	Experimental and density functional study on electronic structure and electronic circular dichroism of the phenylpyrazole insecticides enantiomers and the probable chiral catabolites. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	5
8666	DFT study of the mechanism of manganese quercetin 2,3-dioxygenase: quest for origins of enzyme unique nitroxygenase activity and regioselectivity. <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 475-489.	1.1	14
8667	Gold-Mediated Isomerization of Cyclooctyne to Ring Fused Olefinic Bicycles. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 995-1001.	1.0	6
8668	Enantiopure Chiral Concave 1,10-Phenanthrolines. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 1119-1131.	1.2	4
8669	Competition between hydrogen and halogen bonding in halogenated 1-methyluracil: Water systems. <i>Journal of Computational Chemistry</i> , 2016, 37, 763-770.	1.5	21
8670	Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. <i>Journal of Computational Chemistry</i> , 2016, 37, 1887-1896.	1.5	6
8671	Photofragmentation of Serine Following C 1s Core Ionization—Comparison with Cysteine. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5419-5426.	1.1	9
8672	Vibrational Signatures of Conformer-Specific Intramolecular Interactions in Protonated Tryptophan. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5598-5608.	1.1	32
8673	Theoretical study on mechanism of the photochemical ligand substitution of fac-[Re ^I (bpy)(CO) ₃ (PR) ₃] ⁺ complex. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17557-17564.	1.3	16
8674	NMR properties of hydrogen-bonded glycine cluster in gas phase. <i>Journal of Molecular Structure</i> , 2016, 1123, 55-65.	1.8	6

#	ARTICLE	IF	CITATIONS
8675	Anion directed structural diversity in zinc complexes with conformationally flexible quinazoline ligand: structural, spectral and theoretical studies. Dalton Transactions, 2016, 45, 12053-12068.	1.6	10
8676	Photoresponsive Supramolecular Assemblies Based on a C ₃ -Symmetric Benzene-1,3,5-tricarboxamide-Anchored Diarylethene. Advanced Optical Materials, 2016, 4, 840-847.	3.6	36
8677	Click Functionalization of a Dibenzocyclooctyne-Containing Conjugated Polyimine. Angewandte Chemie, 2016, 128, 957-961.	1.6	7
8678	Click Functionalization of a Dibenzocyclooctyne-Containing Conjugated Polyimine. Angewandte Chemie - International Edition, 2016, 55, 945-949.	7.2	28
8679	Mechanistic Study of Photocatalytic Hydrogen Generation with Simple Iron Carbonyls as Water Reduction Catalysts. ChemCatChem, 2016, 8, 404-411.	1.8	16
8680	Reduction Process of Tetraplatin in the Presence of Deoxyguanosine Monophosphate (dGMP): A Computational DFT Study. Chemistry - A European Journal, 2016, 22, 1037-1047.	1.7	12
8681	Rules of Macrocyclic Topology: A [13]-Macrolactone Case Study. Chemistry - A European Journal, 2016, 22, 6001-6011.	1.7	9
8682	Conducting π Columns of Highly Symmetric Coronene, The Smallest Fragment of Graphene. Chemistry - A European Journal, 2016, 22, 6023-6030.	1.7	18
8683	Chiral ferrocene-based P,S ligands for Ir-catalyzed hydrogenation of α -minimally functionalized olefins. Scope and limitations. Tetrahedron, 2016, 72, 2623-2631.	1.0	32
8684	Re-designing the substrate binding pocket of laccase for enhanced oxidation of sinapic acid. Catalysis Science and Technology, 2016, 6, 3900-3910.	2.1	56
8685	Problems, successes and challenges for the application of dispersion-corrected density-functional theory combined with dispersion-based implicit solvent models to large-scale hydrophobic self-assembly and polymorphism. Molecular Simulation, 2016, 42, 494-510.	0.9	13
8686	Theoretical insight into the enhanced hindrance, thermal stability and optical properties of diarylethene with a benzobis(thiadiazole) bridge and benzothiophene rings. Dyes and Pigments, 2016, 125, 348-355.	2.0	10
8687	From Chaos to Order: Chain-Length Dependence of the Free Energy of Formation of Meso-tetraalkylporphyrin Self-Assembled Monolayer Polymorphs. Journal of Physical Chemistry C, 2016, 120, 1739-1748.	1.5	16
8688	Benchmarking DFT and semi-empirical methods for a reliable and cost-efficient computational screening of benzofulvene derivatives as donor materials for small-molecule organic solar cells. Journal of Physics Condensed Matter, 2016, 28, 074005.	0.7	34
8689	DFTB/PCM Applied to Ground and Excited State Potential Energy Surfaces. Journal of Physical Chemistry A, 2016, 120, 771-784.	1.1	16
8690	Inner-Shell Water Rearrangement Following Photoexcitation of Tris(2,2'-bipyridine)iron(II). Journal of Physical Chemistry B, 2016, 120, 206-216.	1.2	21
8691	[Re(CO) ₃ Cl(C ₅ H ₄ ClP) ₂] and [Re(CO) ₂ Cl(C ₅ H ₄ ClP) ₃]: synthesis and characterization of two novel rhenium(κ^1) phosphinine complexes. RSC Advances, 2016, 6, 14134-14139.	1.7	4
8692	Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4(MP2)/G4 theoretical study. Computational and Theoretical Chemistry, 2016, 1075, 30-37.	1.1	5

#	ARTICLE	IF	CITATIONS
8693	Theoretical investigation on the molecular inclusion process of prilocaine into p-sulfonic acid calix[6]arene. <i>Chemical Physics Letters</i> , 2016, 646, 52-55.	1.2	12
8694	Molecular Dynamics Simulations on O ₂ Permeation through Nafion Ionomer on Platinum Surface. <i>Electrochimica Acta</i> , 2016, 188, 767-776.	2.6	198
8695	Curcumin inspired synthesis of unsymmetrical diarylpentanoids with highly potent anti-parasitic activities: in silico studies and DFT-based stereochemical calculation. <i>MedChemComm</i> , 2016, 7, 820-831.	3.5	8
8696	A fluorescent coumarin-thiophene hybrid as a ratiometric chemosensor for anions: Synthesis, photophysics, anion sensing and orbital interactions. <i>Journal of Molecular Structure</i> , 2016, 1108, 269-277.	1.8	34
8697	Theoretical investigation on functional monomer and solvent selection for molecular imprinting of tramadol. <i>Chemical Physics Letters</i> , 2016, 645, 174-179.	1.2	47
8698	New blue light-emitting isocyanobiphenyl based fluorophores: Their solvatochromic and biolabeling properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 318, 124-134.	2.0	4
8699	A Ruthenium Catalyst with Unprecedented Effectiveness for the Coupling Cyclization of β -Amino Alcohols and Secondary Alcohols. <i>ACS Catalysis</i> , 2016, 6, 1247-1253.	5.5	111
8700	Rhodium Oxide Cluster Ions Studied by Thermal Desorption Spectrometry. <i>Journal of Physical Chemistry A</i> , 2016, 120, 356-363.	1.1	21
8701	Behaviour of the surface hydroxide groups of exfoliated kaolinite in the gas phase and during water adsorption. <i>Dalton Transactions</i> , 2016, 45, 2523-2535.	1.6	9
8702	The multi-channel reaction of the OH radical with 5-hydroxymethylcytosine: a computational study. <i>RSC Advances</i> , 2016, 6, 13349-13357.	1.7	1
8703	Dynamical Correlation Effects on Photoisomerization: Ab Initio Multiple Spawning Dynamics with MS-CASPT2 for a Model <i>trans</i> -Protonated Schiff Base. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1940-1949.	1.2	61
8704	CHARMM force field parameterization protocol for self-assembling peptide amphiphiles: the Fmoc moiety. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4659-4667.	1.3	17
8705	Ternary assemblies comprising metal-salophen complexes and 4,4'-bipyridine. <i>New Journal of Chemistry</i> , 2016, 40, 5714-5721.	1.4	6
8706	Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1660-1669.	1.2	20
8707	A gas-phase ab initio study of the hydrolysis of HCN. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3
8708	Monte Carlo simulation study of the halogenated MIL-47(V) frameworks: influence of functionalization on H ₂ S adsorption and separation properties. <i>Journal of Materials Science</i> , 2016, 51, 2307-2319.	1.7	23
8709	DFT Study on the Mechanism and Stereoselectivity of NHC-Catalyzed Synthesis of Substituted Trifluoromethyl Dihydropyranones with Contiguous Stereocenters. <i>Journal of Organic Chemistry</i> , 2016, 81, 868-877.	1.7	28
8710	Alkyl chain functionalised, cyclometalated platinum(II) complexes: Syntheses, luminescence properties and X-ray crystal structure. <i>Journal of Organometallic Chemistry</i> , 2016, 805, 87-93.	0.8	7

#	ARTICLE	IF	CITATIONS
8711	Raman spectroscopic study of water tetramer in [Cu(3-aminomethyl)pyridine OH 2 oxalate·2H ₂ O] n. <i>Polyhedron</i> , 2016, 105, 200-204.	1.0	3
8712	Acridine-based complex as amino acid anion fluorescent sensor in aqueous solution. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 157, 1-5.	2.0	26
8713	Microscopic Model of the Metal-Organic Framework/Polymer Interface: A First Step toward Understanding the Compatibility in Mixed Matrix Membranes. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 809-819.	4.0	129
8714	Exploring Interfacial Events in Gold-Nanocluster-Sensitized Solar Cells: Insights into the Effects of the Cluster Size and Electrolyte on Solar Cell Performance. <i>Journal of the American Chemical Society</i> , 2016, 138, 390-401.	6.6	137
8715	Unveiling the Catalytic Mechanism of NADP ⁺ -Dependent Isocitrate Dehydrogenase with QM/MM Calculations. <i>ACS Catalysis</i> , 2016, 6, 357-368.	5.5	23
8716	Design of new disulfide-based organic compounds for the improvement of self-healing materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1758-1770.	1.3	139
8717	Quantifying Electron Delocalization in Electrides. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 79-91.	2.3	15
8718	Total Synthesis of (±)-Hymenoseetin. <i>Journal of Organic Chemistry</i> , 2016, 81, 215-228.	1.7	26
8719	TDDFT studies on the chiroptical properties of a chiral inorganic polythioanion Möbius strip. <i>Inorganic Chemistry Frontiers</i> , 2016, 3, 86-91.	3.0	2
8720	Ruthenium-8-quinolinethiolate-phenylterpyridine versus ruthenium-bipyridine-phenyl-terpyridine complexes as homogeneous water and high temperature stable hydrogenation catalysts for biomass-derived substrates. <i>Polyhedron</i> , 2016, 108, 104-114.	1.0	5
8721	Ethyl Nitroacetate in Aza-Henry Addition on Trifluoromethyl Aldimines: A Solvent-Free Procedure To Obtain Chiral Trifluoromethyl (±)-Diamino Esters. <i>Journal of Organic Chemistry</i> , 2016, 81, 2864-2874.	1.7	16
8722	Material Exhibiting Efficient CO ₂ Adsorption at Room Temperature for Concentrations Lower Than 1000 ppm: Elucidation of the State of Barium Ion Exchanged in an MFI-Type Zeolite. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 8821-8833.	4.0	15
8723	A combined computational and experimental investigation of the oxidative ring-opening of cyclic ethers by oxoammonium cations. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3883-3888.	1.5	16
8724	Spectral density mapping at multiple magnetic fields suitable for $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll" \rangle \langle \text{mml:mrow} \langle \text{mml:msup} \langle \text{mml:mrow} / \rangle \langle \text{mml:mrow} \langle \text{mml:mn} \rangle 13 \langle \text{mml:mn} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msup} \langle \text{mml:mtext} \rangle C \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ NMR relaxation studies. <i>Journal of Magnetic Resonance</i> , 2016, 266, 23-40.	1.2	7
8725	Synthesis, characterization, and electronic properties of novel Fc-DCM conjugated system; experimental and computational studies. <i>Journal of Organometallic Chemistry</i> , 2016, 811, 14-19.	0.8	22
8726	Photoluminescence of a New Material: Cyclometalated C ⁺ Thiazole-2-ylidene Platinum(II) Complexes. <i>Organometallics</i> , 2016, 35, 959-971.	1.1	34
8727	Coordination complexes of niobium and tantalum pentahalides with a bulky NHC ligand. <i>Dalton Transactions</i> , 2016, 45, 6939-6948.	1.6	26
8728	High stability of the He atom confined in a U@C ₆₀ fullerene. <i>RSC Advances</i> , 2016, 6, 29288-29293.	1.7	3

#	ARTICLE	IF	CITATIONS
8729	Coumarin Push-Pull NLOphores with Red Emission: Solvatochromic and Theoretical Approach. <i>Journal of Fluorescence</i> , 2016, 26, 949-962.	1.3	32
8730	Connectivity matters – ultrafast isomerization dynamics of bisazobenzene photoswitches. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14795-14804.	1.3	69
8731	<i>Ab initio</i> coupled-cluster and multi-reference configuration interaction studies of the low-lying electronic states of 1,2,3,4-cyclobutanetetraone. <i>Molecular Physics</i> , 2016, 114, 695-708.	0.8	3
8732	Investigation into 9(S)-HPODE-derived allene oxide to cyclopentenone cyclization mechanism via diradical oxyallyl intermediates. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3544-3557.	1.5	10
8733	Catalytic Mechanism of Nitrile Hydratase Subsequent to Cyclic Intermediate Formation: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3259-3266.	1.2	14
8734	Transition-Metal Oxos as the Lewis Basic Component of Frustrated Lewis Pairs. <i>Journal of the American Chemical Society</i> , 2016, 138, 4832-4842.	6.6	42
8735	A phytochemical and computational study on flavonoids isolated from <i>Trifolium resupinatum</i> L. and their novel hepatoprotective activity. <i>Food and Function</i> , 2016, 7, 2094-2106.	2.1	57
8736	Tuning Side Arm Electronics in Unsymmetrical Cyclotriazadisulfonamide (CADA) Endoplasmic Reticulum (ER) Translocation Inhibitors to Improve their Human Cluster of Differentiation 4 (CD4) Receptor Down-Modulating Potencies. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 2633-2647.	2.9	16
8737	Synthesis, electrochemical, spectral and DFT study of novel thiazole-annelated subphthalocyanines with inherent chirality. <i>Dyes and Pigments</i> , 2016, 130, 24-36.	2.0	15
8738	Theoretical investigation on the mechanism of ferrocenecarboxaldehyde-catalyzed direct \hat{I}^2 -alkylation of 1-phenylethanol with benzyl alcohol. <i>Polyhedron</i> , 2016, 111, 179-184.	1.0	3
8739	Four-Component Damped Density Functional Response Theory Study of UV/Vis Absorption Spectra and Phosphorescence Parameters of Group 12 Metal-Substituted Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2324-2334.	2.3	9
8740	Mechanistic Study of Cellulose Hydrolysis by Carbon Catalysts. <i>Springer Theses</i> , 2016, , 77-112.	0.0	2
8741	Evaluation of the relative stabilities of two non-IPR isomers of Sm@C76. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2016, 24, 339-344.	1.0	14
8742	Insights into the use of Au ₁₉ Cu and Au ₁₉ Pd clusters for adsorption of trivalent arsenic. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	11
8743	Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, <i>p</i> -Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1625-1636.	1.1	91
8744	DFT study on the CuBr-catalyzed synthesis of highly substituted furans: effects of solvent DMF, substrate MeOH, trace H ₂ O and the metallic valence state of Cu. <i>RSC Advances</i> , 2016, 6, 20294-20305.	1.7	11
8745	Origin of the Enhanced Reactivity of \hat{I}^4 -Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. <i>ACS Catalysis</i> , 2016, 6, 2230-2243.	5.5	98
8746	The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2016, 138, 3831-3843.	6.6	35

#	ARTICLE	IF	CITATIONS
8747	Configuration Control in the Synthesis of Homo- and Heteroleptic Bis(oxazolinyphenolato/thiazolinyphenolato) Chelate Ligand Complexes of Oxorhenium(V): Isomer Effect on Ancillary Ligand Exchange Dynamics and Implications for Perchlorate Reduction Catalysis. <i>Inorganic Chemistry</i> , 2016, 55, 2597-2611.	1.9	26
8748	Unusual Electrochemical Properties of the Electropolymerized Thin Layer Based on a <i>i>s</i>-Tetrazine-Triphenylamine Monomer. <i>Journal of Physical Chemistry C</i>, 2016, 120, 4382-4391.</i>	1.5	28
8749	Silica-Gel-Supported Dual Acidic Ionic Liquids as Efficient Catalysts for the Synthesis of Polyoxymethylene Dimethyl Ethers. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 1859-1865.	1.8	59
8750	Implementation of High-Order Multireference Coupled-Cluster Methods on Intel Many Integrated Core Architecture. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1129-1138.	2.3	7
8751	Conformational Preferences of a Tropos Biphenyl Phosphinoxazoline—a Ligand with Wide Substrate Scope. <i>ACS Catalysis</i> , 2016, 6, 1701-1712.	5.5	30
8752	Transnitrosylation products of the dipeptide cysteinyl—cysteine: an examination by tandem mass spectrometry and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6047-6052.	1.3	3
8753	Can Nonpolar Polyisobutylenes be Measured by Electrospray Ionization Mass Spectrometry? Anion-Attachment Proved to be an Appropriate Method. <i>Journal of the American Society for Mass Spectrometry</i> , 2016, 27, 432-442.	1.2	4
8754	Synthesis, characterization, photophysics and electrochemistry of hexanuclear silver(I) alkynyl phosphine complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 812, 43-50.	0.8	7
8755	Acid Dissociation of 3-Mercaptopropionic Acid Coated CdSe—CdS/Cd _{0.5} Zn _{0.5} S/ZnS Core—Multishell Quantum Dot and Strong Ionic Interaction with Ca ²⁺ Ion. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3519-3529.	1.5	15
8756	An experimental and theoretical approach on the kinetics and mechanism for the formation of a four-membered (S, S) chelated Pt(<i>scpi</i>) complex. <i>RSC Advances</i> , 2016, 6, 18288-18299.	1.7	7
8757	A Study on Catalytic Conversion of Non-Food Biomass into Chemicals. Springer Theses, 2016, , .	0.0	5
8758	Characteristics of Low-Frequency Molecular Phonon Modes Studied by THz Spectroscopy and Solid-State <i>ab Initio</i> Theory: Polymorphs I and III of Diflunisal. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1698-1710.	1.2	30
8759	Benchmark Theoretical and Experimental Study on ¹⁵ N NMR Shifts of Oxidatively Damaged Guanine. <i>Journal of Physical Chemistry B</i> , 2016, 120, 915-925.	1.2	10
8760	A comparative study on the druggability of Schiff bases and dithiocarbamate derivatives of chitosan. <i>Polymer Bulletin</i> , 2016, 73, 2165-2177.	1.7	3
8761	Theoretical Evidence for Multiple Charge Transfer Pathways in Bacteriorhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1639-1646.	2.3	3
8762	Roles of Water Molecules in Modulating the Reactivity of Dioxygen-Bound Cu-ZSM-5 toward Methane: A Theoretical Prediction. <i>ACS Catalysis</i> , 2016, 6, 2487-2495.	5.5	54
8763	Rhodium-Catalyzed Stitching Reaction: Convergent Synthesis of Quinoidal Fused Oligosiloles. <i>Journal of the American Chemical Society</i> , 2016, 138, 3635-3638.	6.6	29
8764	Theoretical investigation on ratiometric two-photon fluorescent probe for Zn ²⁺ detection based on ICT mechanism. <i>Journal of Molecular Structure</i> , 2016, 1114, 65-77.	1.8	7

#	ARTICLE	IF	CITATIONS
8765	Effects of boryl, phosphino, and phosphonio substituents on optical, electrochemical, and photophysical properties of 2,5-dithienylphospholes and 2-phenyl-5-thienylphospholes. Dalton Transactions, 2016, 45, 2190-2200.	1.6	15
8766	Intramolecular charge transfer in aminobenzonitriles and tetrafluoro counterparts: fluorescence explained by competition between low lying excited states and radiationless deactivation. Part II: influence of substitution on luminescence patterns. Physical Chemistry Chemical Physics, 2016, 18, 6875-6884.	1.3	9
8767	Photodissociation dynamics of propyne at 193 nm: a trajectory surface hopping study. Physical Chemistry Chemical Physics, 2016, 18, 8219-8227.	1.3	5
8768	Mechanisms and reactivity differences for the cobalt-catalyzed enantioselective intramolecular hydroacylation of ketones and alkenes: insights from density functional calculations. Journal of Molecular Modeling, 2016, 22, 60.	0.8	6
8769	Molecular Application of a State Specific Multi-Reference Brillouin-Wigner Perturbation Theory. Chinese Physics Letters, 2016, 33, 023102.	1.3	0
8770	Photophysics of the LOV-Based Fluorescent Protein Variant iLOV-Q489K Determined by Simulation and Experiment. Journal of Physical Chemistry B, 2016, 120, 3344-3352.	1.2	41
8771	How the change of the ligand from L = porphine, P 2 ⁺ , to L = P 4 -substituted porphine, P(P) 4 2 ⁺ , affects the electronic properties and the M ⁺ L binding energies for the first-row transition metals M = Sc ⁺ Zn: Comparative study. Chemical Physics, 2016, 469-470, 38-48.	0.9	8
8772	OH-substituted tridentate ONO Schiff base ligands and related molybdenum(VI) complexes for solvent-free (ep)oxidation catalysis with TBHP as oxidant. Journal of Molecular Catalysis A, 2016, 416, 117-126.	4.8	24
8773	Bis(imino)phosphanes: Synthesis and Coordination Chemistry. Organometallics, 2016, 35, 827-835.	1.1	12
8774	Superlithiation of Organic Electrode Materials: The Case of Dilithium Benzenedipropionate. Chemistry of Materials, 2016, 28, 1920-1926.	3.2	109
8775	Density functional theory prediction of cobalt pincer complexes for catalytic dehydrogenation of ethanol. Journal of Coordination Chemistry, 2016, 69, 1380-1387.	0.8	6
8776	Computational design of zinc-ion-responsive two-photon fluorescent probes with conjugated multi-structures. Journal of Molecular Modeling, 2016, 22, 34.	0.8	2
8777	Broadband terahertz dynamics of propylene glycol monomer and oligomers. Journal of Molecular Structure, 2016, 1126, 127-131.	1.8	3
8778	Computational Study of Fluorinated Diglyoxime-Iron Complexes: Tuning the Electrocatalytic Pathways for Hydrogen Evolution. Inorganic Chemistry, 2016, 55, 2934-2940.	1.9	16
8779	Mechanistic Study of the Direct Intramolecular Allylic Amination Reaction Catalyzed by Palladium(II). ACS Catalysis, 2016, 6, 1772-1784.	5.5	21
8780	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. Physical Chemistry Chemical Physics, 2016, 18, 8701-8709.	1.3	7
8781	Investigation of Electrolyte Concentration Effects on the Performance of Lithium-Oxygen Batteries. Journal of Physical Chemistry C, 2016, 120, 5949-5957.	1.5	22
8782	Probing the reactivity of pentaphenylborole with N-H, O-H, P-H, and S-H bonds. Dalton Transactions, 2016, 45, 9902-9911.	1.6	28

#	ARTICLE	IF	CITATIONS
8783	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. <i>Chemical Society Reviews</i> , 2016, 45, 2516-2543.	18.7	44
8784	Structure and bonding of group 4-nickel heterobimetallics supported by 2-(diphenylphosphino)pyrrolide ligands. <i>Dalton Transactions</i> , 2016, 45, 9892-9901.	1.6	24
8785	Synthesis and characterization of a series of Group 4 phenoxy-thiol derivatives. <i>Polyhedron</i> , 2016, 110, 1-13.	1.0	5
8786	Accelerating <i>Ab Initio</i> Path Integral Simulations via Imaginary Multiple-Timestepping. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1627-1638.	2.3	12
8787	Understanding the mechanism of CO ₂ capture by 1,3 di-substituted imidazolium acetate based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1911-1917.	1.3	37
8788	On the impact of isomer structure and packing disorder in thienoacene organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 4040-4048.	2.7	28
8789	TOWARD THE ASTRONOMICAL DETECTION OF THE PROTON-BOUND COMPLEX NN ⁺ HCO ⁺ : IMPLICATIONS FOR THE SPECTRA OF PROTOPLANETARY DISKS. <i>Astrophysical Journal</i> , 2016, 819, 141.	1.6	14
8790	Theoretical study of microhydrated cyclo(L-pro)4-alkali cation complexes. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 37-46.	1.1	1
8791	Estimation of charge carrier mobility in amorphous organic materials using percolation corrected random-walk model. <i>Organic Electronics</i> , 2016, 29, 50-56.	1.4	42
8792	Experimental and simulation study on structural characterization and hydrogen storage of metal organic structured compounds. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 8256-8263.	3.8	13
8793	Mechanism, chemoselectivity and enantioselectivity for the rhodium-catalyzed desymmetric synthesis of hydrobenzofurans: a theoretical study. <i>Organic Chemistry Frontiers</i> , 2016, 3, 209-216.	2.3	21
8794	Mapping the configuration dependence of electronic coupling in organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3825-3832.	2.7	13
8795	Experimental evidence for the influence of charge on the adsorption capacity of carbon dioxide on charged fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3048-3055.	1.3	19
8796	Efficient Bimolecular Mechanism of Photochemical Hydrogen Production Using Halogenated Boron-Dipyromethene (Bodipy) Dyes and a Bis(dimethylglyoxime) Cobalt(III) Complex. <i>Journal of Physical Chemistry B</i> , 2016, 120, 527-534.	1.2	49
8797	Experimental and computational evaluation of the barrier to torsional rotation in a butadiyne-linked porphyrin dimer. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5264-5274.	1.3	57
8798	Coumarin-based donor-acceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	23
8799	Accessing long lived 1H states via 2H couplings. <i>Journal of Magnetic Resonance</i> , 2016, 263, 108-115.	1.2	8
8800	Similar but Different: The Case of Metoprolol Tartrate and Succinate Salts. <i>Crystal Growth and Design</i> , 2016, 16, 789-799.	1.4	21

#	ARTICLE	IF	CITATIONS
8801	13C Chemical Shift in Natural Gas Hydrates from First-Principles Solid-State NMR Calculations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1130-1136.	1.5	6
8802	Benchmarking semiempirical, Hartree-Fock, DFT, and MP2 methods against the ionization energies and electron affinities of short- through long-chain [n]acenes and [n]phenacenes. <i>Canadian Journal of Chemistry</i> , 2016, 94, 251-258.	0.6	8
8803	Analysis of coordination states for Dy(II) and Dy(III) complexes in ionic liquids by Raman spectroscopy and DFT calculation. <i>Journal of Molecular Liquids</i> , 2016, 215, 308-315.	2.3	10
8804	Internal Conversion and Vibrational Energy Redistribution in Chlorophyll A. <i>Journal of Physical Chemistry B</i> , 2016, 120, 49-58.	1.2	30
8805	Theoretical study of the mechanism of the N-heterocyclic carbene-catalyzed cyclotetramerization of acrylates. <i>Journal of Molecular Modeling</i> , 2016, 22, 16.	0.8	2
8806	Oxidative Dimerization of Triarylaminines Promoted by WCl ₆ , Including the Solid State Isolation and the Crystallographic Characterization of a Triphenylammonium Salt. <i>Inorganic Chemistry</i> , 2016, 55, 887-893.	1.9	15
8807	Calculation on frequency and temperature properties of birefringence of nematic liquid crystal 5CB in terahertz band. <i>Chemical Physics Letters</i> , 2016, 645, 205-209.	1.2	17
8808	Temperature-induced release of crystal water in the Co, Mo and Pt complexes of N,N-diacetatedithiocarbamate. FTIR spectroscopy and quantum chemical study. <i>Journal of Molecular Structure</i> , 2016, 1103, 245-253.	1.8	4
8809	Theoretical study of the catalytic oxidation mechanism of 5-hydroxymethylfurfural to 2,5-diformylfuran by PMo-containing Keggin heteropolyacid. <i>Catalysis Science and Technology</i> , 2016, 6, 3776-3787.	2.1	29
8810	Molecular and electronic structure of 1,3,2-diazaphosphinine derivatives. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 399-404.	0.8	2
8811	Copper(II) complexes of pyridine-oxazoline (Pyox) ligands: Coordination chemistry, ligand stability, and catalysis. <i>Inorganica Chimica Acta</i> , 2016, 441, 86-94.	1.2	26
8812	Buckminster fullerene adhesion on graphene flakes: Numerical accuracy of dispersion corrected DFT. <i>Polyhedron</i> , 2016, 114, 110-117.	1.0	8
8813	Computational assessment of the fluorescence emission of phenol oligomers: A possible insight into the fluorescence properties of humic-like substances (HULIS). <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 315, 87-93.	2.0	41
8814	A radical rebound mechanism for the methane oxidation reaction promoted by the dicopper center of a pMMO enzyme: a computational perspective. <i>Dalton Transactions</i> , 2016, 45, 2492-2504.	1.6	40
8815	Analysis of creatine phosphate disodium salt by ESI-MS/MS: A seven-centered rearrangement mechanism in gas phase. <i>International Journal of Mass Spectrometry</i> , 2016, 394, 42-45.	0.7	1
8816	Accessing Realistic Models for the WO ₃ -SiO ₂ Industrial Catalyst through the Design of Organometallic Precursors. <i>ACS Catalysis</i> , 2016, 6, 1-18.	5.5	54
8817	Reversible hydrogen activation by a bulky haloborane based FLP system. <i>Dalton Transactions</i> , 2016, 45, 6129-6135.	1.6	10
8818	About the electronic and photophysical properties of iridium(III)-pyrazino[2,3-f][1,10]-phenanthroline based complexes for use in electroluminescent devices. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 726-734.	1.3	20

#	ARTICLE	IF	CITATIONS
8819	Comparison of Relative Activation Energies Obtained by Density Functional Theory and the Random Phase Approximation for Several Claisen Rearrangements. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1486-1496.	1.2	10
8820	How carbo-benzenes fit molecules in their inner core as do biologic ion carriers?. <i>Structural Chemistry</i> , 2016, 27, 249-259.	1.0	6
8821	Models of the Ni-L and Ni-SI_a States of the [NiFe]-Hydrogenase Active Site. <i>Inorganic Chemistry</i> , 2016, 55, 419-431.	1.9	56
8822	Surface modification of porous alumina filters for CO2 separation using silane coupling agents. <i>Journal of Membrane Science</i> , 2016, 497, 216-220.	4.1	12
8823	Probing the stability of the M2(Benzene)3 M=Fe, Co, and Ni structures upon electron attachment (deletion) and solvated iron clusters by benzene molecules: Fe2(Benzene)4. <i>Journal of Molecular Structure</i> , 2016, 1103, 295-310.	1.8	5
8824	Solvation of coumarin6 studied by vibrational spectroscopy and density functional theory. <i>Journal of Molecular Structure</i> , 2016, 1106, 170-180.	1.8	2
8825	New heteroscorpionate lanthanide complexes for ring-opening polymerisation of ϵ -caprolactone and rac-lactide. <i>Chemical Papers</i> , 2016, 70, .	1.0	4
8826	A computational study on Ru complexes with bidentate carboxylate ligands: Insights into the photocurrents of dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 314, 171-177.	2.0	5
8827	Investigation of substitution effect on fluorescence properties of Zn2+-selective ratiometric fluorescent compounds: 2-(2-Hydroxyphenyl)benzimidazole derivatives. <i>Talanta</i> , 2016, 146, 575-584.	2.9	22
8828	Structural and optical properties of the M@C59X cages (X=N, B and M=Li, Na). <i>Pramana - Journal of Physics</i> , 2016, 86, 109-116.	0.9	0
8829	Theoretical characterization of first and second generation Grubbs catalysts in styrene cross-metathesis reactions: insights from conceptual DFT. <i>Catalysis Science and Technology</i> , 2016, 6, 755-766.	2.1	16
8830	Molecular structure and vibrational spectroscopic studies of prothionamide by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 152, 262-271.	2.0	4
8831	Elucidating the mechanism responsible for anomalous thermal expansion in a metal-organic framework. <i>Dalton Transactions</i> , 2016, 45, 4141-4149.	1.6	5
8832	Durability improvements of H-ZSM-5 zeolite for ethanol conversion after treatment with chelating agents. <i>Microporous and Mesoporous Materials</i> , 2016, 219, 66-76.	2.2	10
8833	Synthesis, crystal structure, spectral characterization, and theoretical study of glycolato peroxido complexes of vanadium(V). <i>Structural Chemistry</i> , 2016, 27, 605-615.	1.0	5
8834	Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. <i>Molecular Physics</i> , 2017, 115, 39-47.	0.8	12
8835	Functional-Group-Tolerant, Silver-Catalyzed N=C Bond Formation by Nitrene Transfer to Amines. <i>Journal of the American Chemical Society</i> , 2017, 139, 2216-2223.	6.6	62
8836	Kinetics and mechanism of interaction of Pt(II) complex with bio-active ligands and <i>in vitro</i> Pt(II)-sulfur adduct formation in aqueous medium: bio-activity and computational study. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1032-1052.	0.8	1

#	ARTICLE	IF	CITATIONS
8837	Anti-proliferative effects of copper(II) complexes with hydroxyquinoline-thiosemicarbazone ligands. <i>European Journal of Medicinal Chemistry</i> , 2017, 128, 140-153.	2.6	58
8838	Ruthenium complexes bearing a tridentate polypyridyl ligand with non-coordinating donor atoms: Construction of a specific coordination environment involving noncovalent interactions. <i>Journal of Organometallic Chemistry</i> , 2017, 830, 167-174.	0.8	3
8839	Oxygen Atom Transfer Using an Iron(IV)â€Oxo Embedded in a Tetracyclic Nâ€Heterocyclic Carbene System: How Does the Reactivity Compare to Cytochrome P450 Compoundâ€...?. <i>Chemistry - A European Journal</i> , 2017, 23, 2935-2944.	1.7	36
8840	Synthesis and structural characterization of mixed halideâ€N,N-diethylcarbamates of group 4 metals, including a case of unusual tetrahydrofuran activation. <i>New Journal of Chemistry</i> , 2017, 41, 1781-1789.	1.4	14
8841	Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 298-310.	2.5	12
8842	Tuning for Visible Fluorescence and Near-Infrared Phosphorescence on a Unimolecular Mechanically Sensitive Platform via Adjustable CHâ€Iâ€ Interaction. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 3865-3872.	4.0	56
8843	Potential Functional Embedding Theory at the Correlated Wave Function Level. 1. Mixed Basis Set Embedding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1067-1080.	2.3	19
8844	Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1328-1335.	1.1	9
8845	Calculations of One- and Two-Photon Absorption Spectra for Molecular Metal Chalcogenide Clusters with Electron-Acceptor Ligands. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1748-1759.	1.1	5
8846	Formation of Dinuclear Iridium Complexes by NHC-Supported Câ€H Bond Activation. <i>Organometallics</i> , 2017, 36, 699-707.	1.1	15
8847	Computation provides chemical insight into the diverse hydride NMR chemical shifts of [Ru(NHC) ₄ (L)H] ^{0/+} species (NHC = N-heterocyclic carbene; L = vacant,) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50</i>	1.6	22
8848	[Ru(R) ₂ PCH ₂ CH ₂ PR ₂] ₂ (L)H ⁺ congeners. <i>Dalton Transactions</i> , 2017, 46, 2861-2873.		
8848	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. <i>Chemical Reviews</i> , 2017, 117, 6696-6754.	23.0	181
8849	Adamantylidene Addition to M ₃ N@Ihâ€80 (M=Sc, Lu) and Sc ₃ N@D ₅ hâ€80: Synthesis and Crystallographic Characterization of the [5,6]â€Open and [6,6]â€Open Adducts. <i>Chemistry - A European Journal</i> , 2017, 23, 6552-6561.	1.7	18
8850	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2017, , 795-860.		6
8851	Benzimidazolylquinoxalines: novel fluorophores with tuneable sensitivity to solvent effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6095-6104.	1.3	11
8852	An averaged polarizable potential for multiscale modeling in phospholipid membranes. <i>Journal of Computational Chemistry</i> , 2017, 38, 601-611.	1.5	12
8853	Mechanisms of the transfer hydroformylation catalyzed by rhodium, cobalt, and iridium complexes: Insights from density functional theory study. <i>Journal of Organometallic Chemistry</i> , 2017, 833, 71-79.	0.8	8
8854	Triphenylamine-Based Fluorescent Styryl Dyes: DFT, TD-DFT and Non-Linear Optical Property Study. <i>Journal of Fluorescence</i> , 2017, 27, 993-1007.	1.3	21

#	ARTICLE	IF	CITATIONS
8855	On the work function and the charging of small (5 nm) nanoparticles in plasmas. <i>Physics of Plasmas</i> , 2017, 24, .	0.7	11
8856	Ligand Design for Isomer-Selective Oxorhenium(V) Complex Synthesis. <i>Inorganic Chemistry</i> , 2017, 56, 1757-1769.	1.9	12
8857	The Nature of the Chemical Bond from a Quantum Mechanical Interference Perspective. <i>ChemistrySelect</i> , 2017, 2, 604-619.	0.7	20
8858	Highly specific noninvasive photoacoustic and positron emission tomography of brain plaque with functionalized croconium dye labeled by a radiotracer. <i>Chemical Science</i> , 2017, 8, 2710-2716.	3.7	62
8859	In vitro kinetic based adduct formation mechanism of a cytotoxic Pt(II) complex with sulfur containing bio-relevant molecules and a theoretical approach. <i>Polyhedron</i> , 2017, 124, 251-261.	1.0	12
8860	Thiolate-palladium(IV) or sulfonium-palladate(0)? A theoretical study on the mechanism of palladium-catalyzed C-S bond formation reactions. <i>Organic Chemistry Frontiers</i> , 2017, 4, 943-950.	2.3	13
8861	A DFT study of the electronic and magnetic properties of C ₃₆ Si ₂₄ fullerenes. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 1-10.	1.1	12
8862	Impedimetric Enzyme-Free Detection of Glucose via a Computationally-Designed Molecularly Imprinted Electrochemical Sensor Fabricated on Porous Ni Foam. <i>Electroanalysis</i> , 2017, 29, 1243-1251.	1.5	9
8863	Mechanisms for nickel(0)/N-heterocyclic carbene-catalyzed intramolecular alkene hydroacylation: insights from a DFT study. <i>Journal of Molecular Modeling</i> , 2017, 23, 11.	0.8	6
8864	Artificial nodes in the H ₂ + wave functions expanded using Gaussian-type orbitals or Laguerre-type orbitals. <i>Computational and Theoretical Chemistry</i> , 2017, 1103, 17-24.	1.1	2
8865	Protonation Sites of Aromatic Compounds in (+) Atmospheric Pressure Photoionization. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 166-176.	1.0	2
8866	Tunable Approach for the Stereoselective Synthesis of 1-C-Diethylphosphono(difluoromethyl) Iminosugars as Glycosyl Phosphate Mimics. <i>Journal of Organic Chemistry</i> , 2017, 82, 2753-2763.	1.7	26
8867	Reaction Mechanism of Covalent Modification of Phosphatidylethanolamine Lipids by Reactive Aldehydes 4-Hydroxy-2-nonenal and 4-Oxo-2-nonenal. <i>Chemical Research in Toxicology</i> , 2017, 30, 840-850.	1.7	19
8868	Synthesis of Quinoidal Fused Oligosiloles by Rhodium-Catalyzed Stitching Reaction and Theoretical Investigation of Their Properties. <i>Journal of the American Chemical Society</i> , 2017, 139, 3861-3867.	6.6	23
8869	Theoretical study on the bridge comparison of TiO ₂ nanoparticle sensitizers based on phenoxazine in dye-sensitized solar cells. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	9
8870	Catalytic Enantioselective [2,3]-Rearrangements of Allylic Ammonium Ylides: A Mechanistic and Computational Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 4366-4375.	6.6	92
8871	Mesomorphic and DFT studies of terminal ester containing salicylaldehydes and their copper (II) complexes. <i>Molecular Crystals and Liquid Crystals</i> , 2017, 643, 116-128.	0.4	4
8872	An Efficient Synthetic Approach to <i>cis</i> -trans-(NHC) ₂ Pd(R)Br Type Complexes and Their Use in Suzuki-Miyaura Cross-Coupling Reactions. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2144-2154.	1.0	10

#	ARTICLE	IF	CITATIONS
8873	Computational investigation of fullerene-DNA interactions: Implications of fullerene's size and functionalization on DNA structure and binding energetics. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 177-192.	1.3	6
8874	Theoretical insights into the ultrafast excited-state intramolecular proton transfer (ESIPT) mechanism in a series of amide-based N-H...N hydrogen-bonding compounds. <i>Organic Electronics</i> , 2017, 45, 1-8.	1.4	42
8875	Glyphosate binding in soil as revealed by sorption experiments and quantum-chemical modeling. <i>Science of the Total Environment</i> , 2017, 586, 527-535.	3.9	59
8876	Sulfur Groups Improve the Performance of Triazole- and Triazolium-Based Interaction Units in Anion Binding. <i>Journal of Organic Chemistry</i> , 2017, 82, 3341-3346.	1.7	5
8877	Theoretical prediction on the synthesis of 2,3-dihydropyridines through Co(III)-catalysed reaction of unsaturated oximes with alkenes. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25353.	1.0	1
8878	Vibrational frequencies and spectroscopic constants of three, stable noble gas molecules: NeCCH ⁺ , ArCCH ⁺ , and ArCN ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5230-5238.	1.3	16
8879	Quantum-chemistry descriptors for photosensitizers based on macrocycles. <i>Chemical Biology and Drug Design</i> , 2017, 89, 207-220.	1.5	10
8880	Molecule Channels Directed by Cation-Decorated Graphene Oxide Nanosheets and Their Application as Membrane Reactors. <i>Advanced Materials</i> , 2017, 29, 1606093.	11.1	83
8881	Synthesis and Reduction of Uranium(V) Imido Complexes with Redox-Active Substituents. <i>Chemistry - A European Journal</i> , 2017, 23, 5748-5757.	1.7	15
8882	Iminophosphanes: Synthesis, Rhodium Complexes, and Ruthenium(II)-Catalyzed Hydration of Nitriles. <i>Organometallics</i> , 2017, 36, 1079-1090.	1.1	25
8883	Synthesis of Quaternary Ammonium Salts Based on Diketopyrrolopyrroles Skeletons and Their Applications in Copper Electroplating. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 7793-7803.	4.0	44
8884	Mechanism of Dimethylamine-Borane Dehydrogenation Catalyzed by an Iridium(III) PCP-Pincer Complex. <i>ACS Catalysis</i> , 2017, 7, 2325-2333.	5.5	30
8885	Development of Ion-Conductive and Vapoluminescent Porous Coordination Polymers Composed of Ruthenium(II) Metalloligand. <i>Inorganic Chemistry</i> , 2017, 56, 3005-3013.	1.9	19
8886	Rearrangement of vinyl allene oxide geometric isomers to cyclopentenones. Further computational insights with biologically relevant model systems. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 2846-2855.	1.5	12
8887	Computational insights into the mechanisms of Au(I)-catalysed intramolecular addition of the hydroxylamine group onto alkynes. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1130-1136.	2.3	15
8888	QM/MM (ABEEM) Study on the Ligand Substitution Processes of Ruthenium(III) Complex NAMI. <i>Chinese Journal of Chemistry</i> , 2017, 35, 354-362.	2.6	1
8889	Evidence of Oxygen Activation in the Reaction between an N-Heterocyclic Carbene and M ₃ N@Ih(7)-C ₈₀ : An Unexpected Method of Steric Hindrance Release. <i>Journal of Organic Chemistry</i> , 2017, 82, 3500-3505.	1.7	18
8890	Reactivity Patterns of (Protonated) Compound II and Compound I of Cytochrome P450: Which is the Better Oxidant?. <i>Chemistry - A European Journal</i> , 2017, 23, 6406-6418.	1.7	71

#	ARTICLE	IF	CITATIONS
8891	Highly Sensitive and Selective Uranium Detection in Natural Water Systems Using a Luminescent Mesoporous Metal-Organic Framework Equipped with Abundant Lewis Basic Sites: A Combined Batch, X-ray Absorption Spectroscopy, and First Principles Simulation Investigation. <i>Environmental Science & Technology</i> , 2017, 51, 3911-3921.	4.6	331
8892	Computational Study of the Malonic Acid Tautomerization Products in Highly Concentrated Particles. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2259-2264.	1.1	7
8893	Chemiluminogenic acridinium salts: A comparison study. Detection of intermediate entities appearing upon light generation. <i>Journal of Luminescence</i> , 2017, 187, 102-112.	1.5	14
8894	Computational and Experimental Evidence of Emergent Equilibrium Isotope Effects in Anion Receptor Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 3962-3965.	6.6	13
8895	Adsorption and molecular siting of CO ₂ , water, and other gases in the superhydrophobic, flexible pores of FMOF-1 from experiment and simulation. <i>Chemical Science</i> , 2017, 8, 3989-4000.	3.7	60
8896	Isotope exchange reaction in tritium-contaminated vacuum pump oil: mechanism and HTO effect. <i>RSC Advances</i> , 2017, 7, 890-896.	1.7	3
8897	Reactivity of 5-carboxycytosine toward addition and hydrogen abstraction by $\dot{\text{A}}\text{-OH}$ in acetonitrile: a computational study. <i>Molecular Simulation</i> , 2017, 43, 563-567.	0.9	0
8898	Significant electron transfer in heme catalysis: The case of chlorite dismutase. <i>Journal of Catalysis</i> , 2017, 348, 40-46.	3.1	11
8899	Combined powder X-ray diffraction data and quantum-chemical calculations in EXPO2014. <i>Powder Diffraction</i> , 2017, 32, S123-S128.	0.4	7
8900	Synthesis and Structure of 2,5-Bis[<i>N</i> -(2,6-mesityl)iminomethyl]pyrrolylcobalt(II): Evidence for One-Electron-Oxidized, Redox Noninnocent Ligand Behavior. <i>Inorganic Chemistry</i> , 2017, 56, 3377-3385.	1.9	12
8901	Switching of Förster to Dexter Mechanism of Short-Range Energy Transfer in <i>meso</i> -Anthrylporphyrin. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5941-5948.	1.5	22
8902	Quantifying Possible Routes for SpnF-Catalyzed Formal Diels-Alder Cycloaddition. <i>Journal of the American Chemical Society</i> , 2017, 139, 3942-3945.	6.6	39
8903	Synthesis and characterization of a series of nickel(II) alkoxide precursors and their utility for Ni(0) nanoparticle production. <i>Dalton Transactions</i> , 2017, 46, 5806-5815.	1.6	2
8904	Impact of the number of <i>o</i> -carboranyl ligands on the photophysical and electroluminescent properties of iridium(III) cyclometalates. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3024-3034.	2.7	17
8905	Synthesis of three crystalline forms of Al ₂ O ₃ featuring rod-like fibers and their effect on the gaseous degradation of 1-chloronaphthalene. <i>Environmental Science: Nano</i> , 2017, 4, 994-1004.	2.2	9
8906	Utilizing super-atom orbital ideas to understand properties of silver clusters inside ZSM-5 zeolite. <i>RSC Advances</i> , 2017, 7, 4950-4959.	1.7	21
8907	Computational Study of Oxidation of Guanine by Singlet Oxygen (¹ O _g) and Formation of Guanine:Lysine Cross-Links. <i>Chemistry - A European Journal</i> , 2017, 23, 5804-5813.	1.7	34
8908	Characterizing magnesium bonds: main features of a non-covalent interaction. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	21

#	ARTICLE	IF	CITATIONS
8909	Kinetic and mechanistic study of substitution on a cytotoxic Pt II complex with biologically relevant thiols and a density functional study. <i>Polyhedron</i> , 2017, 128, 46-56.	1.0	5
8910	Theoretical prediction of the synthesis of 2,3-dihydropyridines through Ir(III)-catalysed reaction of unsaturated oximes with alkenes. <i>RSC Advances</i> , 2017, 7, 5649-5659.	1.7	0
8911	Molecular aggregation of naphthalimide organic semiconductors assisted by amphiphilic and lipophilic interactions: a joint theoretical and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6206-6215.	1.3	9
8912	On the Detectability of the HSS, HSO, and HOS Radicals in the Interstellar Medium. <i>Astrophysical Journal</i> , 2017, 835, 243.	1.6	36
8913	The reactions of α -amino acids and α -amino acid esters with high valent transition metal halides: synthesis of coordination complexes, activation processes and stabilization of α -ammonium acylchloride cations. <i>RSC Advances</i> , 2017, 7, 10158-10174.	1.7	13
8914	Quantitative Structure-Activity Relationships for the Nucleophilicity of Trivalent Boron Compounds. <i>Chemistry - A European Journal</i> , 2017, 23, 5066-5075.	1.7	15
8915	Thermodynamics and Photodynamics of a Monoprotonated Porphyrin Directly Stabilized by Hydrogen Bonding with Polar Protic Solvents. <i>Chemistry - A European Journal</i> , 2017, 23, 4669-4679.	1.7	13
8916	Density functional theory study of interactions between carbon monoxide and iron tetraaza macrocyclic complexes, FeTAA (X = Cl, OH, OCH ₃ , NH ₂ , and NO ₂). <i>Journal of Molecular Modeling</i> , 2017, 23, 64.	0.8	1
8917	Strong correlation in surface chemistry. <i>Molecular Simulation</i> , 2017, 43, 394-405.	0.9	4
8918	Iridium and Ruthenium Complexes of <i>N</i> -Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal. <i>Organometallics</i> , 2017, 36, 1091-1106.	1.1	94
8919	Theoretical Study on Ruthenium-Catalyzed Hydrocarbamoylative Cyclization of 1,6-Diyne with Dimethylformamide. <i>Organometallics</i> , 2017, 36, 1154-1163.	1.1	6
8920	Redox Control of Aluminum Ring-Opening Polymerization: A Combined Experimental and DFT Investigation. <i>Macromolecules</i> , 2017, 50, 1847-1861.	2.2	56
8921	The reactivity of the 5-formylcytosine with hydroxyl radical: A theoretical perspective. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3691.	0.9	3
8922	Molecular and Electronic Structures of Ruthenium Complexes Containing an ONS-Coordinated Open-Shell π Radical and an Oxidative Aromatic Ring Cleavage Reaction. <i>Inorganic Chemistry</i> , 2017, 56, 3363-3376.	1.9	19
8923	Molecular inclusion process of urease inhibitors into cyclodextrins: A theoretical study. <i>Chemical Physics Letters</i> , 2017, 675, 69-74.	1.2	4
8924	Wavelength-Dependent Photochemistry of Oxime Ester Photoinitiators. <i>Macromolecules</i> , 2017, 50, 1815-1823.	2.2	140
8925	The effect of ring size on the selective carboxylation of cycloalkene oxides. <i>Catalysis Science and Technology</i> , 2017, 7, 1433-1439.	2.1	2
8926	Computational study of one-step polar Diels-Alder reactions using the NEB method for the minimum energy paths search. <i>Molecular Simulation</i> , 2017, 43, 644-655.	0.9	3

#	ARTICLE	IF	CITATIONS
8927	Effect of a σ -Bonded-M-1,2,3-triazole (M = Co, Ru) on the Structure and Reactivity of Group 6 Alkoxy (Fischer) Carbenes. <i>Inorganic Chemistry</i> , 2017, 56, 2801-2811.	1.9	5
8928	Mapping Interaction Energies in Chorismate Mutase with the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1797-1807.	1.1	9
8929	DFT mechanistic study of the selective terminal C-H activation of n-pentane with a tungsten allyl nitrosyl complex. <i>Journal of Saudi Chemical Society</i> , 2017, 21, 558-562.	2.4	3
8930	Bambusuril as a One-Electron Donor for Photoinduced Electron Transfer to Methyl Viologen in Mixed Crystals. <i>Journal of the American Chemical Society</i> , 2017, 139, 2597-2603.	6.6	51
8931	Oxo- and hydroxo-bridged diiron(III) porphyrin dimers: Inorganic and bio-inorganic perspectives and effects of intermacrocylic interactions. <i>Coordination Chemistry Reviews</i> , 2017, 337, 112-144.	9.5	52
8932	Influence of Coupling and Embedding Schemes on QM Size Convergence in QM/MM Approaches for the Example of a Proton Transfer in DNA. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1102-1107.	2.3	71
8933	Unusual (+/-) electro spray ionization induced fragmentation: Structural elucidation of an in-process synthetic intermediate of doravirine (MK-439) using liquid chromatography/high-resolution tandem mass spectrometry and two-dimensional nuclear magnetic resonance. <i>Rapid Communications in Mass Spectrometry</i> , 2017, 31, 719-727.	0.7	1
8934	IRMPD Spectroscopy Sheds New (Infrared) Light on the Sulfate Pattern of Carbohydrates. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2114-2120.	1.1	49
8935	Aggregation-controlled photochromism based on a dithienylethene derivative with aggregation-induced emission. <i>Journal of Materials Chemistry C</i> , 2017, 5, 2717-2722.	2.7	42
8936	Conformational analysis of N^+BH_3 , N^+BF_3 , and $N-CH_3$ complexes with ibuprofen-derivative amides. <i>Heteroatom Chemistry</i> , 2017, 28, e21368.	0.4	1
8937	Mechanism of Organophosphonate Catabolism by Diiron Oxygenase PhnZ: A Third Iron-Mediated O ₂ Activation Scenario in Nature. <i>ACS Catalysis</i> , 2017, 7, 3521-3531.	5.5	27
8938	Salicylaldehyde Hydrazones: Buttressing of Outer-Sphere Hydrogen-Bonding and Copper Extraction Properties. <i>Australian Journal of Chemistry</i> , 2017, 70, 556.	0.5	5
8939	Understanding the Crystal Packing and Organic Thin-Film Transistor Performance in Isomeric Guest-Host Systems. <i>Advanced Materials</i> , 2017, 29, 1700048.	11.1	24
8940	Theoretical Elucidation of Potential Enantioselectivity in a Pd-Catalyzed Aromatic C-H Coupling Reaction. <i>Journal of Organic Chemistry</i> , 2017, 82, 4900-4906.	1.7	13
8941	Reactivity studies on $[Cp^*Fe(\eta^4-L)]_2$: nitrido-, sulfido- and diselenide iron complexes derived from pseudohalide activation. <i>Chemical Science</i> , 2017, 8, 4108-4122.	3.7	25
8942	Development of a ^{13}C NMR Chemical Shift Prediction Procedure Using B3LYP/cc-pVDZ and Empirically Derived Systematic Error Correction Terms: A Computational Small Molecule Structure Elucidation Method. <i>Journal of Organic Chemistry</i> , 2017, 82, 5135-5145.	1.7	58
8943	Potassium <i>tert</i> -Butoxide-Catalyzed Dehydrogenative C-H Silylation of Heteroaromatics: A Combined Experimental and Computational Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2017, 139, 6867-6879.	6.6	160
8944	Hydrogenation of Carbon Dioxide to Methanol Catalyzed by Iron, Cobalt, and Manganese Cyclopentadienone Complexes: Mechanistic Insights and Computational Design. <i>Chemistry - A European Journal</i> , 2017, 23, 8850-8856.	1.7	28

#	ARTICLE	IF	CITATIONS
8945	A comparative study on seniority-based MO and VB calculations of the singlet and triplet energy gaps of open-shell molecules. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 86-91.	1.1	5
8946	Correcting density-driven errors in projection-based embedding. <i>Journal of Chemical Physics</i> , 2017, 146, 084113.	1.2	14
8947	In silico studies of the magnetic octahedral B ₆ cluster nitric oxide and [B ₆ NO] ⁺ O ₂ interactions. <i>Structural Chemistry</i> , 2017, 28, 1757-1764.	1.0	15
8948	Photodebromination behaviors of polybrominated diphenyl ethers in methanol/water systems: Mechanisms and predicting descriptors. <i>Science of the Total Environment</i> , 2017, 595, 666-672.	3.9	17
8949	Ring Opening of Epoxides Induced by Pentaphenylborole. <i>Organometallics</i> , 2017, 36, 2581-2587.	1.1	19
8950	Preparation of Phosphorescent Osmium(IV) Complexes with N,N'-C- and C,N'-Pincer Ligands. <i>Organometallics</i> , 2017, 36, 1848-1859.	1.1	34
8951	Quantification of Lewis acid induced Brønsted acidity of protogenic Lewis bases. <i>Dalton Transactions</i> , 2017, 46, 5976-5985.	1.6	27
8952	On the decay of the triplet state of thionucleobases. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12674-12682.	1.3	38
8953	ZnO nested shell magic clusters as tetrapod nuclei. <i>RSC Advances</i> , 2017, 7, 21933-21942.	1.7	16
8954	Molecular design of porphyrin dyes for dye sensitized solar cells: A quantitative structure property relationship study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25385.	1.0	9
8955	Twisting of Alkynes towards a Carbon Double Helix. <i>Chemistry - A European Journal</i> , 2017, 23, 12190-12197.	1.7	6
8956	A quantum-chemical insight into the tunable fluorescence color and distinct photoisomerization mechanisms between a novel ESIPT fluorophore and its protonated form. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 183, 123-130.	2.0	21
8957	Hydrolysis mechanism of (N, N) chelated cytotoxic Pt/Pd(II)-dichloro complexes: A theoretical approach. <i>Chemical Physics Letters</i> , 2017, 678, 241-249.	1.2	5
8958	Development of an excited-state calculation method for large systems using dynamical polarizability: A divide-and-conquer approach at the time-dependent density functional level. <i>Journal of Chemical Physics</i> , 2017, 146, 124123.	1.2	25
8959	Mechanism for ruthenium hydride-catalyzed regioselective hydroacylation of enones and aldehydes to give 1,3-diketones: Insights from density functional calculations. <i>Molecular Catalysis</i> , 2017, 433, 55-61.	1.0	3
8960	Selective Synthesis and Photophysical Properties of Phosphorescent Heteroleptic Iridium(III) Complexes with Two Different Bidentate Groups and Two Different Monodentate Ligands. <i>Organometallics</i> , 2017, 36, 1743-1755.	1.1	21
8961	Cp*Rh(III)/Bicyclic Olefin Cocatalyzed C-H Bond Amidation by Intramolecular Amide Transfer. <i>Journal of the American Chemical Society</i> , 2017, 139, 6506-6512.	6.6	107
8962	Core-substituted naphthalenediimides anchored on BiVO ₄ for visible light-driven water splitting. <i>Green Chemistry</i> , 2017, 19, 2448-2462.	4.6	11

#	ARTICLE	IF	CITATIONS
8963	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. <i>Journal of Catalysis</i> , 2017, 350, 56-63.	3.1	59
8964	Synthesis, characterization and computational studies of luminescent rhenium(I) tricarbonyl diimine complexes with 8-hydroxyquinoline-containing alkynyl ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 847, 278-288.	0.8	13
8965	Unusual activation pathways of amines in the reactions with molybdenum pentachloride. <i>New Journal of Chemistry</i> , 2017, 41, 4329-4340.	1.4	6
8966	A smart ratiometric red fluorescent chemodosimeter for fluoride based on anthraquinone nosylate. <i>New Journal of Chemistry</i> , 2017, 41, 5098-5104.	1.4	15
8967	Raman intensity and vibrational modes of armchair CNTs. <i>Chemical Physics Letters</i> , 2017, 679, 45-51.	1.2	4
8968	A DFT study of the ring-opening polymerization mechanism of ϵ -lactide and ϵ -caprolactone using aluminium salen-type initiators: Towards an understanding of their reactivities in homo- and copolymerization. <i>Molecular Catalysis</i> , 2017, 436, 145-156.	1.0	24
8969	Switching of Resistive Memory Behavior from Binary to Ternary Logic via Alteration of Substituent Positioning on the Subphthalocyanine Core. <i>Journal of the American Chemical Society</i> , 2017, 139, 7256-7263.	6.6	58
8970	A unified platform for experimental and quantum mechanical study of antibiotic removal from water. <i>Journal of Water Process Engineering</i> , 2017, 17, 207-215.	2.6	18
8971	Structural Investigations on Lithium-Doped Protic and Aprotic Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5279-5292.	1.2	24
8972	Properties of electronically excited states of four squaraine dyes and their complexes with fullerene C 70 : A theoretical investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 184, 82-88.	2.0	4
8973	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. <i>Energy & Fuels</i> , 2017, 31, 6004-6018.	2.5	49
8974	Incipient class II mixed valency in a plutonium solid-state compound. <i>Nature Chemistry</i> , 2017, 9, 856-861.	6.6	28
8975	The open-cubane oxo-oxyl coupling mechanism dominates photosynthetic oxygen evolution: a comprehensive DFT investigation on O-O bond formation in the S4state. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13909-13923.	1.3	31
8976	Synthesis of Structurally Complex Silicon Frameworks through the First Sila-Aldol Reaction. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8089-8093.	7.2	8
8977	Interactions Between Thiocyanate-Free Bis-Tridentate Ru Complexes and Iodide in Dye-Sensitized Solar Cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 344, 134-142.	2.0	1
8978	Azaborininones: Synthesis and Structural Analysis of a Carbonyl-Containing Class of Azaborines. <i>Journal of Organic Chemistry</i> , 2017, 82, 5380-5390.	1.7	18
8979	Reversible multi-electron redox chemistry of π -conjugated N-containing heteroaromatic molecule-based organic cathodes. <i>Nature Energy</i> , 2017, 2, .	19.8	486
8980	Synthesis of Structurally Complex Silicon Frameworks through the First Sila-Aldol Reaction. <i>Angewandte Chemie</i> , 2017, 129, 8201-8205.	1.6	4

#	ARTICLE	IF	CITATIONS
8981	Gold(I)-Catalysed Asymmetric Hydroamination of Alkenes: A Silver- and Solvent-Dependent Enantiodivergent Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 10777-10788.	1.7	31
8982	Interplay Between π -Stacking and Hydrogen Bonding in the Self-Association of Different Isomers of Naphthalenedicarboxylic Acid. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5086-5093.	1.2	6
8983	Nacre-inspired design of graphene oxide-polydopamine nanocomposites for enhanced mechanical properties and multi-functionalities. <i>Nano Futures</i> , 2017, 1, 011003.	1.0	41
8984	Peroxide Activation for Electrophilic Reactivity by the Binuclear Non-heme Iron Enzyme AurF. <i>Journal of the American Chemical Society</i> , 2017, 139, 7062-7070.	6.6	55
8985	Theoretical Studies for Switching Regioselectivity in Ruthenium Hydride-Catalyzed Alkyne Hydroacylation. <i>ChemistrySelect</i> , 2017, 2, 2858-2865.	0.7	1
8986	Ionic and Neutral Mechanisms for C-H Bond Silylation of Aromatic Heterocycles Catalyzed by Potassium <i>tert</i> -Butoxide. <i>Journal of the American Chemical Society</i> , 2017, 139, 6880-6887.	6.6	111
8987	Octahedral iron(II) complexes with pyridyl triazine and bipyridine ligands - synthesis, computational studies, mechanisms and kinetics with 1,10-phenanthroline and 2,2',6,6'-terpyridine. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1893-1909.	0.8	4
8988	Electrostatic Potential Charge including Spatial Electron Density Distribution (SEDD): Application to Biosystems. <i>Bulletin of the Chemical Society of Japan</i> , 2017, 90, 831-837.	2.0	5
8989	Experimental Evidence of Long-Range Intramolecular Vibrational Energy Redistribution through Eight Covalent Bonds: NIR Irradiation Induced Conformational Transformation of <i>E</i> -Glutaconic Acid. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3392-3400.	1.1	9
8990	Experimental and Computational Studies of the Reactions of N and O Atoms with Small Heterocyclic Anions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3655-3661.	1.1	9
8991	The Versatile Behavior of Platinum Alkyne Complexes towards XeF_2 : Formation of Fluorovinyl and Fluorido Complexes. <i>Chemistry - A European Journal</i> , 2017, 23, 8886-8900.	1.7	19
8992	Accurate prediction of emission energies with TD-DFT methods for platinum and iridium OLED materials. <i>Journal of Molecular Modeling</i> , 2017, 23, 174.	0.8	9
8993	A Mechanistic Insight into the Ligand-Controlled Asymmetric Arylation of Aliphatic \pm -Amino Anion Equivalents: Origin of Regio- and Enantioselectivities. <i>Inorganic Chemistry</i> , 2017, 56, 5984-5992.	1.9	6
8994	Low-temperature Synthesis of Heterostructures of Transition Metal Dichalcogenide Alloys ($\text{W}_x\text{Mo}_{1-x}\text{S}_2$) and Graphene with Superior Catalytic Performance for Hydrogen Evolution. <i>ACS Nano</i> , 2017, 11, 5103-5112.	7.3	157
8995	Hydrolysis theory based on density functional studies for cytotoxic Pt(II) and Pd(II) complexes with benzimidazole derivative. <i>Chemical Physics Letters</i> , 2017, 678, 250-258.	1.2	5
8996	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2612-2622.	2.3	13
8997	Coordination of <i>o</i> -benzosemiquinonate, <i>o</i> -iminobenzosemiquinonate and aldimine anion radicals to oxidovanadium(IV). <i>New Journal of Chemistry</i> , 2017, 41, 4564-4572.	1.4	11
8998	Preparation, Structural Determination, and Characterization of Electronic Properties of [5,6]- and [6,6]-Carbosilylated $\text{Sc}_3\text{N@hC}_{80}$. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1391-1399.	1.7	7

#	ARTICLE	IF	CITATIONS
8999	Formic acid catalyzed isomerization of protonated cytosine: a lower barrier reaction for tautomer production of potential biological importance. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13515-13523.	1.3	5
9000	A theoretical study of ascorbic acid oxidation and $\text{HOO}^{\bullet}/\text{O}^{\bullet-}$ radical scavenging. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 4417-4431.	1.5	108
9001	A multifunctional catalyst that stereoselectively assembles prodrugs. <i>Science</i> , 2017, 356, 426-430.	6.0	116
9002	Strategy for the Realization of Efficient Solution-Processable Phosphorescent Organic Light-Emitting Devices: Design and Synthesis of Bipolar Alkynylplatinum(II) Complexes. <i>Journal of the American Chemical Society</i> , 2017, 139, 6351-6362.	6.6	73
9003	Generalized Self-Energy Embedding Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2200-2205.	2.1	45
9004	Quantum-classical calculations of X-ray photoelectron spectra of polymers—Polymethyl methacrylate revisited. <i>Journal of Chemical Physics</i> , 2017, 146, 124902.	1.2	4
9005	A Theoretical Study on the Mechanism of Methylation of <i>N</i> -methylaniline with CO_2 and Silyl Hydrides. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 12-18.	1.0	10
9006	<i>O</i> -Acetyl Side-Chains in Monosaccharides: Redundant NMR Spin-Couplings and Statistical Models for Acetate Ester Conformational Analysis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 66-77.	1.2	25
9007	Cu^{2+} -Selectivity gated photochromism in Schiff-modified diarylethenes with a star-shaped structure. <i>Journal of Materials Chemistry C</i> , 2017, 5, 282-289.	2.7	34
9008	A theoretical study on the unusual square-planar structure of bis(imino)pyridine-ligated Group 13 complexes. <i>Dalton Transactions</i> , 2017, 46, 106-115.	1.6	5
9009	Rhodium(I) macrocyclic and cage-like structures containing diphosphine bridging ligands. <i>Transition Metal Chemistry</i> , 2017, 42, 57-67.	0.7	0
9010	High performance solid-state dye-sensitized solar cells based on organic blue-colored dyes. <i>Journal of Materials Chemistry A</i> , 2017, 5, 1242-1247.	5.2	35
9011	A comparative study on the N-heterocyclic carbene adducts of Ih-C_{60} , $\text{D}_{5h}\text{-C}_{70}$ and $\text{Sc}_3\text{N@Ih-C}_{80}$. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17598-17606.	1.3	5
9012	Comparative study on N,N-di-p-tolylaniline-based D-A1-A2 sensitizers by tuning the auxiliary acceptor for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2017, 145, 427-435.	2.0	15
9013	Understanding the effects of electronic polarization and delocalization on charge-transport levels in oligoacene systems. <i>Journal of Chemical Physics</i> , 2017, 146, 224705.	1.2	16
9014	DFT Studies of Dimerization Reactions of Boroles. <i>Chemistry - A European Journal</i> , 2017, 23, 11587-11597.	1.7	11
9015	A Blocked Linear Method for Optimizing Large Parameter Sets in Variational Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2604-2611.	2.3	20
9016	Molecular Characteristics of a Mixed-Valence Polyoxovanadate $\{\text{V}^{IV/V}_{18}\text{O}_{42}\}$ in Solution and at the Liquid-Surface Interface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 10419-10429.	1.5	28

#	ARTICLE	IF	CITATIONS
9017	Strong van der Waals Adhesion of a Polymer Film on Rough Substrates. <i>Langmuir</i> , 2017, 33, 5298-5303.	1.6	7
9018	Interplay between Terminal and Bridging Diiron Hydrides in Neutral and Oxidized States. <i>Organometallics</i> , 2017, 36, 2245-2253.	1.1	26
9019	Iron Hydroperoxide Intermediate in Superoxide Reductase: Protonation or Dissociation First? MM Dynamics and QM/MM Metadynamics Study. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2987-3004.	2.3	10
9020	Theoretical insights into the selectivity of 1,6-enyne cycloisomerization on gold clusters: Orbital interaction role. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 94-100.	1.1	1
9021	Transferable Atom-Centered Potentials for the Correction of Basis Set Incompleteness Errors in Density-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3505-3524.	2.3	29
9022	Charge-Shift Corrected Electronegativities and the Effect of Bond Polarity and Substituents on Covalent σ -Ionic Resonance Energy. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5190-5195.	1.1	10
9023	Alkaline Earth-Centered CO Homologation, Reduction, and Amine Carbonylation. <i>Journal of the American Chemical Society</i> , 2017, 139, 10036-10054.	6.6	78
9024	Switching Process Consisting of Three Isomeric States of an Azobenzene Unit. <i>Journal of the American Chemical Society</i> , 2017, 139, 9708-9713.	6.6	32
9025	Optimization and transferability of non- σ -electrostatic repulsion in the polarizable density embedding model. <i>Journal of Computational Chemistry</i> , 2017, 38, 2108-2117.	1.5	4
9026	Theoretical study on electronic and vibrational properties of hydrogen bonds in glycine-water clusters. <i>Chemical Physics Letters</i> , 2017, 684, 53-59.	1.2	17
9027	Unusual solvent effect of molecular charge transfer complexes: Stacking/non-stacking interaction revealed by characterization of structure and photophysical aspects. <i>Journal of Luminescence</i> , 2017, 190, 403-412.	1.5	7
9028	Ruthenium(II) Bipyridyl Complexes with Cyclometalated NHC Ligands. <i>Inorganic Chemistry</i> , 2017, 56, 7217-7229.	1.9	33
9029	Reduction of carbon dioxide and organic carbonyls by hydrosilanes catalysed by the perrhenate anion. <i>Catalysis Science and Technology</i> , 2017, 7, 2838-2845.	2.1	42
9030	4,5-Substituted C^*C^* cyclometalated thiazol-2-ylidene platinum(ii) complexes σ synthesis and photophysical properties. <i>Dalton Transactions</i> , 2017, 46, 7800-7812.	1.6	13
9031	A fluorescent photochromic diarylethene based on naphthalic anhydride with strong solvatochromism. <i>RSC Advances</i> , 2017, 7, 29854-29859.	1.7	13
9032	On the spectroscopic constants, first electronic state, vibrational frequencies, and isomerization of hydroxymethylene ($HCOH$). http://www.w3.org/1998/Math/MathML Tj ETQq1 1 0.784314,rgBT /Overlock 10	1.7	4
9033	One-pot synthesis of aryl-substituted 1,2,3-triphospholide anions. <i>Journal of Organometallic Chemistry</i> , 2017, 844, 1-7.	0.8	14
9034	Stability of the Parent Anion of the Potential Radiosensitizer 8-Bromo adenine Formed by Low-Energy (3 eV) Electron Attachment. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5730-5734.	1.2	29

#	ARTICLE	IF	CITATIONS
9035	Density-based errors in mixed-basis mean-field electronic structure, with implications for embedding and QM/MM methods. <i>Chemical Physics Letters</i> , 2017, 683, 375-382.	1.2	4
9036	Vacuum ultraviolet spectroscopy of the lowest-lying electronic state in subcritical and supercritical water. <i>Nature Communications</i> , 2017, 8, 15435.	5.8	20
9037	Odd σ Electron Bonds. <i>ChemPhysChem</i> , 2017, 18, 2766-2771.	1.0	21
9038	A quantum chemical investigation of the solvatochromism of a phthalocyanine within a lipid bilayer: Comparison between continuum and atomistic models. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 344, 42-48.	2.0	4
9039	Structure and spin state of nonheme Fe ^{IV} O complexes depending on temperature: predictive insights from DFT calculations and experiments. <i>Chemical Science</i> , 2017, 8, 5460-5467.	3.7	25
9040	Synthesis, characterization, photophysics, and a ligand rearrangement of CCC-NHC pincer nickel complexes: Colors, polymorphs, emission, and Raman spectra. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 258-265.	0.8	17
9041	Exceptional Perrhenate/Pertechnetate Uptake and Subsequent Immobilization by a Low-Dimensional Cationic Coordination Polymer: Overcoming the Hofmeister Bias Selectivity. <i>Environmental Science and Technology Letters</i> , 2017, 4, 316-322.	3.9	181
9042	Improved pK_a Prediction of Substituted Alcohols, Phenols, and Hydroperoxides in Aqueous Medium Using Density Functional Theory and a Cluster-Continuum Solvation Model. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4698-4706.	1.1	77
9043	Overcoming the crystallization and designability issues in the ultrastable zirconium phosphonate framework system. <i>Nature Communications</i> , 2017, 8, 15369.	5.8	366
9044	A theoretical study on the mechanism of ruthenium(η^2)-catalyzed phosphoryl-directed α -ortho-selective C-H bond activations: the phosphoryl hydroxy group triggered Ru(η^2)/Ru(O) catalytic cycle. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1482-1492.	2.3	14
9045	Dithiafulvenyl-Extended α -Heterotriangulenes and Their Interaction with C ₆₀ : Cooperative Fluorescence. <i>Chemistry - A European Journal</i> , 2017, 23, 12353-12362.	1.7	8
9046	Structural and thermodynamic investigation of pentoxifylline-cyclodextrin inclusion complex. <i>Chemical Physics Letters</i> , 2017, 682, 43-48.	1.2	10
9047	Polarizable and Non-Polarizable Force Field Representations of Ferric Cation and Validations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5718-5729.	1.2	7
9048	Effect of the Metal-Support Interaction on the Adsorption of NO on Pd ₄ /Al ₂ O ₃ : A Density Functional Theory and Natural Bond Orbital Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14147-14155.	1.5	3
9049	Propane CH activation by palladium complexes bearing ligands with Charge-shift bonding characteristics: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 30-36.	1.1	7
9050	Selective Dehydration of Mannitol to Isomannide over H ⁺ Zeolite. <i>ACS Catalysis</i> , 2017, 7, 4828-4834.	5.5	26
9051	Dimension reduction in conformational analysis: a two-rotor mathematical model of amino acid diamide conformational potential energy surface. <i>Canadian Journal of Chemistry</i> , 2017, 95, 830-836.	0.6	2
9052	CO ₂ Sequestration by Triazolylidene-Derived N-Heterocyclic Olefins: A Computational Study. <i>ChemistrySelect</i> , 2017, 2, 4648-4654.	0.7	9

#	ARTICLE	IF	CITATIONS
9053	Methane Oxidation to Methanol Catalyzed by Cu-Oxo Clusters Stabilized in NU-1000 Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2017, 139, 10294-10301.	6.6	282
9054	Catalytic N ₂ Reduction to Silylamines and Thermodynamics of N ₂ Binding at Square Planar Fe. <i>Journal of the American Chemical Society</i> , 2017, 139, 9291-9301.	6.6	72
9055	On the feasibility of reactions through the fullerene wall: a theoretical study of NH _x @C ₆₀ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17199-17209.	1.3	4
9056	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH ₃ MgCl in Tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4226-4237.	1.2	63
9057	(Oligo)aromatic species with one or two conjugated Si-Si bonds: near-IR emission of anthracenyl-bridged tetrasiladiene. <i>Dalton Transactions</i> , 2017, 46, 8839-8848.	1.6	23
9058	The effect of dynamical fluctuations of hydration structures on the absorption spectra of oxyluciferin anions in an aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10028-10035.	1.3	7
9059	N-annulated perylene diimide dimers: the effect of thiophene bridges on physical, electronic, optical, and photovoltaic properties. <i>Sustainable Energy and Fuels</i> , 2017, 1, 1137-1147.	2.5	36
9060	Exact roles of individual chemical forms of nitrogen in the photoluminescent properties of nitrogen-doped carbon dots. <i>Applied Materials Today</i> , 2017, 7, 190-200.	2.3	44
9061	Redox behavior and biological properties of ferrocene bearing porphyrins. <i>Journal of Inorganic Biochemistry</i> , 2017, 171, 76-89.	1.5	13
9062	Side-by-Side Comparison of Hydroperoxide and Corresponding Alcohol as Hydrogen-Bond Donors. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2951-2959.	1.1	29
9063	Brick by brick computation of the gibbs free energy of reaction in solution using quantum chemistry and COSMO-RS. <i>AIChE Journal</i> , 2017, 63, 3944-3954.	1.8	56
9064	Theoretical study on the formation process of Cross-Linked β -Cyclodextrin molecular tubes. <i>Chemical Physics Letters</i> , 2017, 677, 13-18.	1.2	4
9065	Green synthesis and photophysical properties of novel 1 H-imidazo[4,5-f][1,10]phenanthroline derivatives with blue/cyan two-photon excited fluorescence. <i>Tetrahedron</i> , 2017, 73, 2886-2893.	1.0	5
9066	Quantum Chemical Strain Analysis For Mechanochemical Processes. <i>Accounts of Chemical Research</i> , 2017, 50, 1041-1048.	7.6	35
9067	Lattice energetics and thermochemistry of acridine derivatives and substituted acridinium trifluoromethanesulphonates. <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 129, 1613-1624.	2.0	3
9068	Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca ²⁺ and Sr ²⁺ : a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10377-10394.	1.3	6
9069	Mechanistic insight into the regioselectivity of Pd-catalyzed C-H functionalization of N-methoxy cinnamamide. <i>Dalton Transactions</i> , 2017, 46, 5288-5296.	1.6	5
9070	Polarizable charge equilibration model for predicting accurate electrostatic interactions in molecules and solids. <i>Journal of Chemical Physics</i> , 2017, 146, 124117.	1.2	43

#	ARTICLE	IF	CITATIONS
9071	Computational contribution to the electrophoretic enantiomer separation mechanism and migration order using modified β -cyclodextrins. <i>Electrophoresis</i> , 2017, 38, 1860-1868.	1.3	23
9072	Defining the molecular properties of N-nitrosodimethylamine (NDMA) precursors using computational chemistry. <i>Environmental Science: Water Research and Technology</i> , 2017, 3, 502-512.	1.2	9
9073	Comparison of Intramolecular and Intermolecular Ammonium and Phosphonium Borohydrides in Hydrogen \rightarrow Proton \rightarrow and Hydride \rightarrow Transfer Reactions. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2032-2039.	1.0	10
9074	Isomerization of Second-Generation Isoprene Peroxy Radicals: Epoxide Formation and Implications for Secondary Organic Aerosol Yields. <i>Environmental Science & Technology</i> , 2017, 51, 4978-4987.	4.6	53
9075	Studies on hydrolysis mechanism of anticancer ruthenium drug ImH[trans-Ru(Im) ₂ Cl ₄] via ABEEM's polarizable force field combined with QM and MD-FEP. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 239-247.	1.3	3
9076	Identification of a mammalian silicon transporter. <i>American Journal of Physiology - Cell Physiology</i> , 2017, 312, C550-C561.	2.1	45
9077	Evaluation of the restricted virtual space approximation in the algebraic diagrammatic construction scheme for the polarization propagator to speed up excited state calculations. <i>Journal of Computational Chemistry</i> , 2017, 38, 1528-1537.	1.5	10
9078	Bio-inspired Herringbone Foldamers: Strategy for Changing the Structure of Helices. <i>Journal of Organic Chemistry</i> , 2017, 82, 4203-4215.	1.7	4
9079	Novel nickel(II) complexes of sterically modified linear N ₄ ligands: effect of ligand stereoelectronic factors and solvent of coordination on nickel(II) spin-state and catalytic alkane hydroxylation. <i>Dalton Transactions</i> , 2017, 46, 7181-7193.	1.6	30
9080	Improved Infrared Spectra Prediction by DFT from a New Experimental Database. <i>Chemistry - A European Journal</i> , 2017, 23, 8414-8423.	1.7	50
9081	Singlet open-shell diradical nature and redox properties of conjugated carbonyls: a quantum chemical study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
9082	Investigating cyclic sotolon, maple furanone and their dimers in solution using optical rotation, electronic circular dichroism and vibrational circular dichroism. <i>Tetrahedron</i> , 2017, 73, 2432-2438.	1.0	5
9083	The Elephant in the Room of Density Functional Theory Calculations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1449-1457.	2.1	88
9084	Theoretical Study of Addition Reactions of L ₄ M (M = Rh, Ir) and L ₂ M (M = Pd, Pt) Tj ETQq1 1_0,784314_rgBT/Over	1.1	5
9085	Rovibrational Characterization and Interstellar Implications of the Proton-Bound, Noble Gas Complexes: ArHAr ⁺ , NeHNe ⁺ , and ArHNe ⁺ . <i>ACS Earth and Space Chemistry</i> , 2017, 1, 60-69.	1.2	31
9086	TD-DFT benchmark: Excited states of atoms and atomic ions. <i>Computational and Theoretical Chemistry</i> , 2017, 1108, 50-56.	1.1	12
9087	Conformational Populations of β -(1 \rightarrow 4)-Glycosidic Linkages Using Redundant NMR $\langle i \rangle$ -Couplings and Circular Statistics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3042-3058.	1.2	39
9088	Covalent Metal-Metal-Bonded Mn ₄ Tetrahedron Inscribed within a Four-Coordinate Manganese Cubane Cluster, As Evidenced by Unexpected Temperature-Independent Diamagnetism. <i>Inorganic Chemistry</i> , 2017, 56, 3733-3737.	1.9	5

#	ARTICLE	IF	CITATIONS
9089	Computationally Designed 1,2,4-Triazolylidene-Derived N-Heterocyclic Olefins for CO ₂ Capture, Activation, and Storage. <i>ACS Omega</i> , 2017, 2, 299-307.	1.6	16
9090	Exact exchange with non-orthogonal generalized Wannier functions. <i>Journal of Chemical Physics</i> , 2017, 146, 104108.	1.2	8
9091	Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. <i>Inorganic Chemistry</i> , 2017, 56, 4148-4156.	1.9	15
9092	Computational Study on the Mechanisms of Multiple Complexation of CO and Isonitrile Ligands to Boron. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2688-2697.	1.1	4
9093	Structural and Electronic Properties of Hydrated VnH ₂ O and Vn+H ₂ O, n = 13, Systems. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4635-4649.	1.5	10
9094	Photoswitching of azobenzene-containing self-assembled monolayers as a tool for control over silicon surface electronic properties. <i>Journal of Chemical Physics</i> , 2017, 146, 104703.	1.2	15
9095	Synthesis and Reduction of Sterically Encumbered Mesoionic Carbene-Stabilized Aryldihaloboranes. <i>Chemistry - A European Journal</i> , 2017, 23, 12210-12217.	1.7	28
9096	Substitution Kinetics of [Fe(PDT/PPDT) _n (phen) _m] ²⁺ (n+m; n,m= 1,2) with 2,2'-Bipyridine, 1,10-Phenanthroline, and 2,2',6,6'-Terpyridine. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 182-196.	1.0	6
9097	Ruthenium(II) DMSO complexes with C [†] C* cyclometalated phenylimidazol NHC ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 829, 101-107.	0.8	12
9098	Assessing the electrochemical properties of polypyridine and polythiophene for prospective applications in sustainable organic batteries. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3307-3314.	1.3	15
9099	Why So Slow? Mechanistic Insights from Studies of a Poor Catalyst for Polymerization of μ -Caprolactone. <i>Inorganic Chemistry</i> , 2017, 56, 725-728.	1.9	20
9100	Mechanistic Study of Cp*Co ^{III} /Rh ^{III} -Catalyzed Directed C-H Functionalization with Diazo Compounds. <i>Journal of Organic Chemistry</i> , 2017, 82, 1195-1204.	1.7	55
9101	Systematic investigation of the excited-state properties of anthracene-dicarboxylic acids. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 337, 207-215.	2.0	17
9102	Integrating ion mobility spectrometry into mass spectrometry-based exposome measurements: what can it add and how far can it go?. <i>Bioanalysis</i> , 2017, 9, 81-98.	0.6	66
9103	Helical Self-Assembly-Induced Singlet-Triplet Emissive Switching in a Mechanically Sensitive System. <i>Journal of the American Chemical Society</i> , 2017, 139, 785-791.	6.6	153
9104	Bioluminescence of Firefly Squid via Mechanism of Single Electron-Transfer Oxygenation and Charge-Transfer-Induced Luminescence. <i>Journal of the American Chemical Society</i> , 2017, 139, 1106-1119.	6.6	70
9105	Prediction of Minimum Ignition Energy from Molecular Structure Using Quantitative Structure-Property Relationship (QSPR) Models. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 47-51.	1.8	53
9106	Rational design of model Pd-catalysts for C-H activation involving ligands with charge-shift bonding characteristics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2417-2424.	1.3	8

#	ARTICLE	IF	CITATIONS
9107	Machine Learning Methods to Predict Density Functional Theory B3LYP Energies of HOMO and LUMO Orbitals. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 11-21.	2.5	129
9108	Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: I. <i>Ab Initio</i> Calculations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 208-220.	1.2	22
9109	The mechanism of selective catalytic reduction of NO _x on Cu-SSZ-13 – a computational study. <i>Dalton Transactions</i> , 2017, 46, 369-377.	1.6	6
9110	On the role of the termolecular reactions 2O ₂ + H ₂ → 2HO ₂ and 2O ₂ + H ₂ → H + HO ₂ + O ₂ in formation of the first radicals in hydrogen combustion: <i>ab initio</i> predictions of energy barriers. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2175-2185.	1.3	20
9111	The nature of the light absorption and emission transitions of 4-hydroxybenzophenone in different solvents. A combined computational and experimental study. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 527-538.	1.6	7
9112	Hydrosilylation of RN=CH Imino-Substituted Pyridines without a Catalyst. <i>Chemistry - A European Journal</i> , 2017, 23, 3074-3083.	1.7	7
9113	Probing a General Rule towards Thermodynamic Stabilities of Mono BN-doped Lower Polyenes. <i>Chemistry - an Asian Journal</i> , 2017, 12, 605-614.	1.7	5
9114	¹³ C-Labeled Idohexopyranosyl Rings: Effects of Methyl Glycosidation and C6 Oxidation on Ring Conformational Equilibria. <i>Journal of Organic Chemistry</i> , 2017, 82, 1356-1370.	1.7	16
9115	Aromatic and antiaromatic ring currents in a molecular nanoring. <i>Nature</i> , 2017, 541, 200-203.	13.7	204
9116	<i>mer</i> , <i>fac</i> , and Bidentate Coordination of an Alkyl-POP Ligand in the Chemistry of Nonclassical Osmium Hydrides. <i>Inorganic Chemistry</i> , 2017, 56, 676-683.	1.9	29
9117	Automated Fragmentation Polarizable Embedding Density Functional Theory (PE-DFT) Calculations of Nuclear Magnetic Resonance (NMR) Shielding Constants of Proteins with Application to Chemical Shift Predictions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 525-536.	2.3	18
9118	Characterization of the binding of six actinyls AnO ₂ ²⁺ (An = U/Np/Pu) with three expanded porphyrins by density functional theory. <i>New Journal of Chemistry</i> , 2017, 41, 63-74.	1.4	10
9119	Potential use of small basis set on the calculations of electronic properties of some four-membered heterocycles: a conformational study. <i>Molecular Physics</i> , 2017, 115, 261-277.	0.8	5
9120	Characterization of dye-sensitized solar cells using five pure anthocyanidin 3-O-glucosides possessing different chromophores. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 335, 230-238.	2.0	11
9121	Millimeter-wave spectroscopy of <i>syn</i> formyl azide (HC(O)N ₃) in seven vibrational states. <i>Journal of Molecular Spectroscopy</i> , 2017, 331, 71-81.	0.4	4
9122	Glyoxalbis(2-methylmercaptoanil) complexes of nickel and ruthenium: radical versus non-radical states. <i>New Journal of Chemistry</i> , 2017, 41, 1149-1159.	1.4	3
9123	Simulation of NMR chemical shifts in heterocycles: a method evaluation. <i>Journal of Molecular Modeling</i> , 2017, 23, 9.	0.8	5
9124	Understanding the Scarcity of Thorium Peroxide Clusters. <i>Inorganic Chemistry</i> , 2017, 56, 12692-12694.	1.9	6

#	ARTICLE	IF	CITATIONS
9125	A theoretical investigation on bio-transformation of third generation anti-cancer drug Heptaplatin and its interaction with DNA purine bases. <i>Chemical Physics Letters</i> , 2017, 690, 105-115.	1.2	3
9126	Experimental and Theoretical Studies on Iron-Promoted Oxidative Annulation of Arylglyoxal with Alkyne: Unusual Addition and Migration on the Aryl Ring. <i>Journal of the American Chemical Society</i> , 2017, 139, 17015-17021.	6.6	26
9127	Biotransformation of Isoniazid by Cytochromes P450: Analyzing the Molecular Mechanism using Density Functional Theory. <i>Chemical Research in Toxicology</i> , 2017, 30, 2060-2073.	1.7	11
9128	Deconstructing the Confinement Effect upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials: Lessons Learned from Zeolites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22015-22024.	1.5	27
9129	Relevance of the DFT method to study expanded porphyrins with different topologies. <i>Journal of Computational Chemistry</i> , 2017, 38, 2819-2828.	1.5	64
9130	Intermolecular magnetic interactions in stacked DNA base pairs. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27817-27827.	1.3	5
9131	Visualizing spatially decomposed intermolecular correlations in the infrared spectra of aprotic liquids. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 148-157.	1.3	3
9132	Vanadium(IV) oxoanions in basic water solution: a simple oxidative system for the one pot selective conversion of L-proline to pyrroline-2-carboxylate. <i>Dalton Transactions</i> , 2017, 46, 15059-15069.	1.6	8
9133	Binary Blends of Polyimide and Benzothienobenzothiophene for High-Performance Solution-Processed Organic Phototransistors. <i>Advanced Electronic Materials</i> , 2017, 3, 1700284.	2.6	14
9134	Speed-Up of the Excited-State Benchmarking: Double-Hybrid Density Functionals as Test Cases. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5539-5551.	2.3	33
9135	Silica-Grafted Lanthanum Benzyl Species: Synthesis, Characterization, and Catalytic Applications. <i>Organometallics</i> , 2017, 36, 3912-3920.	1.1	10
9136	Efficient Solar Cells Based on Porphyrin Dyes with Flexible Chains Attached to the Auxiliary Benzothiadiazole Acceptor: Suppression of Dye Aggregation and the Effect of Distortion. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 36875-36885.	4.0	84
9137	HOMO inversion as a strategy for improving the light-absorption properties of Fe(II) chromophores. <i>Chemical Science</i> , 2017, 8, 8115-8126.	3.7	52
9138	Synthesis and characterization of chiral and achiral diamines containing one or two BODIPY molecules. <i>New Journal of Chemistry</i> , 2017, 41, 14370-14378.	1.4	13
9139	Enhancing solution-phase supramolecular interactions between monomeric porphyrins and [60]fullerene by simple chemical modification. <i>Tetrahedron Letters</i> , 2017, 58, 4514-4518.	0.7	10
9140	Comparative Assessment of Computational Methods for Free Energy Calculations of Ionic Hydration. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2763-2775.	2.5	20
9141	Structure, antioxidative potency and potential scavenging of OH and OOH of phenylethyl-3,4-dihydroxyhydrocinnamate in protic and aprotic media: DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 221-233.	1.3	7
9142	Absolute configuration assignment of (+)-fluralaner using vibrational circular dichroism. <i>Chirality</i> , 2017, 29, 854-864.	1.3	8

#	ARTICLE	IF	CITATIONS
9143	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5343-5353.	2.3	40
9144	Electronic Band Structure of Helical Polyisocyanides. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7993-8002.	1.1	1
9145	Interconversion between 4-Imidazolone Ions; Isomers of [b ₄] ⁺ Derived from Protonated Tetraglycine. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9541-9547.	1.2	5
9146	Dual-Phase Mechanism for the Catalytic Conversion of <i>n</i> -Butane to Maleic Anhydride by the Vanadyl Pyrophosphate Heterogeneous Catalyst. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24069-24076.	1.5	14
9147	Phosphoramidate hydrolysis catalyzed by human histidine triad nucleotide binding protein 1 (hHint1): a cluster-model DFT computational study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8661-8668.	1.5	7
9148	Quantum Chemical Rovibrational Analysis of the HOSO Radical. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8108-8114.	1.1	14
9149	Preparation of metalated azine complexes of iridium(III). <i>New Journal of Chemistry</i> , 2017, 41, 12976-12988.	1.4	8
9150	Hydrolysis of Dimethyl Methylphosphonate by the Cyclic Tetramer of Zirconium Hydroxide. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7690-7696.	1.1	26
9151	Evaluation of the Factors Impacting the Accuracy of ¹³ C NMR Chemical Shift Predictions using Density Functional Theory: The Advantage of Long-Range Corrected Functionals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5798-5819.	2.3	77
9152	Quantitative DFT modeling of product concentration in organometallic reactions: Cu-mediated pentafluoroethylation of benzoic acid chlorides as a case study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29344-29353.	1.3	22
9153	Exploring the origins of selectivity in soluble epoxide hydrolase from <i>Bacillus megaterium</i> . <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8827-8835.	1.5	14
9154	Change in Luminescence Induced by Solution-Mediated Phase-Transition of Cyclometalated Platinum(II) Complex with Isoquinoline Carboxylate. <i>Inorganic Chemistry</i> , 2017, 56, 12158-12168.	1.9	15
9155	Blue Fluorescence from BF ₂ Complexes of <i>N,O</i> -Benzamide Ligands: Synthesis, Structure, and Photophysical Properties. <i>Inorganic Chemistry</i> , 2017, 56, 12514-12519.	1.9	25
9156	Reduction of Diphenylacetylene Mediated by Rare-Earth Ferrocene Diamide Complexes. <i>Organometallics</i> , 2017, 36, 4643-4648.	1.1	20
9157	Calculating the geometry and Raman spectrum of physiological bis(<i>l</i> -histidinato)copper(II): an assessment of DFT functionals for aqueous and isolated systems. <i>Journal of Molecular Modeling</i> , 2017, 23, 290.	0.8	9
9158	Pseudo Jahn-Teller effect in control and rationalization of chemical transformations in two-dimensional compounds. <i>Journal of Physics: Conference Series</i> , 2017, 833, 012010.	0.3	11
9159	A full pivoting algorithm for the Cholesky decomposition of two-electron repulsion and spin-orbit coupling integrals. <i>Journal of Computational Chemistry</i> , 2017, 38, 2775-2783.	1.5	5
9160	Excited-state absorption in tetrapyrrolyl porphyrins: comparing real-time and quadratic-response time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27452-27462.	1.3	32

#	ARTICLE	IF	CITATIONS
9161	Investigation into the molecular structure, electronic properties, and energetic stability of endohedral (TM@C ₂₀) and exohedral (TM-C ₂₀) metallofullerene derivatives of C ₂₀ : TM = Group 11 and 12 transition metal atoms/ions. <i>Computational and Theoretical Chemistry</i> , 2017, 1119, 32-44.	1.1	16
9162	Two-dimensional second-order nonlinear optical spectra: landscape of second-order nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29315-29320.	1.3	22
9163	Photochromic Heterocycle-Fused Thieno[3,2- <i>b</i>]phosphole Oxides as Visible Light Switches without Sacrificing Photoswitching Efficiency. <i>Journal of the American Chemical Society</i> , 2017, 139, 15142-15150.	6.6	81
9164	Some Hydrated Molecular Complexes of 4-Cyanophenylboronic Acid: Significance of Water in the Structure Stabilization by Theoretical Investigation. <i>Crystal Growth and Design</i> , 2017, 17, 6247-6254.	1.4	10
9165	Cobalt Ion Promoted Redox Cascade: A Route to Spiro Oxazine-Oxazepine Derivatives and a Dinuclear Cobalt(III) Complex of an <i>N</i> -(1,4-Naphthoquinone)- <i>o</i> -aminophenol Derivative. <i>Inorganic Chemistry</i> , 2017, 56, 13194-13204.	1.9	11
9166	Benchmarking of Computational Methods for Creation of Retention Models in Quantitative Structure–Retention Relationships Studies. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2754-2762.	2.5	10
9167	Boron and nitrogen co-doped single-layered graphene quantum dots: a high-affinity platform for visualizing the dynamic invasion of HIV DNA into living cells through fluorescence resonance energy transfer. <i>Journal of Materials Chemistry B</i> , 2017, 5, 8719-8724.	2.9	48
9168	Understanding the function of cetyltrimethyl ammonium bromide in lithium/sulfur cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 23094-23102.	5.2	3
9169	Polyradical PROXYL/TEMPO–Derived Amides: Synthesis, Physicochemical Studies, DFT Calculations, and Antimicrobial Activity. <i>ChemPlusChem</i> , 2017, 82, 1326-1340.	1.3	4
9170	Cluster decomposition of full configuration interaction wave functions: A tool for chemical interpretation of systems with strong correlation. <i>Journal of Chemical Physics</i> , 2017, 147, 154105.	1.2	25
9171	Yttrium nitrate catalyzed synthesis, photophysical study, and TD–DFT calculation of 2,3-dihydroquinazolin-4(1H)-ones. <i>Heteroatom Chemistry</i> , 2017, 28, .	0.4	11
9172	Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory. <i>Computer Physics Communications</i> , 2017, 221, 42-52.	3.0	11
9173	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4442-4451.	2.3	12
9174	Pair 2-electron reduced density matrix theory using localized orbitals. <i>Journal of Chemical Physics</i> , 2017, 147, 084101.	1.2	27
9175	Role of Coordination Number, Geometry, and Local Disorder on ²⁷ Al NMR Chemical Shifts and Quadrupolar Coupling Constants: Case Study with Aluminosilicates. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19946-19957.	1.5	28
9176	Intermetallic Cooperation in C–H Activation Involving Transient Titanium-Alkylidene Species: A Synthetic and Mechanistic Study. <i>Organometallics</i> , 2017, 36, 3076-3083.	1.1	14
9177	Intrinsic self-healing polymers with a high E-modulus based on dynamic reversible urea bonds. <i>NPG Asia Materials</i> , 2017, 9, e420-e420.	3.8	97
9178	Importance of the alignment of polar π -conjugated molecules inside carbon nanotubes in determining second-order non-linear optical properties. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24819-24828.	1.3	17

#	ARTICLE	IF	CITATIONS
9179	Theoretical study on the reaction of Cp* (pentamethylcyclopentadienyl)(Cl)Zr(diene) with isonitriles. Computational and Theoretical Chemistry, 2017, 1117, 177-187.	1.1	1
9180	Theoretical and experimental study of fenofibrate and simvastatin. Journal of Molecular Structure, 2017, 1149, 683-693.	1.8	4
9181	Highly Efficient Proton Conduction in a Three-Dimensional Titanium Hydrogen Phosphate. Chemistry of Materials, 2017, 29, 7263-7271.	3.2	35
9182	Modeling Optical Spectra of Large Organic Systems Using Real-Time Propagation of Semiempirical Effective Hamiltonians. Journal of Chemical Theory and Computation, 2017, 13, 4410-4420.	2.3	16
9183	Intense and Stable Near-Infrared Emission from Light-Emitting Electrochemical Cells Comprising a Metal-Free Indacenodithieno[3,2- <i>b</i>]thiophene-Based Copolymer as the Single Emitter. Chemistry of Materials, 2017, 29, 7750-7759.	3.2	49
9184	Tunable regiodivergent phosphine-catalyzed [3 + 2] cycloaddition of alkynones and trifluoroacetyl phenylamides. Organic Chemistry Frontiers, 2017, 4, 2392-2402.	2.3	18
9185	Relation Between Ring Currents and Hydrogenation Enthalpies for Assessing the Degree of Aromaticity. Journal of Physical Chemistry A, 2017, 121, 7282-7289.	1.1	37
9186	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2017, 19, 25662-25670.	1.3	36
9187	Hydration Control Through Intramolecular Degrees of Freedom: Molecular Dynamics of [Cu(II)(Imidazole) ₄]. Journal of Physical Chemistry B, 2017, 121, 9024-9031.	1.2	4
9188	Spin the light off: rapid internal conversion into a dark doublet state quenches the fluorescence of an RNA spin label. Physical Chemistry Chemical Physics, 2017, 19, 26255-26264.	1.3	8
9189	Thermal and Mechanochemical Syntheses of Luminescent Mononuclear Copper(I) Complexes. European Journal of Inorganic Chemistry, 2017, 2017, 5134-5142.	1.0	18
9190	Supramolecular Interaction-Assisted Fluorescence and Tunable Stimuli-Responsiveness of α -Phenylalanine-Based Polymers. Langmuir, 2017, 33, 10588-10597.	1.6	8
9191	Molecular-Level Insights into Oxygen Reduction Catalysis by Graphite-Conjugated Active Sites. ACS Catalysis, 2017, 7, 7680-7687.	5.5	33
9192	How to Control Inversion vs Retention Transmetalation between Pd ^{II} -Phenyl and Cu ^I -Alkyl Complexes: Theoretical Insight. Journal of the American Chemical Society, 2017, 139, 14065-14076.	6.6	13
9193	Conformational landscape of isolated capped amino acids: on the nature of non-covalent interactions. European Physical Journal D, 2017, 71, 1.	0.6	3
9194	Reactivity of Cyclic Silenolates Revisited. Organometallics, 2017, 36, 3765-3773.	1.1	8
9195	Size-Dependent Reactivity of Nano-Sized Neutral Manganese Oxide Clusters toward Ethylene. Chemistry - A European Journal, 2017, 23, 15820-15826.	1.7	13
9196	Bond dissociation energy controlled σ -bond metathesis in alkaline-earth-metal hydride catalyzed dehydrocoupling of amines and boranes: a theoretical study. Inorganic Chemistry Frontiers, 2017, 4, 1813-1820.	3.0	18

#	ARTICLE	IF	CITATIONS
9197	Axially chiral benzimidazolium based silver(I) and gold(I) bis-NHC complexes of R-BINOL scaffold: synthesis, characterization and DFT studies. <i>Journal of Chemical Sciences</i> , 2017, 129, 1491-1498.	0.7	0
9198	Binding and electrophilic activation of ethylene by zinc(II), cadmium(II), and mercury(II) complexes: A theoretical investigation. <i>Journal of Organometallic Chemistry</i> , 2017, 851, 122-135.	0.8	3
9199	Effects of base strength on the copper-catalyzed cycloisomerization of propargylic acetates to form indolizines: A DFT study. <i>Tetrahedron</i> , 2017, 73, 6092-6100.	1.0	11
9200	Photoelectron Spectroscopy and Density Functional Theory Studies of Iron Sulfur (FeS) _m (m= 2-8) Cluster Anions: Coexisting Multiple Spin States. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7362-7373.	1.1	11
9201	λ -Arene Complexes as Intermediates in the Preparation of Molecular Phosphorescent Iridium(III) Complexes. <i>Chemistry - A European Journal</i> , 2017, 23, 15729-15737.	1.7	22
9202	It Is Not Just Up to the Substrate: Palladium(0) Cyclizes Nazarov Substrates through Intramolecular Allylic Alkylation. <i>Organometallics</i> , 2017, 36, 3589-3596.	1.1	7
9203	Mild sp ² Carbon-Oxygen Bond Activation by an Isolable Ruthenium(II) Bis(dinitrogen) Complex: Experiment and Theory. <i>Organometallics</i> , 2017, 36, 3654-3663.	1.1	13
9204	The Role of Weak Interactions in Supramolecular Compounds: A Synthetic and Theoretical Study of Novel Elongated Cavitands. <i>ChemistrySelect</i> , 2017, 2, 8337-8345.	0.7	5
9205	Palladium-Catalyzed Hydroxycarbonylation of Pentenoic Acids. Computational and Experimental Studies on the Catalytic Selectivity. <i>ACS Catalysis</i> , 2017, 7, 7070-7080.	5.5	27
9206	Computational characterization of the mechanism for the light-driven catalytic trichloromethylation of acylpyridines. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8641-8647.	1.5	22
9207	Theoretical insights into the reaction of Cp*(Cl)Hf(diene) with isonitriles. <i>RSC Advances</i> , 2017, 7, 44979-44989.	1.7	2
9208	Conformational Preference and Spectroscopical Characteristics of the Active Pharmaceutical Ingredient Levetiracetam. <i>Journal of Pharmaceutical Sciences</i> , 2017, 106, 3564-3573.	1.6	2
9209	Peering into the Mechanism of Low-Temperature Synthesis of Bronze-type TiO ₂ in Ionic Liquids. <i>Crystal Growth and Design</i> , 2017, 17, 5586-5601.	1.4	21
9210	The fluorescence properties of tiara like structural thiolated palladium clusters. <i>Dalton Transactions</i> , 2017, 46, 12964-12970.	1.6	9
9211	Implementation and Application of the Frozen Density Embedding Theory with the Algebraic Diagrammatic Construction Scheme for the Polarization Propagator up to Third Order. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4711-4725.	2.3	21
9212	Partial density of states ligand field theory (PDOS-LFT): Recovering a LFT-like picture and application to photoproperties of ruthenium(II) polypyridine complexes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 348, 305-325.	2.0	4
9213	The influence of hydrogen bonds on NIAD-4 for use in the optical imaging of amyloid fibrils. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15849-15855.	1.3	5
9214	Computational Linker Design for Highly Crystalline Metal-Organic Framework NU-1000. <i>Chemistry of Materials</i> , 2017, 29, 8073-8081.	3.2	40

#	ARTICLE	IF	CITATIONS
9215	Synthetic and Computational Studies on the Thermal and Photochemical Reactions of [NPN]TaMe ₃ (NPN = PhP(CH ₂) ₂ SiMe ₂ NPh) ₂ and [^{Mes} NPN]TaMe ₃ (^{Mes} NPN =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 737 Tdi(PhP(CH ₂) ₂ /su Organometallics, 2017, 36, 3564-3572.		
9216	Optical determination of the electronic coupling and intercalation geometry of thiazole orange homodimer in DNA. Journal of Chemical Physics, 2017, 147, 055101.	1.2	17
9217	Influence of Base Strength on the Protonâ€¢Transfer Reaction by Density Functional Theory. European Journal of Organic Chemistry, 2017, 2017, 3947-3956.	1.2	15
9218	A â€œUniversalâ€ Spectroscopic Map for the OH Stretching Mode in Alcohols. Journal of Physical Chemistry A, 2017, 121, 5823-5833.	1.1	11
9219	Diruthenium Carbido Complexes as <i>N</i> -Heterocyclic Carbene Like C-Donor Ligands to Group 11 Metals. Organometallics, 2017, 36, 3686-3691.	1.1	28
9220	Aluminium complexes containing salicylbenzothiazole ligands and their application in the ring-opening polymerisation of rac-lactide and μ -caprolactone. Dalton Transactions, 2017, 46, 11013-11030.	1.6	22
9221	Density Functional Approach and Random Matrix Theory in Proteogenesis. Journal of the Physical Society of Japan, 2017, 86, 023801.	0.7	0
9222	Mechanistic insights into the biomimetic catalytic hydroxylation of arenes by a molecular Fe(NHC) complex. Journal of Catalysis, 2017, 352, 599-605.	3.1	13
9223	New ruthenium compounds bearing semicarbazone 2-formylpyridine moiety: Playing with auxiliary ligands for tuning the mechanism of biological activity. Journal of Inorganic Biochemistry, 2017, 175, 80-91.	1.5	20
9224	Competition between the Hydride Ligands of Two Types in Proton Transfer to [P(CH ₃) ₃ CH ₃ C(CH ₂ CH ₂ PPh ₂) ₃]RuH(<i>l</i> -2-BH ₄). European Journal of Inorganic Chemistry, 2017, 2017, 4673-4682.	1.0	11
9225	Hexagonal Boron Nitride for Adsorption of Saccharides. Journal of Physical Chemistry C, 2017, 121, 17332-17338.	1.5	19
9226	Selected configuration interaction method using sampled first-order corrections to wave functions. Journal of Chemical Physics, 2017, 147, 034102.	1.2	27
9227	Edges of graphene and carbon nanotubes with high catalytic performance for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2017, 19, 21003-21011.	1.3	15
9228	Synthesis, structural analyses and antimicrobial activity of the water soluble 1D coordination polymer [Ag(3-aminopyridine)]ClO ₄ . Journal of Molecular Structure, 2017, 1149, 58-68.	1.8	15
9229	Facile and Rapid Visualization of Colorless Endocrine Disruptor Bisphenol A by Interfacial Chargeâ€¢Transfer Transitions with TiO ₂ Nanoparticles. ChemistrySelect, 2017, 2, 6097-6099.	0.7	22
9230	A Combined Experimental/Computational Study of the Mechanism of a Palladiumâ€¢Catalyzed Boraâ€¢Negishi Reaction. Chemistry - A European Journal, 2017, 23, 12655-12667.	1.7	8
9231	Theoretical study on selectivity trends in (<i>N</i> -heterocyclic carbene)â€¢Pd catalyzed mizorokiâ€¢heck reactions: Exploring density functionals methods and molecular models. Journal of Computational Chemistry, 2017, 38, 2371-2377.	1.5	13
9232	Conformational preferences of protonated N-acetylated hexosamines probed by InfraRed Multiple Photon Dissociation (IRMPD) spectroscopy and ab initio calculations. International Journal of Mass Spectrometry, 2017, 421, 116-123.	0.7	27

#	ARTICLE	IF	CITATIONS
9233	Accurate DFT-D3 Calculations in a Small Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3575-3585.	2.3	70
9234	Regioselective Diversification of 2,1-Borazaronaphthalenes: Unlocking Isosteric Space via C-H Activation. <i>Journal of Organic Chemistry</i> , 2017, 82, 8072-8084.	1.7	24
9235	Radical reactions of diamine bis(phenolate) vanadium(III) complexes. Solid state binding of O ₂ to form a vanadium(V) peroxy complex. <i>Dalton Transactions</i> , 2017, 46, 9692-9704.	1.6	6
9236	Contorted tetrabenzoacenes of varied conjugation: charge transport study with single-crystal field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7935-7943.	2.7	19
9237	Kinetics of Uncatalyzed Reactions of 2,4- and 4,4-Diphenylmethane-Diisocyanate with Primary and Secondary Alcohols. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 643-655.	1.0	13
9238	The effect of external forces on the initial dissociation of RDX (1,3,5-trinitro-1,3,5-triazine): A mechanochemical study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25426.	1.0	9
9239	Predicting optimal finite field strengths for calculating the first and second hyperpolarizabilities using simple molecular descriptors. <i>Chemical Physics Letters</i> , 2017, 682, 160-167.	1.2	4
9240	Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 314002.	0.7	19
9241	Ruthenium(II) pentamethylcyclopentadienyl half-sandwich carbene complexes with polypyridyl ligands. <i>Journal of Organometallic Chemistry</i> , 2017, 848, 1-9.	0.8	5
9242	Absorption Spectra for Disordered Aggregates of Chromophores Using the Exciton Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3787-3801.	2.3	21
9243	Oxazine Ring-Related Vibrational Modes of Benzoxazine Monomers Using Fully Aromatically Substituted, Deuterated, ¹⁵ N Isotope Exchanged, and Oxazine-Ring-Substituted Compounds and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6269-6282.	1.1	198
9244	Using non-empirically tuned range-separated functionals with simulated emission bands to model fluorescence lifetimes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21046-21057.	1.3	12
9245	Protective effects of 4-methylcoumarins and related compounds as radical scavengers and chain-breaking antioxidants. <i>Biochimie</i> , 2017, 140, 133-145.	1.3	9
9246	The VN ₃ H defect in diamond: a quantum-mechanical characterization. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22221-22229.	1.3	20
9247	Synthesis and Characterization of Luminescent Cyclometalated Platinum(II) Complexes with Tunable Emissive Colors and Studies of Their Application in Organic Memories and Organic Light-Emitting Devices. <i>Journal of the American Chemical Society</i> , 2017, 139, 10750-10761.	6.6	110
9248	Experimental and Theoretical Quantification of the Lewis Acidity of Iodine(III) Species. <i>Journal of Organic Chemistry</i> , 2017, 82, 11891-11896.	1.7	49
9249	Visible-to-Near-IR Wide-Range Light Harvesting by Interfacial Charge-Transfer Transitions between TiO ₂ and <i>p</i> -Aminophenol and Evidence of Direct Electron Injection to the Conduction Band of TiO ₂ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 18710-18716.	1.5	20
9250	Selective Decarbonylation of Fatty Acid Esters to Linear α -Olefins. <i>Organometallics</i> , 2017, 36, 2956-2964.	1.1	29

#	ARTICLE	IF	CITATIONS
9251	Mechanisms and Specificity of Phenazine Biosynthesis Protein PhzF. <i>Scientific Reports</i> , 2017, 7, 6272.	1.6	12
9252	Influence of intramolecular vs. intermolecular phosphonium-borohydrides in catalytic hydrogen, hydride, and proton transfer reactions. <i>Dalton Transactions</i> , 2017, 46, 9382-9393.	1.6	8
9253	A comparative study of DFT calculated and experimental UV/Visible spectra for thirty carboline and carbazole based compounds. <i>Journal of Molecular Structure</i> , 2017, 1149, 282-298.	1.8	51
9254	Optimizing the Accuracy and Computational Cost in Theoretical Squaramide Catalysis: The Henry Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 15336-15347.	1.7	18
9255	Singlet L _a and L _b Bands for N-Acenes ($N = 2-7$): A CASSCF/CASPT2 Study. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4297-4306.	2.3	30
9256	Analysis and design of resonance Raman reporter molecules by density functional theory. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 1196-1200.	1.2	15
9257	A Multi-Level Theoretical Study to Disclose the Binding Mechanisms of Gold(III)-Bipyridyl Compounds as Selective Aquaglyceroporin Inhibitors. <i>Chemistry - A European Journal</i> , 2017, 23, 13802-13813.	1.7	31
9258	Theoretical reflections on the structural polymorphism of the oxygen-evolving complex in the S ₂ state and the correlations to substrate water exchange and water oxidation mechanism in photosynthesis. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2017, 1858, 833-846.	0.5	7
9259	Combining active-space coupled-cluster approaches with moment energy corrections via the CC(<i>P</i> ; <i>Q</i>) methodology: connected quadruple excitations. <i>Molecular Physics</i> , 2017, 115, 2860-2891.	0.8	35
9260	“Push-Pull” π - π^* Systems in Catalysis. <i>ACS Catalysis</i> , 2017, 7, 6430-6439.	5.5	24
9261	Accurate potential energy surfaces for hydrogen abstraction reactions: A benchmark study on the XYG3 doubly hybrid density functional. <i>Journal of Computational Chemistry</i> , 2017, 38, 2326-2334.	1.5	4
9262	Computational study of fluoroquinolone binding to Mg(H ₂ O) ₆ ²⁺ and its applicability to future drug design. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25428.	1.0	5
9263	Theoretical Insights into the Electronic Structures and Stability of Dimetallofullerenes M ₂ @I _h C ₈₀ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 18169-18177.	1.5	14
9264	Computerized implementation of higher-order electron correlation methods and their linear scaling divide-and-conquer extensions. <i>Journal of Computational Chemistry</i> , 2017, 38, 2520-2527.	1.5	11
9265	Modelling charge transport of discotic liquid-crystalline triindoles: the role of peripheral substitution. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24202-24208.	1.3	8
9266	Mechanistic Insights into Alkane Metathesis Catalyzed by Silica-Supported Tantalum Hydrides: A DFT Study. <i>Inorganic Chemistry</i> , 2017, 56, 10458-10473.	1.9	14
9267	Even and odd oligothiophene-bridged bis-naphthalimides for n-type and ambipolar organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2017, 5, 9439-9450.	2.7	8
9268	Aliphatic C(sp ³)-H Bond Activation Using Nickel Catalysis: Mechanistic Insights on Regioselective Arylation. <i>Journal of Organic Chemistry</i> , 2017, 82, 9619-9626.	1.7	32

#	ARTICLE	IF	CITATIONS
9269	Estimation of optical rotation of β -alkylidenebutenolide, cyclopropylamine, cyclopropylmethanol and cyclopropanone based compounds by a Density Functional Theory (DFT) approach. <i>Chirality</i> , 2017, 29, 634-647.	1.3	1
9270	Electronic Structure and Properties of Berkelium Iodates. <i>Journal of the American Chemical Society</i> , 2017, 139, 13361-13375.	6.6	25
9271	Toward the laboratory identification of the not-so-simple NS2 neutral and anion isomers. <i>Journal of Chemical Physics</i> , 2017, 147, 074303.	1.2	5
9272	Covalent functionalization of octagraphene with magnetic octahedral B_6 and non-planar C_6 clusters. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2017, 94, 196-203.	1.3	12
9273	Towards completing the cyclopropenylidene cycle: rovibrational analysis of cyclic N_3^+ , CNN , $HCNN$, and CNC . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22860-22869.	1.3	4
9274	A comparative study of inter- and intramolecular C-H aminations: mechanism and site selectivity. <i>RSC Advances</i> , 2017, 7, 34783-34794.	1.7	12
9275	Reductive Eliminations from Diarylpalladium(II) Complexes: A Combined Experimental and Computational Investigation. <i>Chemistry - A European Journal</i> , 2017, 23, 15116-15123.	1.7	9
9276	Prediction of the reduction potential in transition metal containing complexes: How expensive? For what accuracy?. <i>Journal of Computational Chemistry</i> , 2017, 38, 2430-2438.	1.5	23
9277	Hybrid visible-light responsive Al_2O_3 particles. <i>Chemical Physics Letters</i> , 2017, 685, 416-421.	1.2	14
9278	Conformation of some 2,4,6-trisubstitued pyridinium salts. <i>Journal of Molecular Structure</i> , 2017, 1149, 640-644.	1.8	0
9279	Efficient Phosphorescence from Naphthalenebenzimidazole Coordinated Iridium(III) Chromophores. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5238-5245.	1.0	14
9280	Calix[n]arene-based polyradicals: enhancing ferromagnetism by avoiding edge effects. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24264-24270.	1.3	6
9281	Design of Helical M π Topological Switches with High Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19348-19357.	1.5	34
9282	Stability Study of Hypervalent Tellurium Compounds in Aqueous Solutions. <i>ACS Omega</i> , 2017, 2, 4431-4439.	1.6	16
9283	RT-TDDFT study of hole oscillations in B-DNA monomers and dimers. <i>Cogent Physics</i> , 2017, 4, 1361077.	0.7	16
9284	How do ligands influence the quantum yields of cyclometalated platinum(II) complexes, a theoretical research study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23454-23460.	1.3	5
9285	Multiscale time-dependent density functional theory: Demonstration for plasmons. <i>Journal of Chemical Physics</i> , 2017, 147, 054102.	1.2	1
9286	Quantum Chemical Study on Endohedral Heteronuclear Dimetallofullerene $M_1M_2@C_{80}$ toward Molecular Design. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27700-27708.	1.5	6

#	ARTICLE	IF	CITATIONS
9287	Computational Insight Into the Hydroamination of an Activated Olefin, As Catalyzed by a 1,2,4-Triazole-Derived Nickel(II) N-Heterocyclic Carbene Complex. <i>Inorganic Chemistry</i> , 2017, 56, 14859-14869.	1.9	14
9288	Studies on the Reactivity of the $[W_3S_4Br_3(edpp)_3]^+$ [edpp = (2-aminoethyl)diphenylphosphine] Cluster Cation towards Bases: The Active Role of the Amino Group. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 5006-5014.	1.0	2
9289	Coordination Structure and Fragmentation Chemistry of the Tripositive Lanthanide-Thio-Diglycolamide Complexes. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9429-9434.	1.1	8
9290	Chiral intertwined spirals and magnetic transition dipole moments dictated by cylinder helicity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 13097-13101.	3.3	210
9291	Sub-500 fs electronically nonadiabatic chemical dynamics of energetic molecules from the S1 excited state: <i>Ab initio</i> multiple spawning study. <i>Journal of Chemical Physics</i> , 2017, 147, 204302.	1.2	10
9292	Organocalcium-mediated nucleophilic alkylation of benzene. <i>Science</i> , 2017, 358, 1168-1171.	6.0	180
9293	Structural Variability of 4f and 5f Thiocyanate Complexes and Dissociation of Uranium(III)-Thiocyanate Bonds with Increased Ionicity. <i>Inorganic Chemistry</i> , 2017, 56, 14426-14437.	1.9	16
9294	Improved Electrostatic Embedding for Fragment-Based Chemical Shift Calculations in Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6043-6051.	2.3	32
9295	Spectral properties of ionic benzotriazole based donor-acceptor NLO-phores in polymer matrices and their one- and two-photon cellular imaging ability. <i>Photochemical and Photobiological Sciences</i> , 2017, 16, 1832-1844.	1.6	3
9296	Exploring the Mechanism and Stereoselectivity in Chiral Cinchona-Catalyzed Heterodimerization of Ketenes. <i>Journal of Organic Chemistry</i> , 2017, 82, 13449-13458.	1.7	10
9297	Keto-Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. <i>Journal of the American Chemical Society</i> , 2017, 139, 18328-18338.	6.6	66
9298	Engineering of Solvatomorphs of the Luminescent Complex of <i>ortho</i> -Phenylenediboronic Acid and 8-Hydroxyquinoline. <i>Crystal Growth and Design</i> , 2017, 17, 6836-6851.	1.4	9
9299	Structure and electronic states of a graphene double vacancy with an embedded Si dopant. <i>Journal of Chemical Physics</i> , 2017, 147, 194702.	1.2	9
9300	Computational Exploration of Concerted and Zwitterionic Mechanisms of Diels-Alder Reactions between 1,2,3-Triazines and Enamines and Acceleration by Hydrogen-Bonding Solvents. <i>Journal of the American Chemical Society</i> , 2017, 139, 18213-18221.	6.6	35
9301	Design of a catalyst through Fe doping of the boron cage B10H14 for CO2 hydrogenation and investigation of the catalytic character of iron hydride (Fe-H). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32723-32732.	1.3	1
9302	All-boron fullerene B40: a superatomic structure. <i>Science China Materials</i> , 2017, 60, 1264-1268.	3.5	12
9303	Adsorption Forms of NO on Rh _n ($n = 6-16$) Revealed by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27417-27426.	1.5	21
9304	Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. <i>ACS Nano</i> , 2017, 11, 12402-12410.	7.3	550

#	ARTICLE	IF	CITATIONS
9305	Theoretical design of conjugated diradicaloids as singlet fission sensitizers: quinones and methylene derivatives. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30227-30238.	1.3	29
9308	Performance of tertiary amines as the absorbents for CO ₂ capture: Quantum mechanics and molecular dynamics studies. <i>Journal of Natural Gas Science and Engineering</i> , 2017, 47, 154-166.	2.1	19
9309	Nonconventional Hydrogen Bonds between Silver Anion and Nucleobases: Size-Selected Anion Photoelectron Spectroscopy and Density Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8973-8981.	1.1	10
9310	Chloride Maintains a Protonated Internal Water Network in the Photosynthetic Oxygen Evolving Complex. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10327-10337.	1.2	14
9311	A mesoporous cationic thorium-organic framework that rapidly traps anionic persistent organic pollutants. <i>Nature Communications</i> , 2017, 8, 1354.	5.8	296
9312	Mechanistic Studies of Redox-Switchable Copolymerization of Lactide and Cyclohexene Oxide by a Zirconium Complex. <i>Organometallics</i> , 2017, 36, 4451-4457.	1.1	36
9313	Synthesis, computational, and spectroscopic analysis of tunable highly fluorescent BN-1,2-azaborine derivatives containing the N-BOH moiety. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 10172-10183.	1.5	9
9314	Reactions of Sulfur- and Oxygen-Containing Anions with Hydrogen Atoms: A Comparative Study. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5725-5729.	2.1	3
9315	Charge redistribution in the SpnF-catalyzed Diels-Alder reaction. <i>Mendeleev Communications</i> , 2017, 27, 500-502.	0.6	0
9316	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted \hat{I}^3 -Keggin Polyoxotungstate. <i>ACS Catalysis</i> , 2017, 7, 8514-8523.	5.5	23
9317	Hydration of iron-porphyrins: <i>ab initio</i> quantum mechanical charge field molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30822-30833.	1.3	3
9318	Theoretical study on electron structure and charge transport properties of tetraazapentacene derivatives. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 535-542.	1.3	3
9319	Formation of Aza-ortho-quinone Methides Under Room Temperature Conditions: Cs ₂ CO ₃ Effect. <i>Journal of Organic Chemistry</i> , 2017, 82, 7183-7189.	1.7	25
9320	Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. <i>ACS Catalysis</i> , 2017, 7, 5294-5307.	5.5	38
9321	Tanshinone I and isotanshinone I: The effects of media, isomerization and complexation on structural and electronic parameters. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 276-283.	1.1	1
9322	A Redox-Active Cascade Precursor: Isolation of a Zwitterionic Triphenylphosphonio-Hydrazyl Radical and an Indazolo-Indazole Derivative. <i>Inorganic Chemistry</i> , 2017, 56, 8878-8888.	1.9	7
9323	Ultraviolet Spectroscopy of the Gas Phase Hydration of Methylglyoxal. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 345-352.	1.2	19
9324	Ionization of pyridine: Interplay of orbital relaxation and electron correlation. <i>Journal of Chemical Physics</i> , 2017, 146, 244307.	1.2	24

#	ARTICLE	IF	CITATIONS
9325	Bridged HPSi and Linear HSiP as Probes of the SiP Radical in Astrophysical/Interstellar Media. <i>Astrophysical Journal</i> , 2017, 843, 124.	1.6	4
9326	PyrrylBODIPYs: Syntheses, Properties, and Application as Environment-Sensitive Fluorescence Probes. <i>ACS Omega</i> , 2017, 2, 3551-3561.	1.6	17
9327	Exploring the effect of hydroxylic and non-hydroxylic solvents on the reaction of [VIVO(I^2 -diketonate) $_2$] with 2-aminobenzoylhydrazide in aerobic and anaerobic conditions. <i>Dalton Transactions</i> , 2017, 46, 10963-10985.	1.6	8
9328	Theoretical insights into C-C bond formation through isonitrile insertion into a Cp*Ti complex. <i>RSC Advances</i> , 2017, 7, 34816-34829.	1.7	2
9329	ONIOM(QM:AMOEBA09) Study on Binding Energies and Binding Preference of OH, HCO, and CH $_3$ Radicals on Hexagonal Water Ice (I $_h$). <i>Journal of Physical Chemistry C</i> , 2017, 121, 15223-15232.	1.5	19
9330	Electronic Delocalization in the Radical Cations of Porphyrin Oligomer Molecular Wires. <i>Journal of the American Chemical Society</i> , 2017, 139, 10461-10471.	6.6	67
9331	Hybrid organic-inorganic lead and tin halide perovskites with saturated heterocyclic cations (CH $_2$) $_n$ NH $_2^+$ and (CH $_2$) $_n$ OH $_+$, (n = 2-6): Ab initio study. <i>Computational Materials Science</i> , 2017, 138, 99-104.	1.4	5
9332	Combined Experimental and Computational Study on Ruthenium(II)-Catalyzed Reactions of Dienes with Aldehydes and N-Dimethylformamide. <i>Journal of Organic Chemistry</i> , 2017, 82, 7964-7973.	1.7	8
9333	Theoretical investigations on the methylation of N-H bond using CO $_2$ and hydrosilane catalyzed by Zinc II complexes: Mechanism and ligand effect. <i>Journal of CO$_2$ Utilization</i> , 2017, 20, 178-189.	3.3	11
9334	The interstellar formation and spectra of the noble gas, proton-bound HeHHe $_+$, HeHNe $_+$ and HeHAr $_+$ complexes. <i>Monthly Notices of the Royal Astronomical Society</i> , 2017, 469, 339-346.	1.6	24
9335	Two small molecular propellers and their rotational potential energy surfaces. <i>Structural Chemistry</i> , 2017, 28, 1653-1662.	1.0	3
9336	Insight into substituent effects on the hydrolysis of amidines by a microhydration model. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	2
9337	The [3+2] cycloaddition reaction in CpRu(allyl)(acetylene). <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	0
9338	Understanding the Lewis Acidity of Co(II) Sites on a Silica Surface. <i>Inorganic Chemistry</i> , 2017, 56, 7731-7736.	1.9	13
9339	Versatile Design Strategy for Highly Luminescent Vacuum-Evaporable and Solution-Processable Tridentate Gold(III) Complexes with Monoaryl Auxiliary Ligands and Their Applications for Phosphorescent Organic Light Emitting Devices. <i>Journal of the American Chemical Society</i> , 2017, 139, 9341-9349.	6.6	76
9340	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd II , Mn II , and Zn II -Fe II Promiscuous Organophosphate-Degrading Enzyme: Reaction Mechanisms. <i>Chemistry - A European Journal</i> , 2017, 23, 13742-13753.	1.7	8
9341	Engineering Redox Potential of Lithium Clusters for Electrode Material in Lithium-Ion Batteries. <i>Journal of Cluster Science</i> , 2017, 28, 2779-2793.	1.7	13
9342	Light absorption and photoluminescence due to interfacial charge-transfer transitions in aromatic amine-functionalized silicon nanoparticles. <i>Chemical Physics Letters</i> , 2017, 684, 285-289.	1.2	1

#	ARTICLE	IF	CITATIONS
9343	Anharmonicity of Coupled Torsions: The Extended Two-Dimensional Torsion Method and Its Use To Assess More Approximate Methods. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3478-3492.	2.3	30
9344	Multifunctional Desferrichrome Analogues as Versatile Zr(IV) Chelators for ImmunoPET Probe Development. <i>Molecular Pharmaceutics</i> , 2017, 14, 2831-2842.	2.3	41
9345	Frustrated Lewis Pair Catalyzed C-H Bond Borylation. <i>Organometallics</i> , 2017, 36, 2870-2876.	1.1	18
9346	Electrochemical and structural investigation of the interactions between naphthalene diimides and metal cations. <i>Dalton Transactions</i> , 2017, 46, 9472-9480.	1.6	12
9347	Solvolysis of organophosphorus pesticide parathion with simple and α nucleophiles: a theoretical study. <i>Journal of Chemical Sciences</i> , 2017, 129, 1301-1317.	0.7	7
9348	Assessing the performance of ab initio classical valence bond methods for hydrogen transfer reactions. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 234-241.	1.1	6
9349	Reaction of 1,5-diphenyl-3-arylverdazoles with D ₂ O-acids. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 764-768.	0.3	3
9350	Branched and linear alkoxy chains-wrapped push-pull porphyrins for developing efficient dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2017, 137, 421-429.	2.0	34
9351	Theoretical Insights into the Synthesis of 2,3-dihydropyridines from Unsaturated Oximes by Rh ^{III} -Catalyzed C-H Activation – A DFT Study. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 397-408.	1.2	1
9352	Modulation of π -spacer of carbazole-carbazole based organic dyes toward high efficient dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 174, 7-16.	2.0	26
9353	A Light- and Electricity-Driven Molecular Pushing Motor. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 1308-1317.	1.2	16
9354	Molecular engineering and sequential cosensitization for preventing the "trade-off" effect with photovoltaic enhancement. <i>Chemical Science</i> , 2017, 8, 2115-2124.	3.7	41
9355	Crystal and molecular structures, IR and Raman spectra, vibrational dynamics of aquo 7-methyl-1H-[1,2,3]triazolo[4,5-c]pyridinium nitrate – a new composite material. <i>Journal of Molecular Structure</i> , 2017, 1133, 9-17.	1.8	4
9356	Binding free energies in the SAMPL5 octa-acid host-guest challenge calculated with DFT-D3 and CCSD(T). <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 87-106.	1.3	21
9357	Unveiling the three-center hydrogen bond dynamic behavior in ground and excited states. <i>Journal of Luminescence</i> , 2017, 182, 15-21.	1.5	7
9358	Theoretical and experimental study of a new thiosulfonate derivative: Methyl trifluoromethanethiosulfonate, CF ₃ SO ₂ SCH ₃ . Conformational transferability in CX ₃ SO ₂ S-R compounds. <i>Inorganica Chimica Acta</i> , 2017, 455, 254-261.	1.2	4
9359	³¹ P-Solid-State NMR Characterization and Catalytic Hydrogenation Tests of Novel heterogenized Iridium-Catalysts. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 653-669.	1.4	9
9360	Newly designed manganese and cobalt complexes with pendant amines for the hydrogenation of CO ₂ to methanol: a DFT study. <i>Catalysis Science and Technology</i> , 2017, 7, 348-355.	2.1	22

#	ARTICLE	IF	CITATIONS
9361	Modulation of the structures and properties of bidipyrrin zinc complexes by introducing terminal $\hat{\pm}$ -methoxy groups. <i>Dyes and Pigments</i> , 2017, 137, 430-436.	2.0	10
9362	Mild activation of Ir Cl bond upon the interaction of pincer iridium hydride (BuPCP)IrH(Cl) with acids and bases. <i>Journal of Organometallic Chemistry</i> , 2017, 827, 86-95.	0.8	8
9363	Single and double carbon vacancies in pyrene as first models for graphene defects: A survey of the chemical reactivity toward hydrogen. <i>Chemical Physics</i> , 2017, 482, 346-354.	0.9	9
9364	A new solvatochromic linear $\hat{\text{I}}\text{C}$ -conjugated dye based on phenylene-(poly)ethynylene as supersensitive low-level water detector in organic solvents. <i>Dyes and Pigments</i> , 2017, 136, 873-880.	2.0	34
9365	The IPEA dilemma in CASPT2. <i>Chemical Science</i> , 2017, 8, 1482-1499.	3.7	194
9366	Planar-Chiral Secondary Ferrocenylphosphanes. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 256-262.	1.0	4
9367	Synthesis and characterization of triply-bonded titanium-iron complexes supported by 2-(diphenylphosphino)pyrrolide ligands. <i>Inorganica Chimica Acta</i> , 2017, 460, 43-48.	1.2	10
9368	Synthesis and photovoltaic performance of the porphyrin based sensitizers with 2H-[1,2,3]triazolo[4,5-c]pyridine and benzotriazole as auxiliary acceptors. <i>Dyes and Pigments</i> , 2017, 137, 143-151.	2.0	23
9369	Mechanistic Studies on Gold-Catalyzed Direct Arene C-H Bond Functionalization by Carbene Insertion: The Coinage-Metal Effect. <i>Organometallics</i> , 2017, 36, 172-179.	1.1	52
9370	A computational study of ion speciation in mixtures of protic ionic liquids with various molecular solvents: Insight into the solvent polarity and anion basicity. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 170-179.	1.0	4
9371	Synthesis of first ever 4-quinolone-3-carboxylic acid-appended spirooxindole-pyrrolidine derivatives and their biological applications. <i>Molecular Diversity</i> , 2017, 21, 37-52.	2.1	19
9372	Computational model for the acylation step of the $\hat{2}$ -lactam ring: Potential application for l,d-transpeptidase 2 in mycobacterium tuberculosis. <i>Journal of Molecular Structure</i> , 2017, 1128, 94-102.	1.8	41
9373	Cu(I) complexes of bis(methyl)(thia/selena) salen ligands: Synthesis, characterization, redox behavior and DNA binding studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 18-24.	2.0	30
9374	Synthesis, structural, spectroscopic, computational and cytotoxic studies of BODIPY dyes. <i>Sensors and Actuators B: Chemical</i> , 2017, 238, 548-555.	4.0	24
9375	Citral stabilization and characterization of nanoemulsions stabilized by a mixture of gelatin and Tween 20 in an acidic system. <i>Journal of the Science of Food and Agriculture</i> , 2017, 97, 2991-2998.	1.7	25
9376	Computational Design of a Pincer Phosphinito Vanadium ((OPO)V) Propane Monooxygenation Homogeneous Catalyst Based on the Reduction-Coupled Oxo Activation (ROA) Mechanism. <i>ACS Catalysis</i> , 2017, 7, 356-364.	5.5	10
9377	Theory-Driven Insight into the Crystal Packing of Trialkylsilylethynyl Pentacenes. <i>Chemistry of Materials</i> , 2017, 29, 2502-2512.	3.2	30
9378	Sc ₂ O@C ₇₈ : Calculations of the yield ratio for two observed isomers. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2017, 25, 124-127.	1.0	10

#	ARTICLE	IF	CITATIONS
9379	Changing the Emission Properties of Phosphorescent C ² C ¹ -Cyclometalated Thiazolâ€¦ylidene Platinum(II) Complexes by Variation of the Î²â€¦diketonate Ligands. Chemistry - A European Journal, 2017, 23, 1118-1128.	1.7	27
9380	Modulating hydrogen-bond basicity within the context of protein-ligand binding: A case study with thrombin inhibitors thatÂreveals a dominating role for desolvation. European Journal of Medicinal Chemistry, 2017, 125, 975-991.	2.6	6
9381	Analysis of Cathodic Reaction Process of SiCl ₄ during Si Electrodeposition in Ionic Liquids. Journal of the Electrochemical Society, 2017, 164, D994-D998.	1.3	11
9382	A new structural arrangement in proteins involving lysine NH ₃ ⁺ group and carbonyl. Scientific Reports, 2017, 7, 16402.	1.6	10
9383	Synthesis, X-ray analysis, and quantum-chemical DFT study of features in formation of a binuclear phenanthroline complex with a VIVâ€¦Oâ€¦VV core. Russian Journal of General Chemistry, 2017, 87, 2612-2619.	0.3	4
9384	Testing a simple approach for theoretical evaluation of radiolysis products in extraction systems. A case of AN,O-donor ligands for Am/Eu separation. RSC Advances, 2017, 7, 55441-55449.	1.7	14
9385	Propagator quantum chemical study of S-cis-(Z)-2-(2-formylethenyl)pyrrole: electronic structure and aspects of intramolecular hydrogen bond manifestation in ionization spectra. Russian Chemical Bulletin, 2017, 66, 2241-2247.	0.4	0
9386	Accurate and balanced anisotropic Gaussian type orbital basis sets for atoms in strong magnetic fields. Journal of Chemical Physics, 2017, 147, 244108.	1.2	9
9387	Surface-modified TiO ₂ powders with phenol derivatives: A comparative DFT and experimental study. Chemical Physics Letters, 2017, 686, 167-172.	1.2	29
9388	Experimental and theoretical study of bifunctionalized PEOâ€¦PPOâ€¦PEO triblock copolymers with applications as dehydrating agents for heavy crude oil. Arabian Journal of Chemistry, 2017, 10, 410-419.	2.3	12
9389	Reaction Mechanisms of CO ₂ Reduction to Formaldehyde Catalyzed by Hourglass Ru, Fe, and Os Complexes: A Density Functional Theory Study. Catalysts, 2017, 7, 5.	1.6	17
9390	BET & ELF Quantum Topological Analysis of Neutral 2-Aza-Cope Rearrangement of Î³ ³ -Alkenyl Nitrones. Molecules, 2017, 22, 1371.	1.7	4
9391	Biodegradation of Cosmetics Products: A Computational Study of Cytochrome P450 Metabolism of Phthalates. Inorganics, 2017, 5, 77.	1.2	16
9392	Extending the Characteristic Polynomial for Characterization of C ₂₀ Fullerene Congeners. Mathematics, 2017, 5, 84.	1.1	22
9393	Photoreactions of Endohedral Metallofullerene with Siliranes: Electronic Properties of Carbosilylated Lu ₃ N@Ih-C ₈₀ . Molecules, 2017, 22, 850.	1.7	3
9394	Theoretical Confirmation of the Quinone Methide Hypothesis for the Condensation Reactions in Phenol-Formaldehyde Resin Synthesis. Polymers, 2017, 9, 45.	2.0	11
9395	New Mechanism Proposed for the Base-Catalyzed Ureaâ€¦Formaldehyde Condensation Reactions: A Theoretical Study. Polymers, 2017, 9, 203.	2.0	13
9396	Mechanism of Base-Catalyzed Resorcinol-Formaldehyde and Phenol-Resorcinol-Formaldehyde Condensation Reactions: A Theoretical Study. Polymers, 2017, 9, 426.	2.0	36

#	ARTICLE	IF	CITATIONS
9397	Quantitative Structure-Thermostability Relationship of Late Transition Metal Catalysts in Ethylene Oligo/Polymerization. <i>Catalysts</i> , 2017, 7, 120.	1.6	10
9398	Binuclear Copper(I) Borohydride Complex Containing Bridging Bis(diphenylphosphino) Methane Ligands: Polymorphic Structures of $[(\mu_2\text{-dppm})_2\text{Cu}_2(\text{I-2-BH}_4)_2]$ Dichloromethane Solvate. <i>Crystals</i> , 2017, 7, 318.	1.0	13
9399	Switching Activity of Allosteric Modulators Controlled by a Cluster of Residues Forming a Pressure Point in the mGluR5 GPCR. <i>Advances in Quantum Chemistry</i> , 2017, 75, 147-174.	0.4	0
9400	Five Regioisomers of Dimethyl Dodecahedrane Derivatives: A Hybrid DFT B3LYP Study. <i>Journal of Chemistry</i> , 2017, 2017, 1-7.	0.9	1
9401	Quantum Chemical Investigation on the Antioxidant Activity of Neutral and Anionic Forms of Juglone: Metal Chelation and Its Effect on Radical Scavenging Activity. <i>Journal of Chemistry</i> , 2017, 2017, 1-14.	0.9	4
9402	Synthesis, Crystal Structure, DFT Study of <i>m</i> -Methoxy- <i>N</i> -(3-Methoxybenzoyl)- <i>N</i> -Phenylbenzohydrazide. <i>Crystals</i> , 2017, 7, 19.	1.0	5
9403	Explicitly Correlated Orbital Optimized Contracted Pair Correlation Methods: A Short Overview. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4707-4711.	1.1	2
9404	Halogen-containing thiazole orange analogues – new fluorogenic DNA stains. <i>Beilstein Journal of Organic Chemistry</i> , 2017, 13, 2902-2914.	1.3	18
9405	(OC-6-35-A)-Aquadicarbonylchlorido[2-(2-pyridyl)-1,8-naphthyridine- κ^2 ;2N1,N2]ruthenium(II) hexafluoridophosphate 2,2'-Bipyridine. <i>MolBank</i> , 2017, 2017, M950.	0.2	1
9406	Symmetry breaking and spectral considerations of the surprisingly floppy $\langle i \rangle \langle /i \rangle$ -C ₃ H radical and the related dipole-bound excited state of $\langle i \rangle \langle /i \rangle$ -C ₃ H ⁺ . <i>Journal of Chemical Physics</i> , 2017, 146, 224303.	1.2	22
9407	Targeting ideal acceptor-donor materials based on hexabenzocoronene. <i>Journal of Molecular Structure</i> , 2018, 1161, 442-452.	1.8	5
9408	Fabrication of a magnetite/diazonium functionalized-reduced graphene oxide hybrid as an easily regenerated adsorbent for efficient removal of chlorophenols from aqueous solution. <i>RSC Advances</i> , 2018, 8, 7351-7360.	1.7	11
9409	NMR spin-spin coupling constants in hydrogen-bonded glycine clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25608.	1.0	4
9410	A molecular modeling study of combretastatin-like chalcones as anticancer agents using PLS, ANN and consensus models. <i>Structural Chemistry</i> , 2018, 29, 957-965.	1.0	5
9411	Crystal structures and DFT calculations of mixed chloride-azide zinc(II) and chloride-isocyanate cadmium(II) complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent. <i>Journal of Molecular Structure</i> , 2018, 1162, 63-70.	1.8	8
9412	Calculated relative populations of Sm@C ₈₂ isomers. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2018, 26, 233-238.	1.0	13
9413	Adsorption and dissociation of carbon monoxide on iron and iron-carbon clusters: Fe _n +2CO and Fe _n Ca+2CO, n=4 and 7. A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1129, 37-47.	1.1	16
9414	Mechanistic insights into the different chemoselectivities of Rh ₂ ($\langle scpi \rangle$)-catalyzed ring expansion of cyclobutanol-substituted aryl azides and C-H bond amination of cyclopentanol-substituted aryl azides: a DFT study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1471-1482.	2.3	14

#	ARTICLE	IF	CITATIONS
9415	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold–Thiolate Linkers Innocent?. <i>Journal of the American Chemical Society</i> , 2018, 140, 4354-4362.	6.6	66
9416	Computer-Aided Drug Discovery: Molecular Docking of Diminazene Ligands to DNA Minor Groove. <i>Journal of Chemical Education</i> , 2018, 95, 882-887.	1.1	16
9417	Methanol-Assisted Phthalimide Ring Opening: Concerted or Stepwise Mechanism?. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3115-3119.	1.1	4
9418	Disilarylthene- and Ferracyclic Complexes Containing Isocyanide Ligands as Effective Catalysts for Hydrogenation of Unfunctionalized Sterically Hindered Alkenes. <i>Journal of the American Chemical Society</i> , 2018, 140, 4119-4134.	6.6	38
9419	Porphyrin sensitizers with modified indoline donors for dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2018, 6, 3927-3936.	2.7	48
9420	Simple electron donor molecules based on triphenylamine and carbazole derivatives. <i>Dyes and Pigments</i> , 2018, 153, 275-283.	2.0	23
9421	The characterization of the VN H defects in diamond through the infrared vibrational spectrum. A quantum mechanical investigation. <i>Carbon</i> , 2018, 132, 210-219.	5.4	20
9422	Integrative mass spectrometry strategy for fingerprinting and tentative structural characterization of asphaltenes. <i>Fuel</i> , 2018, 220, 717-724.	3.4	10
9423	Synthesis, Characterization, and Reactivity of a <i>High-Spin</i> Iron(II) Hydrido Complex Supported by a PNP Pincer Ligand and Its Application as a Homogenous Catalyst for the Hydrogenation of Alkenes. <i>Inorganic Chemistry</i> , 2018, 57, 3183-3191.	1.9	35
9424	Structure and Energetics of (111) Surface of Al_2O_3 : Insights from DFT Including Periodic Boundary Approach. <i>ACS Omega</i> , 2018, 3, 1881-1888.	1.6	34
9425	Positional Effects from f -Bonded Platinum(II) on Intersystem Crossing Rates in Perylenediimide Complexes: Synthesis, Structures, and Photophysical Properties. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13848-13862.	1.5	18
9426	Influence of Lewis acid strength on hydride transfer to unsaturated substrates. <i>Dalton Transactions</i> , 2018, 47, 3985-3991.	1.6	12
9427	Automated error control in divide-and-conquer self-consistent field calculations. <i>Journal of Computational Chemistry</i> , 2018, 39, 909-916.	1.5	11
9428	Sterically Induced Ligand Framework Distortion Effects on Catalytic Cyclic Ester Polymerizations. <i>Inorganic Chemistry</i> , 2018, 57, 3451-3457.	1.9	20
9429	Hydrogel-Embedded Model Photocatalytic System Investigated by Raman and IR Spectroscopy Assisted by Density Functional Theory Calculations and Two-Dimensional Correlation Analysis. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2677-2687.	1.1	7
9430	The quest for determining one-electron redox potentials of azulene-1-carbonitriles by calculation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7438-7446.	1.3	12
9431	A Conducting Poly(N-(1-Naphthyl)ethylenediamine dihydrochloride) Nanofibers for the Sensitive and Interference-Free Detection of Dopamine. <i>Journal of the Electrochemical Society</i> , 2018, 165, B89-B95.	1.3	14
9432	Computed thermodynamic stabilities of silylium Lewis base adducts. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2318-2323.	1.5	5

#	ARTICLE	IF	CITATIONS
9433	Theoretical study on the mechanism and enantioselectivity of NHC-catalyzed intramolecular S _N 2 nucleophilic substitution: what are the roles of NHC and DBU?. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1493-1501.	2.3	26
9434	Assessment of Fragmentation Strategies for Large Proteins Using the Multilayer Molecules-in-Molecules Approach. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1383-1394.	2.3	29
9435	NMR, Raman, and DFT Study of Lyotropic Chromonic Liquid Crystals of Biomedical Interest: Tautomeric Equilibrium and Slow Self-Assembling in Sunset Yellow Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3047-3055.	1.2	11
9436	Effect of surface vacancies on the adsorption of Pd and Pb on MgO(100). <i>Monatshefte für Chemie</i> , 2018, 149, 1009-1015.	0.9	0
9437	Uniform two-dimensional square assemblies from conjugated block copolymers driven by π - π interactions with controllable sizes. <i>Nature Communications</i> , 2018, 9, 865.	5.8	103
9438	Unraveling the effects of amino acid substitutions enhancing lipase resistance to an ionic liquid: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9600-9609.	1.3	22
9439	Multi-State VALBOND for Atomistic Simulations of π -conjugated Molecules, Metal Complexes, and Reactions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3565-3578.	2.3	9
9440	Conformational study of C ₂₄ cyclic polyene clusters. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25614.	1.0	15
9441	Projection-Based Correlated Wave Function in Density Functional Theory Embedding for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1928-1942.	2.3	70
9442	The missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 128-135.	0.8	4
9443	Ultrafast Dynamics of the Metal-to-Ligand Charge Transfer Excited States of Ir(III) Proteo and Deutero Dihydrides. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4430-4436.	1.1	7
9444	Anticorrelated Contributions to Pre-edge Features of Aluminate Near-Edge X-ray Absorption Spectroscopy in Concentrated Electrolytes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2444-2449.	2.1	9
9445	Ultrafast photochemistry of free-base porphyrin: a theoretical investigation of B ₁₀ Q internal conversion mediated by dark states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12483-12492.	1.3	14
9446	Solution and Solid-State Ligand K-Edge XAS Studies of PdCl ₂ Diphosphine Complexes with Phenyl and Cyclohexyl Substituents. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 2267-2276.	1.0	9
9447	Simplified DFT methods for consistent structures and energies of large systems. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 213001.	0.7	42
9448	Guanidine: A Highly Efficient Stabilizer in Atmospheric New-Particle Formation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4717-4729.	1.1	32
9449	Unique Proton Transportation Pathway in a Robust Inorganic Coordination Polymer Leading to Intrinsically High and Sustainable Anhydrous Proton Conductivity. <i>Journal of the American Chemical Society</i> , 2018, 140, 6146-6155.	6.6	181
9450	Joint refinement model for the spin resolved one-electron reduced density matrix of YTiO ₃ using magnetic structure factors and magnetic Compton profiles data. <i>Journal of Chemical Physics</i> , 2018, 148, 164106.	1.2	7

#	ARTICLE	IF	CITATIONS
9451	Conformationally-restricted bicarbazoles with phenylene bridges displaying deep-blue emission and high triplet energies: systematic structure–property relationships. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11867-11875.	1.3	10
9452	Relationship between x-ray emission and absorption spectroscopy and the local H-bond environment in water. <i>Journal of Chemical Physics</i> , 2018, 148, 144507.	1.2	37
9453	Photophysical features of naphthols having esters, formyl and acetyl groups and the difluoroboronated complex in solution and the solid state. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 360, 204-209.	2.0	5
9454	A Mononuclear Tungsten Photocatalyst for H ₂ Production. <i>ACS Catalysis</i> , 2018, 8, 4838-4847.	5.5	21
9455	Flexible proton-responsive ligand-based Mn(<i>scp</i>) complexes for CO ₂ hydrogenation: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12535-12542.	1.3	11
9456	Synthesis and Structural Characterization of Non-Homoleptic Carbamate Complexes of W ^V and W ^{VI} and Their Facile Implantation onto Silica Surfaces. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1176-1184.	1.0	6
9457	Thermodynamic compatibility between cyclodextrin supramolecular complexes and surfactant. <i>International Journal of Pharmaceutics</i> , 2018, 544, 203-212.	2.6	4
9458	Molecular Engineering of Quinoxaline-Based D–A Organic Sensitizers: Taking the Merits of a Large and Rigid Auxiliary Acceptor. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 13635-13644.	4.0	45
9459	Cyclopropenylgold(I) Complexes as Aurated Carbenoids or Quasi-Carbenes. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 1810-1821.	2.1	29
9460	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2570-2585.	2.3	16
9461	Vibrational spectroscopy of hydrogens in diamond: a quantum mechanical treatment. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11930-11940.	1.3	17
9462	Diaryl-1,2,3-Triazolylidene Platinum(II) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 5584-5590.	1.7	40
9463	Development of paper-based chemosensor for the detection of mercury ions using mono- and tetra-sulfur bearing phenanthridines. <i>New Journal of Chemistry</i> , 2018, 42, 8530-8536.	1.4	25
9464	<i>N</i> -Aryl Imidazole Platforms – Synthesis and Structural Investigation. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 2193-2203.	1.2	2
9465	Solution and solid-state characterization of Zn(II) complexes containing a new tridentate N ₂ S ligand. <i>Polyhedron</i> , 2018, 147, 131-141.	1.0	1
9466	Mechanistic insights into Pd(0)-catalyzed intermolecular and intramolecular hydroamination of methylenecyclopropanes: a computational study. <i>Dalton Transactions</i> , 2018, 47, 5660-5669.	1.6	9
9467	Computational Insights into the Gold-Catalyzed Ring-Opening of Methylenecyclopropanes and Vinylcyclopropanes with Sulfonamides. <i>ChemCatChem</i> , 2018, 10, 2817-2825.	1.8	19
9468	Unusual Photooxidation of S-Bonded Mercaptopyridine in a Mixed Ligand Ruthenium(II) Complex with Terpyridine and Bipyridine Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 4898-4905.	1.9	14

#	ARTICLE	IF	CITATIONS
9469	Immobilization of dextranucrase on functionalized TiO ₂ supports. <i>International Journal of Biological Macromolecules</i> , 2018, 114, 1216-1223.	3.6	18
9470	Synthesis of 3,5-Disubstituted BODIPYs Bearing <i>N</i> -Containing Five-Membered Heteroaryl Groups via Nucleophilic C–N Bond Formation. <i>Journal of Organic Chemistry</i> , 2018, 83, 5274-5281.	1.7	11
9471	Reactivity of a Silica-Supported Mo Alkylidene Catalyst toward Alkanes: A DFT Study on the Metathesis of Propane. <i>Organometallics</i> , 2018, 37, 2023-2036.	1.1	9
9472	Theoretical Studies on the Catalytic Mechanism and Substrate Diversity for Macrocyclization of Pikromycin Thioesterase. <i>ACS Catalysis</i> , 2018, 8, 4323-4332.	5.5	42
9473	Cobalt–Carbon Bond Formation Reaction via Ligand Reduction of Porphycene–Cobalt(II) Complex and Its Noninnocent Reactivity. <i>ACS Omega</i> , 2018, 3, 4027-4034.	1.6	17
9474	A transition state “trapped” QM-cluster models of engineered threonyl-tRNA synthetase. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 4090-4100.	1.5	6
9475	Two-body Schrödinger wave functions in a plane-wave basis via separation of dimensions. <i>Journal of Chemical Physics</i> , 2018, 148, 104101.	1.2	10
9476	The Alexandria library, a quantum-chemical database of molecular properties for force field development. <i>Scientific Data</i> , 2018, 5, 180062.	2.4	45
9477	Is the choice of a standard zeroth-order hamiltonian in CASPT2 ansatz optimal in calculations of excitation energies in protonated and unprotonated schiff bases of retinal?. <i>Journal of Computational Chemistry</i> , 2018, 39, 1470-1480.	1.5	3
9478	Unveiling the mechanism of the promising two-dimensional photoswitch “Hemithioindigo. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 200, 1-9.	2.0	3
9479	Comprehensive Mechanistic Insight into Cooperative Lewis Acid/Cp*CoIII-Catalyzed C–H/N–H Activation for the Synthesis of Isoquinolin-3-ones. <i>Inorganic Chemistry</i> , 2018, 57, 2804-2814.	1.9	26
9480	Enriched optimization of molecular properties under constraints: an electrochromic example. <i>Molecular Systems Design and Engineering</i> , 2018, 3, 485-495.	1.7	4
9481	Structural Characterization of a Fluorido–Amide of Niobium, and Facile CO ₂ Incorporation Affording a Fluorido–Carbamate. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 999-1006.	1.0	4
9482	Rapid Convergence of Energy and Free Energy Profiles with Quantum Mechanical Size in Quantum Mechanical–Molecular Mechanical Simulations of Proton Transfer in DNA. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1695-1705.	2.3	34
9483	Synthesis and characterization of thallium–salen derivatives for use as underground fluid flow tracers. <i>Dalton Transactions</i> , 2018, 47, 4162-4174.	1.6	9
9484	Subphthalocyanine-radiannulene scaffold “a multi-electron acceptor and strong chromophore. <i>Chemical Communications</i> , 2018, 54, 2763-2766.	2.2	6
9485	A multidisciplinary study of 3-(β -D-glucopyranosyl)-5-substituted-1,2,4-triazole derivatives as glycogen phosphorylase inhibitors: Computation, synthesis, crystallography and kinetics reveal new potent inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2018, 147, 266-278.	2.6	22
9486	Synthesis, structure and catalytic activities of nickel(II) complexes bearing N ₄ tetradentate Schiff base ligand. <i>Journal of Molecular Structure</i> , 2018, 1160, 9-19.	1.8	14

#	ARTICLE	IF	CITATIONS
9487	Effect on absorption and electron transfer by using Cd(ii) or Cu(ii) complexes with phenanthroline as auxiliary electron acceptors (A) in Dâ€“Aâ€“Iâ€“A motif sensitizers for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6688-6697.	1.3	4
9488	A Luminescent Manganese PhotoCORM for CO Delivery to Cellular Targets under the Control of Visible Light. <i>Inorganic Chemistry</i> , 2018, 57, 1766-1773.	1.9	58
9489	Structure and vibrational spectroscopic study of phthalimido-functionalized N-heterocyclic palladium complexes. Correlations between structure and catalytic activity. <i>Journal of Organometallic Chemistry</i> , 2018, 869, 233-250.	0.8	2
9490	Ancistrocyclinones A and B, unprecedented pentacyclic <i>N</i>,<i>C</i>-coupled naphthylisoquinoline alkaloids, from the Chinese liana <i>Ancistrocladus tectorius</i>. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 1581-1590.	1.5	10
9491	Mechanistic insight into the ruthenium-catalyzed cycloaddition of diynes with 2,3-diphenyl-2H-azirines: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1127, 16-21.	1.1	5
9492	Substituent Effects at the $\hat{2}$ -Positions of the Nonfused Pyrroles in a Quadruply Fused Porphyrin on the Structure and Optical and Electrochemical Properties. <i>Inorganic Chemistry</i> , 2018, 57, 1106-1115.	1.9	11
9493	Rhodium(III) and Iridium(III) Bipyridine Complexes: Syntheses, Structures, and Properties. <i>Inorganic Chemistry</i> , 2018, 57, 1840-1845.	1.9	3
9494	A magnetic controllable tool for the selective enrichment of dimethoate from olive oil samples: A responsive molecular imprinting-based approach. <i>Food Chemistry</i> , 2018, 254, 309-316.	4.2	21
9495	Origin of $\hat{2}$ -agostic interaction in d0 transition metal alkyl complexes: Influence of ligands. <i>Journal of Organometallic Chemistry</i> , 2018, 865, 37-44.	0.8	7
9496	Computation of Molecular Spectra on a Quantum Processor with an Error-Resilient Algorithm. <i>Physical Review X</i> , 2018, 8, .	2.8	281
9497	Polarizable Density Embedding Coupled Cluster Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1351-1360.	2.3	20
9498	Explicit Solvation Matters: Performance of QM/MM Solvation Models in Nucleophilic Addition. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1841-1852.	2.3	40
9499	Infrared Spectroscopic Study of Vibrational Modes across the Orthorhombicâ€“Tetragonal Phase Transition in Methylammonium Lead Halide Single Crystals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5227-5237.	1.5	61
9500	Chemical Understanding of the Limited Site-Specificity in Molecular Inner-Shell Photofragmentation. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1156-1163.	2.1	31
9501	UV-induced long-lived decays in solvated pyrimidine nucleosides resolved at the MS-CASPT2/MM level. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6877-6890.	1.3	46
9502	Toward a muon-specific electronic structure theory: effective electronic Hartreeâ€“Fock equations for muonic molecules. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4466-4477.	1.3	3
9503	On the regioselectivity of the Dielsâ€“Alder cycloaddition to C₆₀ in high spin states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11577-11585.	1.3	10
9504	Quantum chemical studies of redox properties and conformational changes of a four-center iron CO₂ reduction electrocatalyst. <i>Chemical Science</i> , 2018, 9, 2645-2654.	3.7	6

#	ARTICLE	IF	CITATIONS
9505	Hydrolytic Stability of Boronate Ester-Linked Covalent Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2018, 1, 1700015.	1.3	57
9506	Comparison of Interfacial Electron Transfer Efficiency in [Fe(CTP) ₂] ²⁺ -TiO ₂ and [Fe(CNC) ₂] ²⁺ -TiO ₂ Assemblies: Importance of Conformational Sampling. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1821-1830.	1.1	9
9507	Boron-Doped C ₂₄ Fullerenes for Alkyl Functionalization or Potential Polymerization. <i>ACS Omega</i> , 2018, 3, 1001-1006.	1.6	4
9508	Au-Catalyzed Hexannulation and Pt-Catalyzed Pentannulation of Propargylic Ester Bearing a 2-Alkynyl-phenyl Substituent: A Comparative DFT Study. <i>ACS Omega</i> , 2018, 3, 1159-1169.	1.6	9
9509	Asymmetric triphenylamine-phenothiazine based small molecules with varying terminal acceptors for solution processed bulk-heterojunction organic solar cells. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6390-6400.	1.3	16
9510	Reactivity of amino acid anions with nitrogen and oxygen atoms. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4990-4996.	1.3	10
9511	Zn(II) Byproduct Enhances the Cu-Catalyzed Cross-Coupling of Bromozinc Difluorophosphonate with Iodobenzoates: A DFT Study. <i>Organometallics</i> , 2018, 37, 327-336.	1.1	8
9512	A novel pyrene based highly selective reversible fluorescent-colorimetric sensor for the rapid detection of Cu ²⁺ ions: application in bio-imaging. <i>Analytical Methods</i> , 2018, 10, 1063-1073.	1.3	35
9513	Reconsideration of the Detection and Fluorescence Mechanism of a Pyrene-Based Chemosensor for TNT. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1400-1405.	1.1	32
9514	Molecular electrostatic potential on the proton-donating atom as a theoretical descriptor of excited state acidity. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4351-4359.	1.3	10
9515	Computational elucidation of the reaction mechanism for synthesis of pyrrolidinedione derivatives via Nef-type rearrangement cyclization reaction. <i>RSC Advances</i> , 2018, 8, 3178-3188.	1.7	4
9516	Enantioselective Synthesis of Aminodiols by Sequential Rhodium-Catalysed Oxyamination/Kinetic Resolution: Expanding the Substrate Scope of Amidine-Based Catalysis. <i>Chemistry - A European Journal</i> , 2018, 24, 4635-4642.	1.7	15
9517	Small Alcohols Revisited: CCSD(T) Relative Potential Energies for the Minima, First- and Second-Order Saddle Points, and Torsion-Coupled Surfaces. <i>ACS Omega</i> , 2018, 3, 419-432.	1.6	13
9518	Protective effects of new antioxidant compositions of 4-methylcoumarins and related compounds with dl-α-tocopherol and l-ascorbic acid. <i>Journal of the Science of Food and Agriculture</i> , 2018, 98, 3784-3794.	1.7	8
9519	Chiro-magnetic nanoparticles and gels. <i>Science</i> , 2018, 359, 309-314.	6.0	201
9520	A numerical and experimental study of the decomposition pathways of guanidinium nitrate. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 131, 427-441.	2.0	7
9521	The Nature of the Heavy Alkaline Earth Metal-Hydrogen Bond: Synthesis, Structure, and Reactivity of a Cationic Strontium Hydride Cluster. <i>Journal of the American Chemical Society</i> , 2018, 140, 3403-3411.	6.6	58
9522	Dianionic Carbon-Bridged Scandium-Copper/Silver Heterobimetallic Complexes: Synthesis, Bonding, and Reactivity. <i>Chemistry - A European Journal</i> , 2018, 24, 5637-5643.	1.7	13

#	ARTICLE	IF	CITATIONS
9523	Experimental and theoretical studies of structural and photophysical properties of a novel heteroleptic cyclometalated iridium(III) complex with 8-hydroxyquinoline-phenylazo ligand. <i>Journal of Molecular Structure</i> , 2018, 1158, 122-132.	1.8	6
9524	Role of Solvent Polarity and Hydrogen-Bonding on Excited-State Fluorescence of 3-[(E)-{4-[Dimethylamino]benzylidene}amino]-2-naphthoic Acid (DMAMN): Isomerization vs Rotomerization. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1838-1854.	1.1	6
9525	Steric and Acidity Control in Hydrogen Bonding and Proton Transfer to <i>trans</i> -W(N ₂) ₂ (dppe) ₂ . <i>Inorganic Chemistry</i> , 2018, 57, 1656-1664.	1.9	7
9526	Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2018, 148, 034105.	1.2	23
9527	A combined experimental and computational study on the reaction of fluoroarenes with Mg ⁺ Mg, Mg ⁺ Zn, Mg ⁺ Al and Al ⁺ Zn bonds. <i>Chemical Science</i> , 2018, 9, 2348-2356.	3.7	86
9528	Prediction of lower flammability limits of blended gases based on quantitative structure–property relationship. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 132, 1125-1130.	2.0	17
9529	Closed-Shell Organic Compounds Might Form Dimers at the Surface of Molecular Clusters. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1771-1780.	1.1	16
9530	Assessing ionicity of protic ionic liquids by far IR spectroscopy. <i>Journal of Molecular Liquids</i> , 2018, 252, 180-183.	2.3	11
9531	Accurate density functional theory (DFT) protocol for screening and designing chain transfer and branching agents for LDPE systems. <i>Molecular Systems Design and Engineering</i> , 2018, 3, 228-242.	1.7	4
9532	Combined QM/MM and Monte Carlo study for redox leveling in Mn and Fe superoxide dismutase. <i>Journal of Biological Inorganic Chemistry</i> , 2018, 23, 285-293.	1.1	3
9533	A 3D visualization of the substituent effect. <i>Journal of Molecular Modeling</i> , 2018, 24, 31.	0.8	6
9534	Comparative analysis of fluorene and carbazole fused triphenylamine sensitizer donor units with new anchoring mode in dye-sensitized solar cells. <i>Reactive and Functional Polymers</i> , 2018, 122, 123-130.	2.0	5
9535	The influence of the double-ring nanotubules diameter of Bn (n = 14, 20, 24 and 32) on the electronic and structural properties due to lithium atom doping: quantum chemistry approach. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	0
9536	Molecular modeling for the investigation of UV absorbers for sunscreens: Triazine and benzotriazole derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 356, 219-229.	2.0	22
9537	TGA, Hirshfeld, Raman spectroscopy and computational studies of diethylammonium hexachloroplumbate [(C ₂ H ₅) ₂ NH ₂] ₂ PbCl ₆ . <i>Journal of Molecular Structure</i> , 2018, 1157, 621-630.	1.8	5
9538	Patterns of cation binding to the aromatic amino acid R groups in Trp, Tyr, and Phe. <i>Computational Biology and Chemistry</i> , 2018, 72, 11-15.	1.1	4
9539	New electron delocalization tools to describe the aromaticity in porphyrinoids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2787-2796.	1.3	86
9540	Experimental and DFT evaluation of the ¹ H and ¹³ C NMR chemical shifts for calix[4]arenes. <i>Journal of Molecular Structure</i> , 2018, 1157, 97-105.	1.8	9

#	ARTICLE	IF	CITATIONS
9541	Probing the effect of different graphitic nitrogen sites on the aerobic oxidation of thiols to disulfides: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2057-2065.	1.3	2
9542	Rational Density Functional Selection Using Game Theory. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 61-67.	2.5	20
9543	Well-Defined Heterobimetallic Reactivity at Unsupported Ruthenium-Indium Bonds. <i>Chemistry - A European Journal</i> , 2018, 24, 1732-1738.	1.7	16
9544	Cationic λ^5 -C ₅ Me ₄ Rh ^{III} Complexes with Metalated Aryl Phosphines Featuring λ^4 -Phosphorus plus Pseudo-Allylic Coordination. <i>Organometallics</i> , 2018, 37, 11-21.	1.1	10
9545	High-Mobility Self-Assembling Truxenone-Based n-Type Organic Semiconductors. <i>Chemistry - A European Journal</i> , 2018, 24, 3576-3583.	1.7	22
9546	Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case. <i>Journal of Physical Chemistry A</i> , 2018, 122, 375-382.	1.1	12
9547	Preparation of multiblock copolymers <i>via</i> step-wise addition of <i>l</i> -lactide and trimethylene carbonate. <i>Chemical Science</i> , 2018, 9, 2168-2178.	3.7	28
9548	Synthesis, biological evaluation, substitution behaviour and DFT study of Pd(ii) complexes incorporating benzimidazole derivative. <i>New Journal of Chemistry</i> , 2018, 42, 2574-2589.	1.4	32
9549	A C=O... π ...Isothiouonium Interaction Dictates Enantiodiscrimination in Acylative Kinetic Resolutions of Tertiary Heterocyclic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3200-3206.	7.2	102
9550	A C=O... π ...Isothiouonium Interaction Dictates Enantiodiscrimination in Acylative Kinetic Resolutions of Tertiary Heterocyclic Alcohols. <i>Angewandte Chemie</i> , 2018, 130, 3254-3260.	1.6	43
9551	Consensus Conformations of Dinucleoside Monophosphates Described with Well-Converged Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1456-1470.	2.3	21
9552	Density Functional Theory Study on the Demethylation Reaction between Methylamine, Dimethylamine, Trimethylamine, and Tamoxifen Catalyzed by a Fe(IV)=Oxo Porphyrin Complex. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1658-1671.	1.1	8
9553	ESI-MS, UV-Vis, and Theoretical Investigation of Fe ³⁺ -Amoxicillin Complexation during Coagulation. <i>Journal of Environmental Engineering, ASCE</i> , 2018, 144, .	0.7	5
9554	Binuclear Metal Phthalocyanines Catalysis for Li/SOCl ₂ Batteries: An Experimental and Computational Study. <i>Energy Technology</i> , 2018, 6, 1342-1351.	1.8	5
9555	Highly Sensitive Detection of UV Radiation Using a Uranium Coordination Polymer. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 4844-4850.	4.0	52
9556	Ultrasensitive and specific fluorescence detection of a cancer biomarker <i>via</i> nanomolar binding to a guanidinium-modified calixarene. <i>Chemical Science</i> , 2018, 9, 2087-2091.	3.7	113
9557	Dynamic exit-channel pathways of the microsolvated HOO [•] (H ₂ O) + CH ₃ Cl S _N 2 reaction: Reaction mechanisms at the atomic level from direct chemical dynamics simulations. <i>Journal of Chemical Physics</i> , 2018, 148, 014302.	1.2	5
9558	Supramolecular Organization of Solid Azobenzene Chromophore Disperse Orange 3, Its Chloroform Solutions, and PMMA-Based Films. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1779-1785.	1.5	13

#	ARTICLE	IF	CITATIONS
9559	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1392-1399.	1.1	101
9560	Gas-phase spectra of MgO molecules: a possible connection from gas-phase molecules to planet formation. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 474, 2055-2063.	1.6	16
9561	Absolute and relative facial selectivities in organocatalytic asymmetric chlorocyclization reactions. <i>Chemical Science</i> , 2018, 9, 2898-2908.	3.7	22
9562	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 33.	0.8	6
9563	Molecular level investigation of the role of peptide interactions in the glyphosate analytics. <i>Chemosphere</i> , 2018, 196, 129-134.	4.2	15
9564	Degradation of Glyphosate by Mn-Oxide May Bypass Sarcosine and Form Glycine Directly after C-N Bond Cleavage. <i>Environmental Science & Technology</i> , 2018, 52, 1109-1117.	4.6	35
9565	An off-on-fluorescein-based colorimetric and fluorescent probe for the detection of glutathione and cysteine over homocysteine and its application for cell imaging. <i>Sensors and Actuators B: Chemical</i> , 2018, 260, 295-302.	4.0	48
9566	Efficient Implementation of Variation after Projection Generalized Hartree-Fock. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 588-596.	2.3	14
9567	Overview of Computational Methods for Organic Chemists. , 2018, , 31-67.		3
9568	The isomerization of cytosine: Intramolecular hydrogen atom transfer mediated through formic acid. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3831.	0.9	4
9569	A DFT-based mechanistic proposal for the light-driven insertion of dioxygen into Pt(II)-C bonds. <i>Chemical Science</i> , 2018, 9, 5039-5046.	3.7	18
9570	Structural characterization of the P1+ intermediate state of the P-cluster of nitrogenase. <i>Journal of Biological Chemistry</i> , 2018, 293, 9629-9635.	1.6	44
9571	Unravelling Chemical Interactions with Principal Interacting Orbital Analysis. <i>Chemistry - A European Journal</i> , 2018, 24, 9639-9650.	1.7	126
9572	Sulfenamides as Building Blocks for Efficient Disulfide-Based Self-Healing Materials. A Quantum Chemical Study. <i>ChemistryOpen</i> , 2018, 7, 248-255.	0.9	16
9573	Synthesis, structure, theoretical studies and electrochemistry of Ru(II) N heterocyclic carbenes. <i>Inorganica Chimica Acta</i> , 2018, 479, 141-147.	1.2	7
9574	Total Synthesis of Natural Hyacinthacine C ₅ and Six Related Hyacinthacine C ₅ Epimers. <i>Journal of Organic Chemistry</i> , 2018, 83, 5558-5576.	1.7	25
9575	Charge-transfer complexes based on C _{2v} -symmetric benzo[ghi]perylene: comparison of their dynamic and electronic properties with those of D _{6h} -symmetric coronene. <i>Materials Chemistry Frontiers</i> , 2018, 2, 1165-1174.	3.2	6
9576	Explicitly correlated orbital optimized contracted pair correlation methods: Foundations and applications. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850024.	1.8	1

#	ARTICLE	IF	CITATIONS
9577	Theoretical Development of Near-Infrared Bioluminescent Systems. <i>Chemistry - A European Journal</i> , 2018, 24, 9340-9352.	1.7	9
9578	Reprocessable and recyclable crosslinked poly(urea-urethane)s based on dynamic amine/urea exchange. <i>Polymer</i> , 2018, 145, 127-136.	1.8	77
9579	Porphyrin sensitizers containing an auxiliary benzotriazole acceptor for dye-sensitized solar cells: Effects of steric hindrance and cosensitization. <i>Dyes and Pigments</i> , 2018, 155, 323-331.	2.0	35
9580	Theoretical design of new small molecules with a low band-gap for organic solar cell applications: DFT and TD-DFT study. <i>Computational Materials Science</i> , 2018, 150, 54-61.	1.4	41
9581	Self-assembly study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach. <i>Dalton Transactions</i> , 2018, 47, 6304-6313.	1.6	30
9582	Electronic-state-driven adsorption of O ₂ on a nanocrystalline TiO ₂ under "dark" and UV-irradiation conditions: Ab initio study. <i>Chemical Physics Letters</i> , 2018, 698, 97-101.	1.2	0
9583	Investigating the Interaction of Silicon Dioxide Nanoparticles with Human Hemoglobin and Lymphocyte Cells by Biophysical, Computational, and Cellular Studies. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4278-4288.	1.2	36
9584	A Reactive Manganese(IV)-Hydroxide Complex: A Missing Intermediate in Hydrogen Atom Transfer by High-Valent Metal-Oxo Porphyrinoid Compounds. <i>Journal of the American Chemical Society</i> , 2018, 140, 4380-4390.	6.6	52
9585	Effective electronic-only Kohn-Sham equations for the muonic molecules. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8802-8811.	1.3	3
9586	Hybridization of Nitrogen Determines Hydrogen-Bond Acceptor Strength: Gas-Phase Comparison of Redshifts and Equilibrium Constants. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3899-3908.	1.1	8
9587	Computational insights into the mechanisms of Ru-catalyzed cycloisomerization of 2-ethynylaniline and 2-(2-propynyl)tosylanilide: The role of pyridine in assisting the metal-vinylidene formation. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 160-168.	0.8	7
9588	Co(III) Complexes with N ₂ S ₃ -Type Ligands as Structural/Functional Models for the Isocyanide Hydrolysis Reaction Catalyzed by Nitrile Hydratase. <i>Inorganic Chemistry</i> , 2018, 57, 4277-4290.	1.9	3
9589	Combined QSAR, molecular docking and molecular dynamics study on new Acetylcholinesterase and Butyrylcholinesterase inhibitors. <i>Computational Biology and Chemistry</i> , 2018, 74, 304-326.	1.1	68
9590	Basis sets for the calculation of core-electron binding energies. <i>Chemical Physics Letters</i> , 2018, 699, 279-285.	1.2	32
9591	Density functional theory modeling of chromate adsorption onto ferrihydrite nanoparticles. <i>Geochemical Transactions</i> , 2018, 19, 8.	1.8	26
9592	Molecular Modelling of the H ₂ Adsorptive Properties of Tetrazolate-Based Metal-Organic Frameworks: From the Cluster Approach to Periodic Simulations. <i>ChemPhysChem</i> , 2018, 19, 1349-1357.	1.0	6
9593	Computationally Guided Design of a Readily Assembled Phosphite-Thioether Ligand for a Broad Range of Pd-Catalyzed Asymmetric Allylic Substitutions. <i>ACS Catalysis</i> , 2018, 8, 3587-3601.	5.5	27
9594	Isolation of diborenes and their 90°-twisted diradical congeners. <i>Nature Communications</i> , 2018, 9, 1197.	5.8	62

#	ARTICLE	IF	CITATIONS
9595	A Possible Progenitor of the Interstellar Sulfide Bond: Rovibrational Characterization of the Hydrogen Disulfide Cation HSSH ⁺ . <i>Astrophysical Journal</i> , 2018, 856, 30.	1.6	7
9596	Divideâ€“Expandâ€“Consolidate Second-Order MÃ¼llerâ€“Plesset Theory with Periodic Boundary Conditions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2427-2438.	2.3	9
9597	NeON ⁺ : An Atom <i>and</i> a Molecule. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 491-495.	1.2	5
9598	Review of computer simulations on anti-cancer drug delivery in MOFs. <i>Inorganic Chemistry Frontiers</i> , 2018, 5, 1255-1272.	3.0	79
9599	Probing the antioxidant potential of phloretin and phlorizin through a computational investigation. <i>Journal of Molecular Modeling</i> , 2018, 24, 101.	0.8	40
9600	Wave Function Theories and Electronic Structure Methods: Quantum Chemistry, from Atoms to Molecules. , 2018, , 107-220.		0
9601	Detailed characterization of glycosylated sensory-active volatile phenols in smoke-exposed grapes and wine. <i>Food Chemistry</i> , 2018, 259, 147-156.	4.2	29
9602	Computational study of effect of solvents on vibrational spectra of coumarin 500. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 46-57.	1.1	4
9603	One-Photon Absorption Properties from a Hybrid Polarizable Density Embedding/Complex Polarization Propagator Approach for Polarizable Solutions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2145-2154.	2.3	4
9604	Ni(COD) ₂ -Catalyzed <i>ipso</i> -Silylation of 2-Methoxynaphthalene: A Density Functional Theory Study. <i>Organometallics</i> , 2018, 37, 1141-1149.	1.1	26
9605	Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM MD free-energy simulations of sodium and potassium hydration. <i>Journal of Chemical Physics</i> , 2018, 148, 222814.	1.2	71
9606	Multiorientation Model for Planar Ordering of Trimesic Acid Molecules. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7344-7352.	1.5	19
9607	Fused donorâ€“acceptor ï€-conjugated diazatruxenones: synthesis and electronic properties. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1748-1755.	2.3	10
9608	Luminescent ionic liquids based on cyclometalated platinum(ⁱⁱ) complexes exhibiting thermochromic behaviour in different colour regions. <i>Dalton Transactions</i> , 2018, 47, 5589-5594.	1.6	22
9609	Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems. <i>Chemistry - A European Journal</i> , 2018, 24, 12383-12388.	1.7	28
9610	Compact, flexible conducting polymer/graphene nanocomposites for supercapacitors of high volumetric energy density. <i>Composites Science and Technology</i> , 2018, 160, 50-59.	3.8	62
9611	Photophysical and electrochemical properties of organic molecules: Solvatochromic effect and DFT studies. <i>Optical Materials</i> , 2018, 77, 211-220.	1.7	15
9612	Can Density Matrix Embedding Theory with the Complete Activate Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems?. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1960-1968.	2.3	39

#	ARTICLE	IF	CITATIONS
9613	Radical chemistry of alkyl aluminum with quinoxaline ligands. <i>Journal of Coordination Chemistry</i> , 2018, 71, 1234-1249.	0.8	3
9614	Synthesis and characterization of yttrium, europium, terbium and dysprosium complexes containing a novel type of triazolyl-oxazoline ligand. <i>Chemical Papers</i> , 2018, 72, 799-808.	1.0	15
9615	Interplay between salt bridge, hydrogen bond and anion-π interactions in thiocyanate binding. <i>Inorganica Chimica Acta</i> , 2018, 470, 133-138.	1.2	22
9616	Dissociation of [b5] ⁺ ions containing an L-methyltryptophan and four alanine residues; losses of CO ₂ and the oxazolone ring. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 28-38.	0.7	1
9617	Predictions of water/oil interfacial tension at elevated temperatures and pressures: A molecular dynamics simulation study with biomolecular force fields. <i>Fluid Phase Equilibria</i> , 2018, 476, 30-38.	1.4	32
9618	Theoretical investigations of transport properties of organic solvents in cation-functionalized graphene oxide membranes: Implications for drug delivery. <i>Nano Research</i> , 2018, 11, 254-263.	5.8	7
9619	Excited states study reveals the twisted geometry induced large Stokes shift in DCM fluorescent dye. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 354, 127-138.	2.0	14
9620	Hydrogen atom transfer in metal ion complexes of the glutathione thiol radical. <i>International Journal of Mass Spectrometry</i> , 2018, 429, 39-46.	0.7	5
9621	Half-sandwich hydrazine complexes of iridium: Preparation and reactivity. <i>Inorganica Chimica Acta</i> , 2018, 470, 139-148.	1.2	10
9622	Modulating a D-π-A type diarylethene for on-demand Cu ²⁺ check via photo-switchable detection range and sensitivity. <i>Sensors and Actuators B: Chemical</i> , 2018, 257, 77-86.	4.0	9
9623	A chemical kinetic mechanism for the low- and intermediate-temperature combustion of Polyoxymethylene Dimethyl Ether 3 (PODE3). <i>Fuel</i> , 2018, 212, 223-235.	3.4	100
9624	Metal-to-metal charge-transfer transitions in Prussian blue hexacyanochromate analogues. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2018, 227, 28-38.	1.7	11
9625	Crystal structures, magnetic properties and DFT study of cobalt(II) azido complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent. <i>Polyhedron</i> , 2018, 139, 142-147.	1.0	13
9626	Rational design of a molecularly imprinted polymer for dinotefuran: theoretical and experimental studies aimed at the development of an efficient adsorbent for microextraction by packed sorbent. <i>Analyst</i> , 2017, 143, 141-149.	1.7	43
9627	Adsorption of TNT, DNAN, NTO, FOX7, and NQ onto cellulose, chitin, and cellulose triacetate. Insights from Density Functional Theory calculations. <i>Surface Science</i> , 2018, 668, 54-60.	0.8	14
9628	Development of Solid Catalyst-Solid Substrate Reactions for Efficient Utilization of Biomass. <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 29-43.	2.0	63
9629	Understanding the origins of metal-organic framework/polymer compatibility. <i>Chemical Science</i> , 2018, 9, 315-324.	3.7	153
9630	(C ₅ Me ₅) ₂ Y(1/4-H)(1/4-CH ₂ C ₅ Me ₄)Y(C ₅ Me ₅) as a reservoir of electrons for the reduction of PhSSPh and CO ₂ : A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 857, 80-87.	0.8	0

#	ARTICLE	IF	CITATIONS
9631	Highly delocalized endohedral metal in Gd@C _{2v} (9)-C ₈₂ metallofullerenes co-crystallized with $\hat{I}\pm$ -S ₈ . Nano Research, 2018, 11, 2277-2284.	5.8	10
9632	<scp>DFT</scp> study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. International Journal of Quantum Chemistry, 2018, 118, e25497.	1.0	41
9633	Primary Formation Path of Formaldehyde in Hydrothermal Vents. Origins of Life and Evolution of Biospheres, 2018, 48, 1-22.	0.8	6
9634	Synthesis, spatial and electronic structure of 1-(+)-neomenthyl-1,2-diphosphole and 1-(+)-neomenthyl-1,2,4-triphosphole tungstenpentacarbonyl complexes. Journal of Organometallic Chemistry, 2018, 867, 125-132.	0.8	11
9635	Incorporating quinoxaline unit as additional acceptor for constructing efficient donor-free solar cell sensitizers. Dyes and Pigments, 2018, 149, 65-72.	2.0	10
9636	Reduction of Carbonyl Groups by Uranium(III) and Formation of a Stable Amide Radical Anion. Chemistry - A European Journal, 2018, 24, 826-837.	1.7	23
9637	Revised CHARMM force field parameters for iron-containing cofactors of photosystem II. Journal of Computational Chemistry, 2018, 39, 7-20.	1.5	18
9638	Effect of hydrogen-bonded interactions on the energetics and spectral properties of the astromolecule aminoacetonitrile. International Journal of Quantum Chemistry, 2018, 118, e25459.	1.0	1
9639	Preparation and characterization by infrared emission spectroscopy and applications of new mineral-based composite materials of biomedical interest. Applied Spectroscopy Reviews, 2018, 53, 439-485.	3.4	1
9640	Th@C ₇₆ . Computational characterization of larger actinide endohedral fullerenes. International Journal of Quantum Chemistry, 2018, 118, e25501.	1.0	23
9641	Fullerene/cobalt porphyrin charge-transfer cocrystals: Excellent thermal stability and high mobility. Nano Research, 2018, 11, 1917-1927.	5.8	27
9642	Binding affinities of the farnesoid X receptor in the D3R Grand Challenge 2 estimated by free-energy perturbation and docking. Journal of Computer-Aided Molecular Design, 2018, 32, 211-224.	1.3	10
9643	Free methylidyne? CCC-NHC tantalum bis(imido) reactivity: protonation, rearrangement to a mixed unsymmetrical CCC-N-heterocyclic carbene/N-heterocyclic dicarbene (CCC-NHC/NHDC) pincer tantalum bis(imido) complex. Inorganica Chimica Acta, 2018, 469, 164-172.	1.2	10
9644	Immobilization of luminescent Platinum(II) complexes on periodic mesoporous organosilica and their water reduction photocatalysis. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 358, 334-344.	2.0	19
9645	An improved two-rotor function for conformational potential energy surfaces of 20 amino acid diamides. Canadian Journal of Chemistry, 2018, 96, 58-71.	0.6	2
9646	Energetics of van der Waals Adsorption on the Metal-Organic Framework NU-1000 with Zr ₆ -oxo, Hydroxo, and Aqua Nodes. Journal of the American Chemical Society, 2018, 140, 328-338.	6.6	11
9647	Structure-activity relationship on DNA binding and anticancer activities of a family of mixed-ligand oxidovanadium(V) hydrazone complexes. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4143-4155.	2.0	29
9648	Effect of acceptor strength on optical, electrochemical and photovoltaic properties of phenothiazine-based small molecule for bulk heterojunction organic solar cells. Dyes and Pigments, 2018, 149, 830-842.	2.0	26

#	ARTICLE	IF	CITATIONS
9649	A comparative study of the structures and electronic properties of graphene fragments: A DFT and MP2 survey. <i>Chemical Physics Letters</i> , 2018, 691, 291-297.	1.2	5
9650	Mono and dinuclear bis(ortho-tolyl)platinum(II) compounds containing diethyl sulfide ligands: Synthesis, DFT studies and use as precursors in cycloplatination reactions. <i>Journal of Organometallic Chemistry</i> , 2018, 854, 122-130.	0.8	1
9651	Theoretical studies on the reaction kinetics of methyl crotonate with hydroxyl radical. <i>Sustainable Energy and Fuels</i> , 2018, 2, 392-402.	2.5	24
9652	Hydrogen atoms in the diamond vacancy defect. A quantum mechanical vibrational analysis. <i>Carbon</i> , 2018, 129, 349-356.	5.4	18
9653	NH Tautomerism of a Quadruply Fused Porphyrin: Rigid Fused Structure Delays the Proton Transfer. <i>Journal of Physical Chemistry B</i> , 2018, 122, 316-327.	1.2	2
9654	On lithium doping in two stable nano-flakes of the B24: The double-ring versus the quasiplanar configuration. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 213-222.	1.3	0
9655	Theoretical investigation on the molecular inclusion process of urease inhibitors into p-sulfonic acid calix[4,6]arenes. <i>Chemical Physics Letters</i> , 2018, 692, 117-123.	1.2	4
9656	Effects of C5-substituent group on the hydrogen peroxide-mediated tautomerisation of protonated cytosine: a theoretical perspective. <i>Molecular Physics</i> , 2018, 116, 471-481.	0.8	1
9657	<sc>libreta</sc>: Computerized Optimization and Code Synthesis for Electron Repulsion Integral Evaluation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 572-587.	2.3	89
9658	Mechanistic study of CO/CO ₂ conversion catalyzed by a biomimetic Ni(II)-iminothiolate complex. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25555.	1.0	2
9659	Assessment of basis sets for density functional theory-based calculations of core-electron spectroscopies. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	50
9660	Hydrazinylpyridine based highly selective optical sensor for aqueous source of carbonate ions: Electrochemical and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 193, 330-337.	2.0	18
9661	Excited-state intramolecular proton transfer (ESIPT) fluorescence from 3-amidophthalimides displaying RGBY emission in the solid state. <i>Tetrahedron Letters</i> , 2018, 59, 388-391.	0.7	20
9662	Photophysical properties of acetylene-linked <i>syn</i> bimane oligomers: a molecular photonic wire. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1150-1163.	1.3	1
9663	Theoretical study on photo-induced processes of 1-methyl-3-(1,8-naphthalimidyl)ethyl)imidazolium halide species: an application of constrained density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3911-3917.	1.3	5
9664	Mechanistic Study on Aryl-Exchange Reaction of Diaryl- ³ -iodane with Aryl Iodide. <i>Journal of Organic Chemistry</i> , 2018, 83, 289-295.	1.7	14
9665	Solution-processed <i>N</i> -trialkylated triindoles for organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2018, 6, 50-56.	2.7	16
9666	Light Harvesting and Direct Electron Injection by Interfacial Charge-Transfer Transitions between TiO ₂ and Carboxy-Anchor Dye LEG4 in Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8-15.	1.5	41

#	ARTICLE	IF	CITATIONS
9667	Ultrafast Relaxation Dynamics of Luminescent Copper Nanoclusters (Cu ₇ L ₃) and Efficient Electron Transfer to Functionalized Reduced Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13354-13362.	1.5	44
9668	DFT Study of the Strong Solvent Effects in the Cu-Catalyzed Asymmetric Conjugate Addition Reaction. <i>Journal of the Chinese Chemical Society</i> , 2018, 65, 346-351.	0.8	2
9669	Hydrogen bonding cooperation in glycine(water) _n clusters studied by density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25556.	1.0	0
9670	Theoretical study of initial reactions of amine (CH ₃)NH(3 ⁺) (n ⁻ =1, 2, 3) with ozone. <i>Chemical Physics Letters</i> , 2018, 692, 111-116.	1.2	7
9671	Ultrafast Photodynamics of Glucose. <i>Journal of Physical Chemistry B</i> , 2018, 122, 19-27.	1.2	4
9672	Derivatives of 1-benzyl-4-(4-triphenylvinylphenyl) pyridinium bromide: Synthesis, characterization, mechanofluorochromism/aggregation-induced emission (AIE) character and theoretical simulations. <i>Journal of Luminescence</i> , 2018, 195, 14-23.	1.5	10
9673	Ion-pair recognition based on halogen bonding: a case of the crown-ether receptor with iodo-triazole moiety. <i>Structural Chemistry</i> , 2018, 29, 533-540.	1.0	7
9674	Ni(i)-Ni(iii) vs Ni(ii)-Ni(iv): mechanistic study of Ni-catalyzed alkylation of benzamides with alkyl halides. <i>Organic Chemistry Frontiers</i> , 2018, 5, 615-622.	2.3	48
9675	Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. <i>Journal of Computational Chemistry</i> , 2018, 39, 293-306.	1.5	11
9676	Electron-based descriptors in the study of physicochemical properties of compounds. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 1-10.	1.1	11
9677	Theoretical study: Electronic structure and receptor interaction of four type bis-1,4-dihydropyridine molecules. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 102-110.	1.1	3
9678	Research on the thermal behavior of novel heat resistance explosive 5,5-bis(2,4,6-trinitrophenyl)-2,2-bis(1,3,4-oxadiazole). <i>Journal of Analytical and Applied Pyrolysis</i> , 2018, 129, 189-194.	2.6	20
9679	Photoelectron spectroscopy and density functional theory studies of (FeS) _m H ⁻ (m= 2-4) cluster anions: effects of the single hydrogen. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 367-382.	1.3	6
9680	Nitrogen Reduction to Ammonia on a Biomimetic Mononuclear Iron Centre: Insights into the Nitrogenase Enzyme. <i>Chemistry - A European Journal</i> , 2018, 24, 5293-5302.	1.7	44
9681	Studies of lysine cyclodeaminase from <i>Streptomyces pristinaespiralis</i> : Insights into the complex transition NAD ⁺ state. <i>Biochemical and Biophysical Research Communications</i> , 2018, 495, 306-311.	1.0	6
9682	β-cyclodextrin encapsulated polyphenols as effective antioxidants. <i>Biopolymers</i> , 2018, 109, e23084.	1.2	17
9683	Divergent stereoisomers of molybdenum carbonyl complexes of NHC-based pincer ligands. <i>Polyhedron</i> , 2018, 143, 57-61.	1.0	13
9684	Quantum chemical spectral characterization of CH ₂ NH ₂ for remote sensing of Titan's atmosphere. <i>Icarus</i> , 2018, 299, 187-193.	1.1	7

#	ARTICLE	IF	CITATIONS
9685	Actinide endohedral boron clusters: A closed-shell electronic structure of U@B40. <i>Nano Research</i> , 2018, 11, 354-359.	5.8	35
9686	Buckybowl Structure of Sumanenes and Distortions of Thiophenes Induced by the Pseudo Jahn-Teller Effect. <i>Journal of Physics: Conference Series</i> , 2018, 1148, 012005.	0.3	4
9687	The QAIM Approach to Chemical Bonding in Triruthenium Carbonyl Cluster: [Ru ₃ (η^4 -H)(η^4 -C ₃ -H ₂)-Haminox-N,N](CO) ₉ . <i>Journal of Physics: Conference Series</i> , 2018, 1032, 012068.	0.3	2
9688	Density Functional Theory Study on the Mechanisms of Platinum- and Gold-Catalyzed Cycloisomerizations of Biaryl Propargyl Alcohol and Indolyl Allenol to Phenanthrene and Carbazole. <i>ChemistrySelect</i> , 2018, 3, 12093-12107.	0.7	5
9689	Interaction of pyridine π -bridge-based poly(methacrylate) dyes for the fabrication of dye-sensitized solar cells with the influence of different strength phenothiazine, fluorene and anthracene sensitizers as donor units with new anchoring mode. <i>New Journal of Chemistry</i> , 2018, 42, 17939-17949.	1.4	11
9690	Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25518-25530.	1.3	23
9691	<i>Ab initio</i> molecular dynamics study of solvated electrons in methanol clusters. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28741-28750.	1.3	8
9692	Chiral differentiation of <i>d</i> - and <i>l</i> -isoleucine using permethylated β -cyclodextrin: infrared multiple photon dissociation spectroscopy, ion-mobility mass spectrometry, and DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30428-30436.	1.3	24
9693	Cyanine platelet single crystals: growth, crystal structure and optical spectra. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29166-29173.	1.3	5
9694	Tuning the reactivity of copper complexes supported by tridentate ligands leading to two-electron reduction of dioxygen. <i>Dalton Transactions</i> , 2018, 47, 16337-16349.	1.6	14
9695	Humidity-induced CO ₂ capture enhancement in Mg-CUK-1. <i>Dalton Transactions</i> , 2018, 47, 15827-15834.	1.6	29
9696	Hydroboration of carbon dioxide with catechol- and pinacolborane using an Ir ^{III} -CNP* pincer complex. Water influence on the catalytic activity. <i>Dalton Transactions</i> , 2018, 47, 16766-16776.	1.6	18
9697	A 2,2'-bipyridine-containing covalent organic framework bearing rhenium(<i>i</i>) tricarbonyl moieties for CO ₂ reduction. <i>Dalton Transactions</i> , 2018, 47, 17450-17460.	1.6	80
9698	Mechanistic insights into HCO ₂ H dehydrogenation and CO ₂ hydrogenation catalyzed by Ir(Cp*) containing tetrahydroxy bipyrimidine ligand: the role of sodium and proton shuttle. <i>Dalton Transactions</i> , 2018, 47, 17020-17031.	1.6	8
9699	Asymmetric hydrogenation of imines with chiral alkene-derived boron Lewis acids. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 8686-8689.	1.5	18
9700	A quantitative structure-property study of reorganization energy for known p-type organic semiconductors. <i>RSC Advances</i> , 2018, 8, 40330-40337.	1.7	13
9701	9. Complexes between core-modified porphyrins ZnP(X) ₄ (X = P and S) and small semiconductor nanoparticle Zn ₆ S ₆ : are they possible?. , 2018, , 135-146.		3
9702	Computational Exploration of a Pd(II)-Catalyzed β -C-H Arylation Where Stereoselectivity Arises from Attractive Aryl-Aryl Interactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 14786-14790.	1.7	8

#	ARTICLE	IF	CITATIONS
9703	Nuclear Resonance Vibrational Spectroscopy Definition of O ₂ Intermediates in an Extradioxygenase: Correlation to Crystallography and Reactivity. <i>Journal of the American Chemical Society</i> , 2018, 140, 16495-16513.	6.6	14
9704	Independent amplitude approximations in coupled cluster valence bond theory: Incorporation of 3-electron-pair correlation and application to spin frustration in the low-lying excited states of a ferredoxin-type tetrametallic iron-sulfur cluster. <i>Journal of Chemical Physics</i> , 2018, 149, 144103.	1.2	7
9705	Electrocatalytic Water Reduction Beginning with a {Fe(NO) ₂ } ¹⁰⁺ -Reduced Dinitrosyliron Complex: Identification of Nitrogen-Doped FeO _x (OH) _y as a Real Heterogeneous Catalyst. <i>Inorganic Chemistry</i> , 2018, 57, 14715-14726.	1.9	11
9706	Computational Investigation of RO ₂ + HO ₂ and RO ₂ + RO ₂ Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9542-9552.	1.1	19
9707	Dessâ€martin periodinane: The reactivity of a Î»5â€iodane catalyst explained by topological analysis. <i>International Journal of Quantum Chemistry</i> , 2018, 119, e25838.	1.0	2
9708	Inverse Design of a Catalyst for Aqueous CO/CO ₂ Conversion Informed by the Ni ^{II} â€Iminothiolate Complex. <i>Inorganic Chemistry</i> , 2018, 57, 15474-15480.	1.9	13
9709	Synthesis and properties of redoxâ€switchable zinc complexes of 10,15,20â€triarylâ€1,5â€zaâ€5â€oxaporphyrin. <i>Heteroatom Chemistry</i> , 2018, 29, .	0.4	9
9710	Prediction on the Origin of Selectivities in Baseâ€controlled Switchable NHCâ€catalyzed Transformations. <i>Chemistry - an Asian Journal</i> , 2019, 14, 293-300.	1.7	42
9711	Computational study on the hydrolysis of halomethanes. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	1
9712	Can the Radical Channel Contribute to the Catalytic Cycle of <i>N</i> -Heterocyclic Carbene in Benzoin Condensation?. <i>Journal of Organic Chemistry</i> , 2018, 83, 15202-15209.	1.7	10
9713	The Infrared spectrum of very large (periodic) systems: global versus fragment strategiesâ€the case of three defects in diamond. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	10
9714	Ruthenium(II) Bipyridyl Complexes with C ^{âˆš} C* Cyclometalated Mesoionic Carbene Ligands. <i>Organometallics</i> , 2018, 37, 4619-4629.	1.1	16
9715	Monitoring Mechanical, Electronic, and Catalytic Trends in a Titanium Metal Organic Framework Under the Influence of Guest-Molecule Encapsulation Using Density Functional Theory. <i>Scientific Reports</i> , 2018, 8, 16651.	1.6	12
9716	Heterobiaryl synthesis by contractive Câ€C coupling via P(V) intermediates. <i>Science</i> , 2018, 362, 799-804.	6.0	145
9717	Theoretical investigation of auxiliary electronic acceptors in modifying D-D-ï€A sensitizers for dye-sensitized solar cells. <i>Journal of Molecular Modeling</i> , 2018, 24, 339.	0.8	1
9718	Scalars, vectors and tensors evolving from slabs to bulk. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	0
9719	Structural, energetic and spectroscopic studies of new luminescent complexes based on 2-(2â€hydroxyphenyl)imidazo[1,2- <i>a</i>]pyridines and 1,2-phenylenediboronic acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 725-737.	0.5	7
9720	Counter Anion Effect on the Photophysical Properties of Emissive Indolizine-Cyanine Dyes in Solution and Solid State. <i>Molecules</i> , 2018, 23, 3051.	1.7	34

#	ARTICLE	IF	CITATIONS
9721	Photoreactions of Sc ₃ N@h-C ₈₀ and Lu ₃ N@h-C ₈₀ with disilirane: Isolation and characterization of labile 1,2-adducts. <i>Heteroatom Chemistry</i> , 2018, 29, .	0.4	2
9722	Computational Comparative Mechanistic Study of C ⁺ E (E=C,N,O,S) Coupling Reactions through CO ₂ Activation Mediated by Uranium(III) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 19289-19299.	1.7	3
9723	Simulation of Capture and Release Processes of Hydrogen by β^2 -Hydroquinone Clathrate. <i>ACS Omega</i> , 2018, 3, 18771-18782.	1.6	16
9724	Big data analysis of <i>ab Initio</i> molecular integrals in the neglect of diatomic differential overlap approximation. <i>Journal of Computational Chemistry</i> , 2019, 40, 638-649.	1.5	10
9725	Using density based indexes to characterize excited states evolution. <i>Journal of Computational Chemistry</i> , 2019, 40, 650-656.	1.5	6
9726	Zigzag sp ² Carbon Chains Passing through an sp ³ Framework: A Driving Force toward Room-Temperature Ferromagnetic Graphene. <i>ACS Nano</i> , 2018, 12, 12847-12859.	7.3	19
9727	Taking Solution Proton NMR to Its Extreme: Prediction and Detection of a Hydride Resonance in an Intermediate-Spin Iron Complex. <i>Journal of the American Chemical Society</i> , 2018, 140, 17413-17417.	6.6	37
9728	Theoretical Study on the Mechanism of Rearrangement Reactions of Bicyclic Derivatives of Cyclopropane to Monocyclic Derivatives under the Catalysis of Pt-Salt. <i>ACS Omega</i> , 2018, 3, 16165-16174.	1.6	3
9729	Tetramer Compound of Manganese Ions with Mixed Valence [MnII MnIII MnIV] and Its Spatial, Electronic, Magnetic, and Theoretical Studies. <i>Crystals</i> , 2018, 8, 447.	1.0	7
9730	Effective quenching and excited-state relaxation of a Cu(I) photosensitizer addressed by time-resolved spectroscopy and TDDFT calculations. <i>Chemical Physics</i> , 2018, 515, 557-563.	0.9	9
9731	Insights into Ag(<i>scp</i>)-catalyzed addition reactions of amino alcohols to electron-deficient olefins: competing mechanisms, role of catalyst, and origin of chemoselectivity. <i>RSC Advances</i> , 2018, 8, 40338-40346.	1.7	8
9732	Light-Induced Conformational Change of Uracil-Anchored Polythiophene-Regulating Thermo-Responsiveness. <i>Langmuir</i> , 2018, 34, 12401-12411.	1.6	11
9733	Solvation of Piperidine in Nonaqueous Solvents. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2095-2097.	0.1	1
9734	Competitive McLafferty-type rearrangements of sodium adduct of <i>anti</i> -2,3-dihydroxy-1-phenylpentane-1,4-dione compounds in tandem mass spectrometry. <i>European Journal of Mass Spectrometry</i> , 2018, 24, 437-441.	0.5	3
9735	Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor. <i>Journal of the American Chemical Society</i> , 2018, 140, 15241-15251.	6.6	25
9736	Au(I) and Au(III)-Catalyzed Mechanism of the Cyclization Reaction of 3-(Ethylnylamino)-1,3-diphenylprop-2-en-1-one. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 1893-1899.	0.1	0
9737	Exchange-repulsion energy in QM/EFP. <i>Journal of Chemical Physics</i> , 2018, 149, 094103.	1.2	22
9738	Theoretical Study of Protein-Ligand Interactions Using the Molecules-in-Molecules Fragmentation-Based Method. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5143-5155.	2.3	33

#	ARTICLE	IF	CITATIONS
9739	Cooperative Metal-Ligand Hydroamination Catalysis Supported by C-H Activation in Cyclam Zr(IV) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 13034-13045.	1.9	12
9740	Computational design of a molecular triple photoswitch for wavelength-selective control. <i>Chemical Science</i> , 2018, 9, 8665-8672.	3.7	29
9741	Theoretical Study of the Copper-Catalyzed Hydroarylation of (Trifluoromethyl)alkyne with Phenylboronic Acid. <i>Journal of Organic Chemistry</i> , 2018, 83, 12775-12783.	1.7	11
9742	Altered superatomic properties of U@C28 by the electron rearrangement via adatom defects. <i>Chemical Physics Letters</i> , 2018, 712, 20-24.	1.2	3
9743	Synthesis of Tetracyclic 2,3-Dihydro-1,3-diazepines from a Dinitrodibenzothiophene Derivative. <i>Journal of Organic Chemistry</i> , 2018, 83, 12320-12326.	1.7	6
9744	Calculated Hydrogen Shift Rate Constants in Substituted Alkyl Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8665-8673.	1.1	55
9745	A New Dinuclear Cd(II) Macrocyclic Complex of a Schiff Base Ligand: Synthesis, Characterization, NMR and Mass Spectroscopy Investigation and Ab Initio Calculations. <i>Journal of Structural Chemistry</i> , 2018, 59, 968-974.	0.3	0
9746	Uncontracted core Pople basis sets in vibrational frequency calculations. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25761.	1.0	4
9747	Regioselective Palladium-Catalyzed Heterocyclization-Sonogashira Coupling Cascades from 2-Alkynylbenzamides and Terminal Alkynes: Experimental and DFT Studies. <i>Organometallics</i> , 2018, 37, 3813-3826.	1.1	11
9748	Chiral Control in Pentacoordinate Systems: The Case of Organosilicates. <i>Inorganic Chemistry</i> , 2018, 57, 12697-12708.	1.9	16
9749	Insight into the Photocatalytic Mechanism of Tin Dioxide/Polyaniline Nanocomposites for NO Degradation under Solar Light. <i>ACS Applied Nano Materials</i> , 2018, 1, 5786-5794.	2.4	39
9750	Fractional-occupation-number based divide-and-conquer coupled-cluster theory. <i>Chemical Physics Letters</i> , 2018, 712, 184-189.	1.2	5
9751	Fully anharmonic infrared cascade spectra of polycyclic aromatic hydrocarbons. <i>Journal of Chemical Physics</i> , 2018, 149, 134302.	1.2	37
9752	Reduced Occupancy of the Oxygen-Evolving Complex of Photosystem II Detected in Cryo-Electron Microscopy Maps. <i>Biochemistry</i> , 2018, 57, 5925-5929.	1.2	3
9753	Theoretical Investigation of Hydride Insertion into N-Heterocyclic Carbenes Containing N, P, C, O and S Heteroatoms. <i>Chemistry - an Asian Journal</i> , 2018, 13, 3745-3752.	1.7	5
9754	Rhodium(III) and Iridium(III) Complexes of a NHC-Based Macrocyclic: Persistent Weak Agostic Interactions and Reactions with Dihydrogen. <i>Organometallics</i> , 2018, 37, 3963-3971.	1.1	28
9755	Anharmonic vibrational spectroscopy of polycyclic aromatic hydrocarbons (PAHs). <i>Journal of Chemical Physics</i> , 2018, 149, 144102.	1.2	25
9756	The antioxidative activity of piceatannol and its different derivatives: Antioxidative mechanism analysis. <i>Phytochemistry</i> , 2018, 156, 184-192.	1.4	30

#	ARTICLE	IF	CITATIONS
9757	Activation of the Basal Plane in Two Dimensional Transition Metal Chalcogenide Nanostructures. <i>Journal of the American Chemical Society</i> , 2018, 140, 13663-13671.	6.6	38
9758	Computational investigation of intramolecular reorganization energy in diketopyrrolopyrrole (DPP) derivatives. <i>Turkish Journal of Chemistry</i> , 2018, 42, .	0.5	1
9759	Catalytic Role of H ₂ O Molecules in Oxidation of CH ₃ OH in Water. <i>Catalysts</i> , 2018, 8, 157.	1.6	9
9760	Direct observation of the morphology and peeling behavior of poly(vinyl alcohol) derivatives in water by scanning probe microscopy. <i>Journal of the Ceramic Society of Japan</i> , 2018, 126, 839-842.	0.5	0
9761	Molecular Dynamics Simulations of Lithium-Doped Ionic-Liquid Electrolytes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10535-10547.	1.2	28
9762	Davydov-type excitonic effects on the absorption spectra of parallel-stacked and herringbone aggregates of pentacene: Time-dependent density-functional theory and time-dependent density-functional tight binding. <i>Journal of Chemical Physics</i> , 2018, 149, 134111.	1.2	17
9763	A Biphasic Medium Slows Down the Transfer Hydrogenation and Allows a Selective Catalytic Deuterium Labeling of Amines from Imines Mediated by a Ru ^{H/D} Exchange in D ₂ O. <i>ChemCatChem</i> , 2018, 10, 5541-5550.	1.8	11
9764	Quantum chemical calculations support pseudouridine synthase reaction through a glycol intermediate and provide details of the mechanism. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	5
9765	Computational study on ionic and ion pair methylation reactions of enethiolates and their lithium salts. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	0
9766	Computational study of synergistic effects of electron withdrawing groups as catalysts for fullerene formation. <i>Chemical Data Collections</i> , 2018, 17-18, 415-418.	1.1	0
9767	Hydrogen, boron and nitrogen atoms in diamond: a quantum mechanical vibrational analysis. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	16
9768	Detection and identification of genetic material via single-molecule conductance. <i>Nature Nanotechnology</i> , 2018, 13, 1167-1173.	15.6	59
9769	Cyclometalated Ir(III) Complexes Involving Functionalized Terpyridine-Based Ligands Exhibiting Aggregation-Induced Emission and Their Potential Applications in CO ₂ Detection. <i>Organometallics</i> , 2018, 37, 3827-3838.	1.1	12
9770	Theoretical Study of Alkylsulfonic Acids: Force-Field Development and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9747-9756.	1.2	1
9771	Long Chain Branching Detection and Quantification in LDPE with Special Solvents, Polarization Transfer Techniques, and Inverse Gated ¹³ C NMR Spectroscopy. <i>Macromolecules</i> , 2018, 51, 8443-8454.	2.2	19
9772	Phosphorescence Properties of Discrete Platinum(II) Complex Anions Bearing N-Heterocyclic Carbenes in the Solid State. <i>Inorganic Chemistry</i> , 2018, 57, 14086-14096.	1.9	34
9773	Probing the structures and bonding of auropolyyenes, Au ⁺ (C _n) ⁻ Au ⁺ (n = 1-3), using high-resolution photoelectron imaging. <i>Journal of Chemical Physics</i> , 2018, 149, 144307.	1.2	13
9774	Controlling Proton-Coupled Electron Transfer in Bioinspired Artificial Photosynthetic Relays. <i>Journal of the American Chemical Society</i> , 2018, 140, 15450-15460.	6.6	52

#	ARTICLE	IF	CITATIONS
9775	Synthesis of Glycomimetics by Diastereoselective Passerini Reaction. <i>Journal of Organic Chemistry</i> , 2018, 83, 13146-13156.	1.7	17
9776	Stereoselectivity, Different Oxidation States, and Multiple Spin States in the Cyclopropanation of Olefins Catalyzed by Fe ^{II} -Porphyrin Complexes. <i>ACS Catalysis</i> , 2018, 8, 11140-11153.	5.5	27
9777	Orthometalated <i>N</i> -(Benzophenoxazine)- <i>o</i> -aminophenol: Phenolato versus Phenoxy States. <i>ACS Omega</i> , 2018, 3, 13323-13334.	1.6	8
9778	Can a temporary bond between dye and redox mediator increase the efficiency of p-type dye-sensitized solar cells?. <i>Journal of Molecular Modeling</i> , 2018, 24, 317.	0.8	1
9779	ArCH ₂ ⁺ : A Detectable Noble Gas Molecule. <i>ChemPhysChem</i> , 2018, 19, 3388-3392.	1.0	5
9780	Chromism of Tartrate-Bridged Clamshell-like Platinum(II) Complex: Intramolecular Pt ^{II} -Pt Interaction-Induced Luminescence Vapochromism and Intermolecular Interactions-Triggered Thermochromism. <i>Inorganic Chemistry</i> , 2018, 57, 14159-14169.	1.9	31
9781	Theoretical Study of C-H Bond Cleavage via Concerted Proton-Coupled Electron Transfer in Fluorenyl-Benzoates. <i>Journal of the American Chemical Society</i> , 2018, 140, 15641-15645.	6.6	25
9782	Modeling the Oxygen Vacancy at a Molecular Vanadium(III) Silica-Supported Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 14903-14914.	6.6	26
9783	Electronic Effect on the Molecular Motion of Aromatic Amides: Combined Studies Using VT-NMR and Quantum Calculations. <i>Molecules</i> , 2018, 23, 2294.	1.7	7
9784	Phosphorescent Cyclometalated Platinum(II) aNHC Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 15603-15612.	1.7	17
9785	Multipath VTST rate constants for D ⁺ + ⁻ methyl formate reactions: Importance of torsional anharmonicity and conformational flexibility for combustion chemistry. <i>Chemical Physics Letters</i> , 2018, 711, 132-137.	1.2	6
9786	Computational Tools for Calculating log $\hat{\nu}^2$ Values of Geochemically Relevant Uranium Organometallic Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8007-8019.	1.1	10
9787	Electronic Spectroscopies Combined with Quantum Chemistry Calculations: Study of the Interactions of 3-Hydroxyflavone with Copper Ions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8943-8951.	1.2	9
9788	Enhanced quantum yields by sterically demanding aryl-substituted $\hat{\nu}^2$ -diketonate ancillary ligands. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 664-671.	1.3	17
9789	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. <i>ACS Catalysis</i> , 2018, 8, 9298-9311.	5.5	17
9790	Adsorption of Multiple NO Molecules on Rh _{<i>n</i>} ⁺ (<i>n</i> = 6, 7) Investigated by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22884-22891.	1.5	19
9791	Exploring Oxidation State-Dependent Selectivity in Polymerization of Cyclic Esters and Carbonates with Zinc(II) Complexes. <i>IScience</i> , 2018, 7, 120-131.	1.9	13
9792	Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels ⁻ Alder Reactions: Importance of the Molecular Dipole Moment. <i>Journal of the American Chemical Society</i> , 2018, 140, 13350-13359.	6.6	113

#	ARTICLE	IF	CITATIONS
9793	Dramatic rate-enhancement of oxygen atom transfer by an iron(IV)-oxo species by equatorial ligand field perturbations. <i>Dalton Transactions</i> , 2018, 47, 14945-14957.	1.6	32
9794	Enantiodivergent Pd-catalyzed C-C bond formation enabled through ligand parameterization. <i>Science</i> , 2018, 362, 670-674.	6.0	134
9795	Computational Insight into the Activation Mechanism of Carcinogenic N-Nitrosornicotine (NNN) Catalyzed by Cytochrome P450. <i>Environmental Science & Technology</i> , 2018, 52, 11838-11847.	4.6	7
9796	QM/MM Ehrenfest dynamics from first principles: photodissociation of diazine in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	7
9797	Dinitrogen Fixation by Vanadium Complexes with a Triamidoamine Ligand. <i>Inorganic Chemistry</i> , 2018, 57, 11884-11894.	1.9	25
9798	Relevance of Protons in Heterolytic Activation of H ₂ O ₂ over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. <i>ACS Catalysis</i> , 2018, 8, 9722-9737.	5.5	52
9799	Redox Potential-Dependent Formation of an Unusual His-Trp Bond in Bilirubin Oxidase. <i>Chemistry - A European Journal</i> , 2018, 24, 18052-18058.	1.7	14
9800	Mechanistic insight into the ruthenium-catalyzed cycloaddition of enynes with alkynes: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 875, 46-51.	0.8	7
9801	Resonance State Method for Electron Injection in Dye Sensitized Solar Cells. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5090-5104.	2.3	2
9802	Amine Boranes Dehydrogenation Mediated by an Unsymmetrical Iridium Pincer Hydride: (PCN) vs (PCP) Improved Catalytic Performance. <i>Organometallics</i> , 2018, 37, 3142-3153.	1.1	32
9803	Density Functional Theory Investigation on Boron Subphthalocyanine-Ferrocene Dyads. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7620-7627.	1.1	3
9804	Toward quantum-chemical method development for arbitrary basis functions. <i>Journal of Chemical Physics</i> , 2018, 149, 084106.	1.2	10
9805	Design of dendritic core carbazole-based hole transporting materials for efficient and stable hybrid perovskite solar cells. <i>Organic Electronics</i> , 2018, 60, 22-30.	1.4	16
9806	Investigation of metallation/transmetallation reactions to synthesize a series of C-C-NHC Co pincer complexes and their X-ray structures. <i>Polyhedron</i> , 2018, 151, 568-574.	1.0	10
9807	The influence of the position of a chiral substituent on undecathiophene chain. A DFT study. <i>Synthetic Metals</i> , 2018, 242, 73-82.	2.1	6
9808	Th-Based Endohedral Metallofullerenes: Anomalous Metal Position and Significant Metal-Cage Covalent Interactions with the Involvement of Th 5f Orbitals. <i>Inorganic Chemistry</i> , 2018, 57, 7142-7150.	1.9	21
9809	Dimerization of Substituted Arylacetylenes—Quantum Chemical Calculations and Kinetic Studies. <i>Journal of Organic Chemistry</i> , 2018, 83, 7878-7885.	1.7	14
9810	The Vibrational Circular Dichroism Pattern of the $\hat{1}/2$ (C=O) Bands in Isoindolinones. <i>ChemPhysChem</i> , 2018, 19, 2411-2422.	1.0	10

#	ARTICLE	IF	CITATIONS
9811	Possibility of reducing the coordinated dinitrogen into ammonia and hydrazine using [Ru-L] (L =) Tj ETQq0 0 0 rgBT/Qverlock 10 Tf 50 7	0.7	10
9812	How does binuclear zinc amidohydrolase FwdA work in the initial step of methanogenesis: From formate to formyl-methanofuran. <i>Journal of Inorganic Biochemistry</i> , 2018, 185, 71-79.	1.5	2
9813	Mechanism for Co(dppp)-catalyzed regioselective intermolecular hydroacylation of 1,3-dienes and benzaldehydes: Insights from density functional calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 868, 102-111.	0.8	7
9814	Potential Use of Squarates and Croconates as Singlet Fission Sensitizers. <i>ChemPhysChem</i> , 2018, 19, 2224-2233.	1.0	10
9815	Slow-Starter Enzymes: Role of Active-Site Architecture in the Catalytic Control of the Biosynthesis of Taxadiene by Taxadiene Synthase. <i>Biochemistry</i> , 2018, 57, 3773-3779.	1.2	31
9816	Hybrid Correlation Energy (HyCE): An Approach Based on Separate Evaluations of Internal and External Components. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5223-5237.	1.1	3
9817	Pyridyl group design in viologens for anolyte materials in organic redox flow batteries. <i>RSC Advances</i> , 2018, 8, 18762-18770.	1.7	23
9818	N-Annulated perylene-based organic dyes sensitized graphitic carbon nitride to form an amide bond for efficient photocatalytic hydrogen production under visible-light irradiation. <i>Applied Catalysis B: Environmental</i> , 2018, 237, 32-42.	10.8	42
9819	Platinacycles Containing a Primary Amine Platinum(II) Compounds for Treating Cisplatin-Resistant Cancers by Oxidant Therapy. <i>Organometallics</i> , 2018, 37, 3502-3514.	1.1	16
9820	Synthesis, characterization and crystal structure of 2-chloroethyl(methylsulfonyl)methanesulfonate. <i>New Journal of Chemistry</i> , 2018, 42, 11073-11084.	1.4	7
9821	Control of excimer phosphorescence by steric effects in cyclometalated platinum(II) diketonate complexes bearing peripheral carbazole moieties towards application in non-doped white OLEDs. <i>New Journal of Chemistry</i> , 2018, 42, 11583-11592.	1.4	15
9822	Diastereoselectivity in a cyclic secondary amine catalyzed asymmetric Mannich reaction: a model rationalization from DFT studies. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2148-2157.	2.3	5
9823	Cold physics and chemistry: Collisions, ionization and reactions inside helium nanodroplets close to zero K. <i>Physics Reports</i> , 2018, 751, 1-90.	10.3	113
9824	Mechanism of enhanced triplet decay of thionucleobase by glycosylation and rate-modulating strategies. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16428-16436.	1.3	6
9825	Concerted Mechanism of Water Insertion and O ₂ Release during the S ₄ to S ₀ Transition of the Oxygen-Evolving Complex in Photosystem II. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6491-6502.	1.2	21
9826	Computational Analysis of the Intramolecular Oxidative Amination of an Alkene Catalyzed by the Extreme I ⁻ -Loading N-Heterocyclic Carbene Pincer Tantalum(V) Bis(imido) Complex. <i>Organometallics</i> , 2018, 37, 1671-1681.	1.1	11
9827	Experimental and theoretical studies of a greener catalytic system for saturated hydrocarbon chlorination composed by trichloroisocyanuric acid and a copper(II) compound. <i>Applied Catalysis A: General</i> , 2018, 562, 150-158.	2.2	1
9828	Insights into the NHC-catalyzed cascade Michael/aldol/lactamization reaction: mechanism and origin of stereoselectivity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2065-2072.	2.3	35

#	ARTICLE	IF	CITATIONS
9829	Insights into the luminescent properties of anionic cyclometalated iridium(III) complexes with ligands derived from natural products. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25664.	1.0	6
9830	The role of sulfate in the chemical synthesis of graphene oxide. <i>Materials Chemistry and Physics</i> , 2018, 215, 203-210.	2.0	12
9831	Hydrogen Sulfide as a Scavenger of Sulfur Atomic Cation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4983-4987.	1.1	16
9832	Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4790-4800.	1.1	37
9833	Intramolecular Charge Transfer and Local Excitation in Organic Fluorescent Photoredox Catalysts Explained by RASCI-PDFT. <i>Journal of Physical Chemistry C</i> , 2018, 122, 12061-12070.	1.5	16
9834	QM/MM studies on ozonolysis of β -humulene and Criegee reactions with acids and water at air/water/acetonitrile interfaces. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16138-16150.	1.3	9
9835	Mechanistic insights into the iridium catalysed hydrogenation of ethyl acetate to ethanol: a DFT study. <i>Dalton Transactions</i> , 2018, 47, 10172-10178.	1.6	7
9836	Experimental and theoretical investigations on spectroscopic properties of tropicamide. <i>Journal of Molecular Structure</i> , 2018, 1173, 52-62.	1.8	26
9837	Understanding the mechanism of transition metal-free <i>anti</i> addition to alkynes: the selenoboration case. <i>Catalysis Science and Technology</i> , 2018, 8, 3617-3628.	2.1	13
9838	Phenylene-bridged cross-conjugated 1,2,3-trisilacyclopentadienes. <i>Chemical Communications</i> , 2018, 54, 8399-8402.	2.2	10
9839	Mechanism of NO/CO reaction over highly dispersed cuprous oxide on γ -alumina catalyst using a metal support interfacial site in the presence of oxygen: similarities to and differences from biological systems. <i>Catalysis Science and Technology</i> , 2018, 8, 3833-3845.	2.1	16
9840	Enantioselective Synthesis of Sterically Hindered Tertiary β -Aryl Oxindoles via Palladium-Catalyzed Decarboxylative Protonation. An Experimental and Theoretical Mechanistic Investigation. <i>Advanced Synthesis and Catalysis</i> , 2018, 360, 3124-3137.	2.1	11
9841	Energy flow in the Photosystem I supercomplex: Comparison of approximative theories with DM-HEOM. <i>Chemical Physics</i> , 2018, 515, 262-271.	0.9	21
9842	A computational mechanistic study of substrate-controlled competitive O-H and C-H insertion reactions catalyzed by dirhodium(σ -carbenoids): insight into the origin of chemoselectivity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2353-2363.	2.3	9
9843	Photophysical insights on the influence of excited states reorganization processes on the visible and near infra-red luminescence of two-photon quadrupolar chromophores. <i>Dyes and Pigments</i> , 2018, 159, 352-366.	2.0	6
9844	Preparation and reactivity of half-sandwich dioxygen complexes of ruthenium. <i>Dalton Transactions</i> , 2018, 47, 9173-9184.	1.6	6
9845	Gas-phase intramolecular hydroxyl-amino exchange of protonated arginine and verified by the synthetic intermediate compound. <i>Journal of Mass Spectrometry</i> , 2018, 53, 700-704.	0.7	5
9846	Origin of stereoselectivity in the amination of alcohols using cooperative asymmetric dual catalysis involving chiral counter-ions. <i>Chemical Science</i> , 2018, 9, 6126-6133.	3.7	23

#	ARTICLE	IF	CITATIONS
9847	Role of Anation on the Mechanism of Proton Reduction Involving a Pentapyridine Cobalt Complex: A Theoretical Study. <i>Inorganic Chemistry</i> , 2018, 57, 8116-8127.	1.9	6
9848	A reference data set for validating vapor pressure measurement techniques: homologous series of polyethylene glycols. <i>Atmospheric Measurement Techniques</i> , 2018, 11, 49-63.	1.2	41
9849	Kineticomechanistic Study of the Redox pH Cycling Processes Occurring on a Robust Water-Soluble Cyanido-Bridged Mixed-Valence {Co(II)/Fe(II)} ₂ Square. <i>Inorganic Chemistry</i> , 2018, 57, 8465-8475.	1.9	8
9850	Defining the conditional basis of silicon phthalocyanine near-IR ligand exchange. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19030-19036.	1.3	18
9851	Poly(lactic acid), maleic anhydride and dicumyl peroxide: NMR study of the free-radical melt reaction product. <i>Polymer Degradation and Stability</i> , 2018, 155, 1-8.	2.7	9
9852	New insights into the sensing mechanism of a phosphonate pyrene chemosensor for TNT. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19539-19545.	1.3	20
9853	How to engineer glucose oxidase for mediated electron transfer. <i>Biotechnology and Bioengineering</i> , 2018, 115, 2405-2415.	1.7	13
9854	DFT investigation on adsorption of diatomic, triatomic and tetraatomic gases on Sc-doped ZnO sodalite like cage for gas sensing purpose. <i>Materials Chemistry and Physics</i> , 2018, 217, 63-73.	2.0	5
9855	Quantum-Chemical Study of Reaction Laws of 2,4,6-Triphenylpyranil Radical with Oxygen. <i>Russian Journal of Organic Chemistry</i> , 2018, 54, 719-725.	0.3	2
9856	Theoretical and experimental adsorption studies of sulfamethoxazole and ketoprofen on synthesized ionic liquids modified CNTs. <i>Ecotoxicology and Environmental Safety</i> , 2018, 161, 542-552.	2.9	55
9857	Experimental and Theoretical Studies on the Reactivity of Titanium Chelidamate Complexes: the Significant Role of the Hydroxide Pyridine Moiety. <i>Organometallics</i> , 2018, 37, 3515-3523.	1.1	7
9858	A fluorescence resonance energy transfer based pH probe for visualizing acidification in fungal cells. <i>Sensors and Actuators B: Chemical</i> , 2018, 274, 533-540.	4.0	12
9859	Method Calibration or Data Fitting?. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4651-4661.	2.3	27
9860	Sulfoximine-Assisted One-Pot Unsymmetrical Multiple Annulation of Arenes: A Combined Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 9667-9681.	1.7	39
9861	The Acetate Proton Shuttle between Mutually <i>trans</i> Ligands. <i>Organometallics</i> , 2018, 37, 2645-2651.	1.1	9
9862	Conductive Binder for Si Anode with Boosted Charge Transfer Capability via n-Type Doping. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 27795-27800.	4.0	49
9863	Density Functional Modeling of Ligand Effects on Electronic Structure and C-H Bond Activation Activity of Copper(III) Hydroxide Compounds. <i>Inorganic Chemistry</i> , 2018, 57, 9807-9813.	1.9	8
9864	Tunable Binding of Dinitrogen to a Series of Heterobimetallic Hydride Complexes. <i>Organometallics</i> , 2018, 37, 4521-4526.	1.1	18

#	ARTICLE	IF	CITATIONS
9865	Solvation structure for Fe(II), Co(II) and Ni(II) complexes in [P2225][NTf2] ionic liquids investigated by Raman spectroscopy and DFT calculation. <i>Journal of Molecular Liquids</i> , 2018, 269, 8-13.	2.3	3
9866	Vibrational Relaxation in EDTA Is Ion-Dependent. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6585-6592.	1.1	11
9867	Thermal azide-alkene cycloaddition reactions: straightforward multi-gram access to 1,2,3-triazolines in deep eutectic solvents. <i>Green Chemistry</i> , 2018, 20, 4023-4035.	4.6	30
9868	Ligand and solvent control of selectivity in the C-H activation of a pyridylimine-substituted 1-naphthalene; a combined synthetic and computational study. <i>Dalton Transactions</i> , 2018, 47, 11680-11690.	1.6	3
9869	Monomeric Rare-Earth Metal Silyl-Thiophosphinoyl-Alkylidene Complexes: Synthesis, Structure, and Reactivity. <i>Chemistry - A European Journal</i> , 2018, 24, 13903-13917.	1.7	20
9870	Unraveling the Structure of Magic-Size (CdSe) ₁₃ Cluster Pairs. <i>Chemistry of Materials</i> , 2018, 30, 5468-5477.	3.2	37
9871	An uracil-linked hydroxyflavone probe for the recognition of ATP. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 747-755.	1.3	11
9872	Electrochemical studies of a new, low-band gap inherently chiral ethylenedioxythiophene-based oligothiophene. <i>Electrochimica Acta</i> , 2018, 284, 513-525.	2.6	12
9873	Kinetic Control in the Alignment of Polar π -Conjugated Molecules inside Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18151-18160.	1.5	10
9874	Systematic Study of Structure, Stability, and Electronic Absorption of Tetrahedral CdSe Clusters with Carboxylate and Amine Ligands. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6704-6712.	1.1	10
9875	Third-Order Kinetics for Interaction of Glutathione with a Dinuclear Pd(II) Complex and Their Mechanism, DNA Binding and DFT Study. <i>Journal of Solution Chemistry</i> , 2018, 47, 1139-1156.	0.6	1
9876	Spin-Unrestricted Self-Energy Embedding Theory. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4444-4450.	2.1	17
9877	Degradable Carbon Dots with Broad-Spectrum Antibacterial Activity. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 26936-26946.	4.0	246
9878	Co-synthesis of atomically precise nickel nanoclusters and the pseudo-optical gap of Ni ₄ (SR) ₈ . <i>Dalton Transactions</i> , 2018, 47, 11097-11103.	1.6	10
9879	Using reduced density matrix techniques to capture static and dynamic correlation in the energy landscape for the decomposition of the CH ₂ CH ₂ ONO radical and support a non-IRC pathway. <i>Journal of Chemical Physics</i> , 2018, 149, 024302.	1.2	6
9880	Rovibrational analysis of <i>c</i> -SiC ₂ H ₂ : Further evidence for out-of-plane bending issues in correlated methods. <i>Journal of Chemical Physics</i> , 2018, 149, 024303.	1.2	10
9881	Promising pyridinium ylide based anchors towards high-efficiency dyes for dye-sensitized solar cells applications: Insights from theoretical investigations. <i>Electrochimica Acta</i> , 2018, 283, 1798-1805.	2.6	33
9882	The structural model of Zika virus RNA-dependent RNA polymerase in complex with RNA for rational design of novel nucleotide inhibitors. <i>Scientific Reports</i> , 2018, 8, 11132.	1.6	26

#	ARTICLE	IF	CITATIONS
9883	New polymer-matrix nanocomposites based on SWCNTs and PVK-PPV copolymer: Synthesis, functionalization and characterization. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 205, 630-636.	2.0	7
9884	$^{99}\text{TcO}_4^-$ remediation by a cationic polymeric network. <i>Nature Communications</i> , 2018, 9, 3007.	5.8	234
9885	Understanding Trends in ^{27}Al Chemical Shifts and Quadrupolar Coupling Constants in Chloroalkyl Aluminum $[\text{AlCl}_x(\text{Me})_3]_n$ or 2 Compounds. <i>Helvetica Chimica Acta</i> , 2018, 101, e1800120.	1.0	8
9886	Synthesis, biological evaluation, and molecular modelling studies of potent human neutrophil elastase (HNE) inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 1108-1124.	2.5	18
9887	Tuning the Biradicaloid Nature of Polycyclic Aromatic Hydrocarbons: The Effect of Graphitic Nitrogen Doping in Zethrenes. <i>ChemPhysChem</i> , 2018, 19, 2492-2499.	1.0	11
9888	Theoretical study of Sn adsorbed on the MgO(100) surface with defects. <i>Comptes Rendus Chimie</i> , 2018, 21, 669-675.	0.2	5
9889	Synthesis and Reactivity of Low-Valent f-Element Iodide Complexes with Neutral Iminophosphorane Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 9230-9240.	1.9	22
9890	Mechanistic Studies of $[\text{AlCp}^*]_4$ Combustion. <i>Inorganic Chemistry</i> , 2018, 57, 8181-8188.	1.9	4
9891	Comparing Interactions of a Three-Coordinate Pd Cation with Common Weakly Coordinating Anions. <i>Organometallics</i> , 2018, 37, 2376-2385.	1.1	9
9892	Vibrational properties of small rhodium clusters: role of magnetism, charge state, and isomerization effects. <i>European Physical Journal D</i> , 2018, 72, 1.	0.6	4
9893	$\text{S}\ddot{\text{C}}\text{H}$ Bond Activation in Hydrogen Sulfide by NHC-Stabilized Silyliumylidene Ions. <i>Inorganics</i> , 2018, 6, 54.	1.2	18
9894	Direct (Hetero)Arylation for the Synthesis of Molecular Materials: Coupling Thieno[3,4-c]pyrrole-4,6-dione with Perylene Diimide to Yield Novel Non-Fullerene Acceptors for Organic Solar Cells. <i>Molecules</i> , 2018, 23, 931.	1.7	29
9895	Linear response time-dependent density functional theory without unoccupied states: The Kohn-Sham-Sternheimer scheme revisited. <i>Journal of Chemical Physics</i> , 2018, 149, 024105.	1.2	13
9896	Molecular model of J-aggregated pseudoisocyanine fibers. <i>Journal of Chemical Physics</i> , 2018, 149, 024905.	1.2	11
9897	Quantitative studies on the <i>p</i> -substituent effect of the phenolic component on the polymerization of benzoxazines. <i>Polymer Chemistry</i> , 2018, 9, 4194-4204.	1.9	36
9898	Iron(II) Bis(acetylide) Complexes as Key Intermediates in the Catalytic Hydrofunctionalization of Terminal Alkynes. <i>ACS Catalysis</i> , 2018, 8, 7973-7982.	5.5	61
9899	Water-Nucleophilic Attack Mechanism for the Cu^{II} (pyalk) $_2$ Water-Oxidation Catalyst. <i>ACS Catalysis</i> , 2018, 8, 7952-7960.	5.5	37
9900	Competing mechanisms and origins of chemo- and stereo-selectivities of NHC-catalyzed reactions of enals with 2-aminoacrylates. <i>Catalysis Science and Technology</i> , 2018, 8, 4229-4240.	2.1	40

#	ARTICLE	IF	CITATIONS
9901	Mechanochromic Switching between Delayed Fluorescence and Phosphorescence of Luminescent Coordination Polymers Composed of Dinuclear Copper(I) Iodide Rhombic Cores. <i>Chemistry - A European Journal</i> , 2018, 24, 14750-14759.	1.7	75
9902	Synthesis and Reactivity of Methylpalladium Complexes Bearing a Partially Saturated IzQO Ligand. <i>Organometallics</i> , 2018, 37, 2286-2296.	1.1	22
9903	Insights on the Origin of Regiodivergence in the Parallel Kinetic Resolution of <i>rac</i> -Aziridines Using a Chiral Lanthanum–Yttrium Bimetallic Catalyst. <i>ACS Catalysis</i> , 2018, 8, 7633-7644.	5.5	9
9904	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17170-17183.	1.5	33
9905	Synthesis of reaction-adapted zeolites as methanol-to-olefins catalysts with mimics of reaction intermediates as organic structure-directing agents. <i>Nature Catalysis</i> , 2018, 1, 547-554.	16.1	111
9906	Syntheses of Substituted 1,4-Disila-2,5-cyclohexadienes from Cyclic Hexasilane $\text{Si}_6\text{Me}_{12}$ and Alkynes via Successive Si–Si Bond Activation by Pd/Isocyanide Catalysts. <i>Organometallics</i> , 2018, 37, 2531-2543.	1.1	11
9907	Dimethylberyllium + CO_2 Fire! A DFT and <i>ab Initio</i> Study into the Photon Emission Observed in a Gas Phase Carbon Dioxide Activation Reaction. <i>Organometallics</i> , 2018, 37, 2519-2530.	1.1	0
9908	Effects of methyl groups in a pyrimidine-based flexible ligand on the formation of silver(<i>scp</i>) coordination networks. <i>New Journal of Chemistry</i> , 2018, 42, 13998-14008.	1.4	3
9909	Computational modelling of singlet excitation energy transfer: a DFT/TD-DFT study of the ground and excited state properties of a syn bimane dimer system using non-empirically tuned range-separated functionals. <i>New Journal of Chemistry</i> , 2018, 42, 13732-13743.	1.4	2
9910	Conformational analysis of a TADDOL-based phosphoramidite P,N ligand in a palladium(II) η^3 -allyl complex. <i>Computational and Theoretical Chemistry</i> , 2018, 1139, 70-76.	1.1	2
9911	Chloride Ion Transport by the <i>E. coli</i> CLC Cl ⁻ /H ⁺ Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study. <i>Frontiers in Chemistry</i> , 2018, 6, 62.	1.8	10
9912	Multiple Hydrogen-Bond Activation in Asymmetric Brønsted Acid Catalysis. <i>Chemistry - A European Journal</i> , 2018, 24, 7718-7723.	1.7	25
9913	Investigation of the upper rim binding of triphenylpyrylium cation with <i>p</i> -sulfonatocalix[4]arene. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2018, 91, 161-169.	0.9	2
9914	Translating Microscopic Molecular Motion into Macroscopic Body Motion: Reversible Self-Reshaping in the Solid State Transition of an Organic Crystal. <i>Crystal Growth and Design</i> , 2018, 18, 3535-3543.	1.4	11
9915	Colorimetric and fluorometric turn-on sensor for selective detection of fluoride ions: sol-gel transition studies and theoretical insights. <i>New Journal of Chemistry</i> , 2018, 42, 10406-10413.	1.4	7
9916	DFT based vibrational spectroscopic investigations and biological activity of toxic material monocrotophos. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	0
9917	Base Mechanism to the Hydrolysis of Phosphate Triester Promoted by the Cd^{2+} / Cd^{2+} Active site of Phosphotriesterase: A Computational Study. <i>Inorganic Chemistry</i> , 2018, 57, 5888-5902.	1.9	6
9918	Novel Phenothiazine-oxide Based Push-Pull Molecules: Synthesis and Fine-Tuning of Electronic, Optical and Thermal Properties. <i>ChemistrySelect</i> , 2018, 3, 5073-5081.	0.7	9

#	ARTICLE	IF	CITATIONS
9919	A novel potential anticancer chalcone: Synthesis, crystal structure and cytotoxic assay. <i>Journal of Molecular Structure</i> , 2018, 1168, 309-315.	1.8	11
9920	QM/MM Investigation for Protonation States in a Bilin Reductase PcyA-Biliverdin IX ϵ Complex. <i>ChemPhysChem</i> , 2018, 19, 1809-1813.	1.0	3
9921	A computational investigation on the antioxidant potential of myricetin 3,4-di-O- β -L-rhamnopyranoside. <i>Journal of Molecular Modeling</i> , 2018, 24, 133.	0.8	39
9922	Acidic amino acids: A new-type of enzyme mimics with application to biosensing and evaluating of antioxidant behaviour. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 201, 367-375.	2.0	15
9923	Highly porous defective carbons derived from seaweed biomass as efficient electrocatalysts for oxygen reduction in both alkaline and acidic media. <i>Carbon</i> , 2018, 137, 93-103.	5.4	64
9924	Modelling absorption and emission of a <i>meso</i> -aniline-BODIPY based dye with molecular mechanics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14537-14544.	1.3	11
9925	Solvent-Free Thermal Synthesis of Luminescent Dinuclear Cu(I) Complexes with Triarylphosphines. <i>Inorganic Chemistry</i> , 2018, 57, 5929-5938.	1.9	21
9926	Valence and charge-transfer optical properties for some Si $_n$ C $_m$ ($n, m \leq 12$) clusters: Comparing TD-DFT, complete-basis-limit EOMCC, and benchmarks from spectroscopy. <i>Journal of Chemical Physics</i> , 2018, 148, 174309.	1.2	1
9927	Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions. <i>Physical Review A</i> , 2018, 98, .	1.0	214
9928	Twist and Return-Induced Ring Strain Triggers Quick Relaxation of a <i>Z</i> -Stabilized Cyclobisazobenzene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4776-4781.	2.1	17
9929	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. <i>ACS Catalysis</i> , 2018, 8, 8751-8762.	5.5	53
9930	Rovibrational Considerations for the Monomers and Dimers of Magnesium Hydride and Magnesium Fluoride. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7079-7088.	1.1	14
9931	Kinetics of the Reaction of OH with Isoprene over a Wide Range of Temperature and Pressure Including Direct Observation of Equilibrium with the OH Adducts. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7239-7255.	1.1	16
9932	Synthesis and Reactivity of Group Six Metal PCP Pincer Complexes: Reversible CO Addition Across the Metal-C $_2$ aryl Bond. <i>Organometallics</i> , 2018, 37, 3631-3638.	1.1	13
9933	Mechanistic exploration of CpRe(CO) $_3$ -catalyzed coupling of chloromethyloxirane with CO $_2$: Unexpected potentials of CO ligands. <i>Molecular Catalysis</i> , 2018, 458, 25-32.	1.0	2
9934	Synthesis, Characterization, and Nanomaterials Generated from 6,6-((2-Hydroxyethyl)azanediyl)bis(methylene)bis(2,4-di- <i>tert</i> -butylphenol) Modified Group 4 Metal Alkoxides. <i>Inorganic Chemistry</i> , 2018, 57, 11264-11274.	1.9	8
9935	Expanding the Range of Force Fields Available for ONIOM Calculations: The SICTWO Interface. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1828-1835.	2.5	18
9936	Formation and Characterization of Zr $^{4+}$ Stabilized by Neutral Tridentate Ligands in the Gas Phase. <i>Journal of the American Society for Mass Spectrometry</i> , 2018, 29, 2327-2332.	1.2	9

#	ARTICLE	IF	CITATIONS
9937	Position of the anchoring group determined the sensitization efficiency of metal-free D- π -A dyes: Combined experimental and TD-DFT insights. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 367, 128-136.	2.0	7
9938	Time-resolved nuclear dynamics in bound and dissociating acetylene. <i>Structural Dynamics</i> , 2018, 5, 044302.	0.9	8
9939	Linear tricationic ionic liquids: Insights into the structural features using DFT and molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2018, 271, 96-104.	2.3	17
9940	Theoretical Study on the Electronic Structures and Charge Transport Properties of a Series of Rubrene Derivatives. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21226-21238.	1.5	16
9941	Theoretical investigations of the Ir-catalyzed direct borylation of B(3,6)- H of $\text{C}_{10}\text{H}_{12}$ -carborane: the actual catalyst, mechanism, and origin of regioselectivity. <i>Catalysis Science and Technology</i> , 2018, 8, 5165-5177.	2.1	22
9942	to $1 < L >$	0.9	17
9943	A systematic examination of ligand basicity effects on bonding in palladium(0)- and palladium(II)-ethylene complexes. <i>Inorganica Chimica Acta</i> , 2018, 483, 191-202.	1.2	2
9944	The Mechanism of C-H Bond Oxidation by Aqueous Permanganate. <i>Environmental Science & Technology</i> , 2018, 52, 9845-9850.	4.6	11
9945	Highly reversible sorption of H_2S and CO_2 by an environmentally friendly Mg-based MOF. <i>Journal of Materials Chemistry A</i> , 2018, 6, 16900-16909.	5.2	81
9946	Underwater adhesive using solid-liquid polymer mixes. <i>Materials Today Chemistry</i> , 2018, 9, 149-157.	1.7	25
9947	Gas-Phase Reactions of Carbon Dioxide with Copper Hydride Anions Cu_2H_2^+ : Temperature-Dependent Transformation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19379-19384.	1.5	26
9948	New Generation of the Reference Interaction Site Model Self-Consistent Field Method: Introduction of Constrained Spatial Electron Density Distribution (cSED). <i>Bulletin of the Chemical Society of Japan</i> , 2018, 91, 1540-1545.	2.0	20
9949	Reactions of sulfur and oxygen containing anions with nitrogen and oxygen atoms: A comparative study. <i>International Journal of Mass Spectrometry</i> , 2018, 433, 1-6.	0.7	5
9950	Triple resonance EPR spectroscopy determines the Mn^{2+} coordination to ATP. <i>Journal of Magnetic Resonance</i> , 2018, 294, 143-152.	1.2	6
9951	Toward a Predictive Understanding of Phosphine-Catalyzed [3 + 2] Annulation of Allenates with Acrylate or Imine. <i>Journal of Organic Chemistry</i> , 2018, 83, 9729-9740.	1.7	22
9952	Divergent Diels-Alder Reactions in the Biosynthesis and Synthesis of Endiandric-Type Tetracycles: A Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 10941-10947.	1.7	6
9953	DFT study on the Au-catalyzed cyclization of indole-allenoate: counterion and solvent effects. <i>New Journal of Chemistry</i> , 2018, 42, 15618-15628.	1.4	14
9954	Conversion of $\text{N-Acetylglucosamine}$ to Protected Amino Acid over Ru/C Catalyst. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 12411-12418.	3.2	46

#	ARTICLE	IF	CITATIONS
9955	Application of TensorFlow to recognition of visualized results of fragment molecular orbital (FMO) calculations. <i>Chem-Bio Informatics Journal</i> , 2018, 18, 58-69.	0.1	6
9956	Phosphatase-like Activity of Tetranuclear Iron(III) and Zinc(II) Complexes. <i>Inorganic Chemistry</i> , 2018, 57, 10802-10820.	1.9	36
9957	Electrochemical Generation and Spectroscopic Characterization of the Key Rhodium(III) Hydride Intermediates of Rhodium Poly(bipyridyl) H ₂ -Evolving Catalysts. <i>Inorganic Chemistry</i> , 2018, 57, 11225-11239.	1.9	21
9958	Exploring the nature of the clopidogrel-bromocresol green interaction via spectrophotometric measurements and quantum chemical calculations. <i>RSC Advances</i> , 2018, 8, 29104-29114.	1.7	1
9959	Fe ^{IV} sulfur clusters studied through photoelectron spectroscopy and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22610-22622.	1.3	4
9960	Metal-Organic Framework-Inspired Metal-Containing Clusters for High-Resolution Patterning. <i>Chemistry of Materials</i> , 2018, 30, 4124-4133.	3.2	65
9961	Evidence for a Sigmatropic and an Ionic Pathway in the Winstein Rearrangement. <i>Journal of Organic Chemistry</i> , 2018, 83, 8214-8224.	1.7	22
9962	Importance of the Molecular Orientation of an Iridium(III)-Heteroleptic Photosensitizer Immobilized on TiO ₂ Nanoparticles. <i>ACS Applied Energy Materials</i> , 2018, 1, 2882-2890.	2.5	12
9963	A prelude to building mathematical models for polypeptide folding: analysis on the conformational potential energy hypersurface cross-sections of N-acetyl-glycyl-glycine-N ² -methylamide. <i>Canadian Journal of Chemistry</i> , 2018, 96, 912-921.	0.6	0
9964	Dyad Sensitizer of Chlorophyll with Indoline Dye for Panchromatic Photocatalytic Hydrogen Evolution. <i>ACS Applied Energy Materials</i> , 2018, 1, 2813-2820.	2.5	51
9965	Lactamization of sp ² C-H bonds with CO ₂ under transition-metal-free and redox-neutral conditions: a computational mechanistic study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2189-2201.	2.3	8
9966	Beyond the Woodward-Hoffman Rules: What Controls Reactivity in Eliminative Aromatic Ring-Forming Reactions?. <i>Australian Journal of Chemistry</i> , 2018, 71, 249.	0.5	3
9967	Switchable Imidazole Platform Synthesis and Structural Investigation. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 4306-4316.	1.2	4
9968	The role of explicit solvent molecules in the calculation of NMR chemical shifts of glycine in water. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	16
9969	Symmetrical and unsymmetrical substituted 2,5-diarylidene cyclohexanones as anti-parasitic compounds. <i>European Journal of Medicinal Chemistry</i> , 2018, 155, 596-608.	2.6	17
9970	Molecular Electrostatic Potential: A New Tool to Predict the Lithiation Process of Organic Battery Materials. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3573-3579.	2.1	131
9971	Oxidation of Cymantrene Analogues of Ferrocifen: Electrochemical, Spectroscopic, and Computational Studies of the Parent Complex 1,1-Diphenyl-2-cymantrenylbutene. <i>Organometallics</i> , 2018, 37, 1910-1918.	1.1	6
9972	Loss of water from protonated polyglycines: interconversion and dissociation of the product imidazolone ions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18688-18698.	1.3	4

#	ARTICLE	IF	CITATIONS
9973	Iron(III) N^2 -Dialkylcarbamate-Catalyzed Formation of Cyclic Carbonates from CO_2 and Epoxides under Ambient Conditions by Dynamic CO_2 Trapping as Carbamate Ligands. <i>ChemSusChem</i> , 2018, 11, 2737-2743.	3.6	31
9974	Polymeric Copper Oxide: Preparation and Investigation of Its Structure and Optical Properties. <i>Journal of Inorganic and Organometallic Polymers and Materials</i> , 2018, 28, 2328-2335.	1.9	2
9975	Thermodynamics of radical scavenging of symmetric carotenoids and their charged species. <i>Food Chemistry</i> , 2018, 268, 542-549.	4.2	5
9976	Heteroleptic $\text{Cu}(\text{I})$ complexes bearing methoxycarbonyl-imidoylindazole and POP ligands: an experimental and theoretical study of their photophysical properties. <i>New Journal of Chemistry</i> , 2018, 42, 12576-12586.	1.4	12
9977	Molecular quantum cellular automata cell design trade-offs: latching vs. power dissipation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17881-17888.	1.3	18
9978	Theoretical investigation of differences of optical rotation, electronic circular dichroism and vibrational circular dichroism of α -hydroxyl cyclic ketones and esters as monomers or dimers in solution. <i>Tetrahedron</i> , 2018, 74, 4020-4028.	1.0	2
9979	Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 287-294.	0.5	1
9980	A DFT/PCM-based methodology for predicting solvolytic reactivities of organic carbonates. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 4665-4674.	1.5	5
9981	Ring-Opening of Epoxides Mediated by Frustrated Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 12669-12677.	1.7	22
9982	5-Selenocyanato and 5-trifluoromethanesulfonyl derivatives of 2-deoxyuridine: synthesis, radiation and computational chemistry as well as cytotoxicity. <i>RSC Advances</i> , 2018, 8, 21378-21388.	1.7	16
9983	Impact of the Valence Charge of Transition Metals on the Cobalt- and Rhodium-Catalyzed Synthesis of Indenamines, Indenols, and Isoquinolinium Salts: A Catalytic Cycle Involving $\text{M}^{\text{III}}/\text{M}^{\text{V}}$ [$\text{M} = \text{Co}, \text{Rh}$] for [4 + 2] Annulation. <i>Journal of Organic Chemistry</i> , 2018, 83, 7814-7824.	1.7	6
9984	Synthesis of C^1 -Unsubstituted 1,2-Diazetidines and Their Ring-Opening Reactions via Selective N^2 -Bond Cleavage. <i>Journal of Organic Chemistry</i> , 2018, 83, 9497-9503.	1.7	12
9985	Hydrophobic Nanoprecipitates of β -Cyclodextrin/Avermectins Inclusion Compounds Reveal Insecticide Activity against <i>Aedes aegypti</i> Larvae and Low Toxicity against Fibroblasts. <i>Journal of Agricultural and Food Chemistry</i> , 2018, 66, 7275-7285.	2.4	26
9986	Surface enhanced Raman scattering of neutral and zwitterionic α - and β -Proline monomers adsorbed on Au_3 cluster: A DFT study. <i>Vibrational Spectroscopy</i> , 2018, 98, 15-21.	1.2	3
9987	D^2H -benzo[<i>d</i>][1,2,3]triazole derivatives as p-type semiconductors in organic field-effect transistors. <i>RSC Advances</i> , 2018, 8, 21879-21888.	1.7	13
9988	Theoretical Studies on the Hydroaminoalkylation of Alkenes with Primary and Secondary Amines. <i>Chemistry - A European Journal</i> , 2018, 24, 12485-12489.	1.7	9
9989	First-Order Interacting Space Approach to Excited-State Molecular Interaction: Solvatochromic Shift of <i>p</i> -Coumaric Acid and Retinal Schiff Base. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3643-3655.	2.3	3
9990	Vibrational properties and bonding analysis of copper hexacyanoferrate complexes in solid state. <i>Applied Spectroscopy Reviews</i> , 2019, 54, 369-424.	3.4	9

#	ARTICLE	IF	CITATIONS
9991	Visible light absorption of surface-modified Al ₂ O ₃ powders: A comparative DFT and experimental study. <i>Microporous and Mesoporous Materials</i> , 2019, 273, 41-49.	2.2	15
9992	Theoretical studies on the feasibility of the hybrid nanocomposites of graphene quantum dot and phenoxazine-based dyes as an efficient sensitizer for dye-sensitized solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 216-223.	2.0	23
9993	Synthesis and DFT calculations of 2-thioxo-1,2-dihydropyridine-3-carbonitrile as versatile precursors for novel pharmacophoric hybrid molecules. <i>Journal of Molecular Structure</i> , 2019, 1176, 19-30.	1.8	12
9994	Spectroscopic investigation and computational studies on the interaction of Acriflavine with various estrogens. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 622-629.	2.0	5
9995	Computationally Assisted Assessment of the Metal-Organic Framework/Polymer Compatibility in Composites Integrating a Rigid Polymer. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900116.	1.3	5
9996	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. <i>ChemCatChem</i> , 2019, 11, 5068-5076.	1.8	5
9997	Cycloaddition of Nitrile Oxides to Graphene: a Theoretical and Experimental Approach. <i>Chemistry - A European Journal</i> , 2019, 25, 14644-14650.	1.7	9
9998	Systematic optimization of the substituents on the phenothiazine donor of doubly strapped porphyrin sensitizers: an efficiency over 11% unassisted by any cosensitizer or coadsorbent. <i>Journal of Materials Chemistry A</i> , 2019, 7, 20854-20860.	5.2	68
9999	Complementary Synthetic Approaches toward 9-Phosphatriptycene and Structure-Activity Investigations of Its Association with Sterically Hindered Lewis Acids. <i>Journal of Organic Chemistry</i> , 2019, 84, 11268-11274.	1.7	15
10000	A detailed mechanism of the oxidative half-reaction of <i>l</i> -tryptophan oxidase: another route for flavin oxidation. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7973-7984.	1.5	14
10001	In situ surface enhanced infrared absorption spectroscopy study of the adsorption of cytosine on gold electrodes. <i>Journal of Electroanalytical Chemistry</i> , 2019, 849, 113362.	1.9	5
10002	Efficient separation of vitamins mixture in aqueous solution using a stable zirconium-based metal-organic framework. <i>Journal of Colloid and Interface Science</i> , 2019, 555, 714-721.	5.0	18
10003	EnzyDock: Protein-Ligand Docking of Multiple Reactive States along a Reaction Coordinate in Enzymes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5116-5134.	2.3	28
10004	Analytical gradients for projection-based wavefunction-in-DFT embedding. <i>Journal of Chemical Physics</i> , 2019, 151, .	1.2	17
10005	1,2,3-Triazolium-Derived Mesoionic Carbene Ligands Bearing Chiral Sulfur-Based Moieties: Synthesis, Catalytic Properties, and Their Role in Chirality Transfer. <i>ACS Omega</i> , 2019, 4, 12983-12994.	1.6	11
10006	Can Hammett indicators accurately measure the acidity of zeolite catalysts with confined space? Insights into the mechanism of coloration. <i>Catalysis Science and Technology</i> , 2019, 9, 5045-5057.	2.1	11
10007	Exploring the possibilities of double proton transfer in hydrazides: A theoretical approach. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4003.	0.9	5
10008	Why Pore Width of Nanoporous Carbon Materials Determines the Preferred Solvated States of Alkaline Cations: A Density Functional Theory Calculation Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21457-21466.	1.5	8

#	ARTICLE	IF	CITATIONS
10009	Corroleâ€“Fullerene Dyads: Stability, Photophysical, and Redox Properties. <i>Journal of Physical Chemistry C</i> , 2019, 123, 20869-20876.	1.5	10
10010	Catalytic Conversion of a Chitin-Derived Sugar Alcohol to an Amide-Containing Isosorbide Analog. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 14883-14888.	3.2	22
10011	Formation of Metal Complexes with Malate Anions: Quantum-Chemical Modeling. <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 225-229.	0.3	4
10012	Molecular Dynamics Simulation of the Solvated Environment of 18-Crown-6 Ether in Mixed Ethanolâ€“Dimethylsulfoxide. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1513-1518.	0.1	1
10013	Importance of thorough conformational analysis in modelling transition metal-mediated reactions: Case studies on pincer complexes containing phosphine groups. <i>Journal of Saudi Chemical Society</i> , 2019, 23, 1206-1218.	2.4	6
10014	Peroxo-Cerium(IV)-Containing Polyoxometalates: [Ce ^{IV} ₆ (O ₂) ₉ (GeW ₁₀ O ₃₇) ₃] ²⁴⁻ as a Recyclable Homogeneous Oxidation Catalyst. <i>Inorganic Chemistry</i> , 2019, 58, 11300-11307.	1.9	23
10015	9-Cobalt(II)-Containing 27-Tungsto-3-germanate(IV): Synthesis, Structure, Computational Modeling, and Heterogeneous Water Oxidation Catalysis. <i>Inorganic Chemistry</i> , 2019, 58, 11308-11316.	1.9	23
10016	Statistically representative databases for density functional theory <i>via</i> data science. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19092-19103.	1.3	20
10017	Alkylation of 2-oxo(thioxo)-thieno[2,3-d]pyrimidine-4-ones: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2019, 1198, 126858.	1.8	16
10018	Norbornadieneâ€“dihydroazulene conjugates. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7735-7746.	1.5	25
10019	Solvent mediated complete trans-to-cis isomerization of [Ru(polypyridine)(CO)2Cl2] complexes. <i>Journal of Organometallic Chemistry</i> , 2019, 900, 120883.	0.8	1
10020	On the magnetic properties of nanodiamonds: Electronic <i>g</i> -tensor calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 044305.	1.2	4
10021	A stable artificial protective layer for high capacity dendrite-free lithium metal anode. <i>Nano Research</i> , 2019, 12, 2535-2542.	5.8	35
10022	Isosteric expansion of the structural diversity of chiral ligands: Design and application of proline-based N,Nâ€“2-dioxide ligands for copper-catalyzed enantioselective Henry reactions. <i>Tetrahedron</i> , 2019, 75, 130492.	1.0	7
10023	Cooperativity and serial ligand catalysis in an allylic amination reaction by Pd(ⁱⁱ)-bis-sulfoxide and Brønsted acids. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7723-7734.	1.5	2
10024	Synthesis and characterization of hydrazine-appended BODIPY dyes and the related aminomethyl complexes. <i>New Journal of Chemistry</i> , 2019, 43, 13103-13111.	1.4	4
10025	Two single-reference approaches to singlet biradicaloid problems: Complex, restricted orbitals and approximate spin-projection combined with regularized orbital-optimized MÅller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2019, 150, 244106.	1.2	36
10026	Calculating the Gibbs Energies of Solvation of 2,2'-Dipyridyl in Nonaqueous Solvents. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 1206-1208.	0.1	1

#	ARTICLE	IF	CITATIONS
10027	Solar cells sensitized with porphyrin dyes with a carbazole donor: The effects of an auxiliary benzothiadiazole acceptor and bulky substituents on the donor. <i>Dyes and Pigments</i> , 2019, 171, 107776.	2.0	13
10028	Phthalocyanines core-modified by P and S and their complexes with fullerene C60: DFT study. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	2
10029	Mechanistic Features in Al(I)-Mediated Oxidative Addition of Aryl C–F Bonds: Insights From Density Functional Theory Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 596.	1.8	11
10030	A New Look on Larger Sulfur and Selenium Rings – Dispersion Forces and Shapes of Larger Cycles. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 3846-3853.	1.0	15
10031	A DFT-based analysis of adsorption of Cd ²⁺ , Cr ³⁺ , Cu ²⁺ , Hg ²⁺ , Pb ²⁺ , and Zn ²⁺ , on vanillin monomer: a study of the removal of metal ions from effluents. <i>Journal of Molecular Modeling</i> , 2019, 25, 267.	0.8	38
10032	The Design of Quaternary Nitrogen Redox Center for High-Performance Organic Battery Materials. <i>Matter</i> , 2019, 1, 945-958.	5.0	71
10033	Synthesis, characterization and catalytic activity of novel ruthenium complexes bearing NNN click based ligands. <i>Dalton Transactions</i> , 2019, 48, 13580-13588.	1.6	15
10034	Facile preparation of a cationic COF functionalized magnetic nanoparticle and its use for the determination of nine hydroxylated polycyclic aromatic hydrocarbons in smokers'™ urine. <i>Analyst</i> , The, 2019, 144, 5829-5841.	1.7	36
10035	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7057-7074.	1.1	19
10036	Photoinduced Water–Heptazine Electron-Driven Proton Transfer: Perspective for Water Splitting with g-C ₃ N ₄ . <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4310-4316.	2.1	33
10037	Observation of Ultrafast Intersystem Crossing in Thymine by Extreme Ultraviolet Time-Resolved Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6897-6903.	1.1	29
10038	Efficient Protocol for Accurately Calculating ¹³ C Chemical Shifts of Conformationally Flexible Natural Products: Scope, Assessment, and Limitations. <i>Journal of Natural Products</i> , 2019, 82, 2299-2306.	1.5	87
10039	Direct Experimental Observation of in situ Dehydrogenation of an Amine–Borane System Using Gas Electron Diffraction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7104-7112.	1.1	5
10040	On the catalytic transfer hydrogenation of nitroarenes by a cubane-type Mo ₃ S ₄ cluster hydride: disentangling the nature of the reaction mechanism. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17221-17231.	1.3	6
10041	Mechanistic studies on the N-heterocyclic carbene-catalyzed reaction of isatin-derived enals with hydrazones. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 7442-7447.	1.5	25
10042	Computational Modeling for Biomimetic Sensors. <i>Methods in Molecular Biology</i> , 2019, 2027, 195-210.	0.4	4
10043	Detection and Identification of Reaction Intermediates in the Photorearrangement of Pyridazine <i>N</i> -Oxide: Discrepancies between Experiment and Theory. <i>Journal of Organic Chemistry</i> , 2019, 84, 10032-10039.	1.7	4
10044	Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6596-6604.	1.1	35

#	ARTICLE	IF	CITATIONS
10045	Calculations of the relative populations of Lu@C ₈₂ isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 710-714.	1.0	10
10047	Role of the Photosystem II as an Environment in the Oxidation Free Energy of the Mn Cluster from S ₁ to S ₂ . Journal of Physical Chemistry B, 2019, 123, 7081-7091.	1.2	5
10048	Magnetic descriptors of hydrogen bonds in malonaldehyde and its derivatives. Physical Chemistry Chemical Physics, 2019, 21, 19742-19754.	1.3	6
10049	Extent of conjugation in diazonium-derived layers in molecular junction devices determined by experiment and modelling. Physical Chemistry Chemical Physics, 2019, 21, 16762-16770.	1.3	8
10050	In silico analysis of heparin and chondroitin sulfate binding mechanisms of the antiprotozoal drug berenil and pentamidine. Carbohydrate Research, 2019, 482, 107742.	1.1	4
10051	Mechanistic insights into asymmetric transfer hydrogenation of pyruvic acid catalysed by chiral osmium complexes with formic acid assisted proton transfer. Chemical Communications, 2019, 55, 9633-9636.	2.2	8
10052	Bithiophene based red light emitting material - Photophysical and DFT studies. AIP Conference Proceedings, 2019, , .	0.3	2
10053	Structural basis of microcystinase activity for biodegrading microcystin-LR. Chemosphere, 2019, 236, 124281.	4.2	15
10054	Enantioselective Synthesis of \pm -Allyl Amino Esters via Hydrogen-Bond-Donor Catalysis. Journal of the American Chemical Society, 2019, 141, 11414-11419.	6.6	47
10055	Theoretical investigation of the chiral transition of serine and the roles of water, hydroxyl radical and hydroxide ion. New Journal of Chemistry, 2019, 43, 12340-12350.	1.4	1
10056	Vanadium(ν) complexes of mandelic acid. New Journal of Chemistry, 2019, 43, 17696-17702.	1.4	6
10057	Adsorption Forms of Water Molecules on Gas-Phase Platinum Clusters Pt ₃ ⁺ Studied by Vibrational Photodissociation Spectroscopy. Zeitschrift Fur Physikalische Chemie, 2019, 233, 881-894.	1.4	6
10058	Enantioselective Synthesis of β -Heterosubstituted α -Amino Alcohols by Sequential Metal-Free Diene Aziridination/Kinetic Resolution. Chemistry - A European Journal, 2019, 25, 12628-12635.	1.7	4
10059	D ₃ TADF emitters: the role of the density of states for achieving faster triplet harvesting rates. Journal of Materials Chemistry C, 2019, 7, 12942-12952.	2.7	22
10060	Dimethylphenylphosphine oxide coordinated trivalent rhenium featuring pyridylbenzazole chelation: Oxygen atom transfer kinetics, isomer preference, metal oxidation and computational analysis. Polyhedron, 2019, 171, 112-119.	1.0	0
10061	A comparative theoretical study on the optoelectronic and nonlinear optical properties of [Pt(bpy)(qdt)] derivatives with electron-donating and -withdrawing anchors. New Journal of Chemistry, 2019, 43, 12865-12873.	1.4	3
10062	A proposal for the structure of high- and low-density fluctuations in liquid water. Journal of Chemical Physics, 2019, 151, 034508.	1.2	39
10063	Ligands and Bases Mediate Switching between Aminocarbonylations and Alkoxy carbonylations in Coupling of Aminophenols with Iodoarenes. Inorganic Chemistry, 2019, 58, 10217-10226.	1.9	8

#	ARTICLE	IF	CITATIONS
10064	Hydroalkynylation of Enamides Using Iridium or Rhodium Complexes: DFT Study on the Mechanism and Regioselectivity. <i>Organometallics</i> , 2019, 38, 2998-3006.	1.1	17
10065	Determination of ¹³ C NMR Chemical Shift Structural Ranges for Polycyclic Aromatic Hydrocarbons (PAHs) and PAHs in Asphaltenes: An Experimental and Theoretical Density Functional Theory Study. <i>Energy & Fuels</i> , 2019, 33, 7950-7970.	2.5	21
10066	Supported Boron Oxide Catalysts for Selective and Low-Temperature Oxidative Dehydrogenation of Propane. <i>ACS Catalysis</i> , 2019, 9, 8263-8270.	5.5	114
10067	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7087-7103.	1.1	32
10068	U2C Unit in Fullerenes: Robust Multicenter Bonds with a Cluster Shape Controlled by Cage Size and Charge Transfer. <i>Inorganic Chemistry</i> , 2019, 58, 10648-10655.	1.9	10
10069	Ionic liquids from a fragmented perspective. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16878-16888.	1.3	10
10070	Experimental and theoretical insights into spectroscopy and electrochemistry of Re(I) carbonyl with oxazoline-based ligand. <i>Polyhedron</i> , 2019, 171, 551-558.	1.0	8
10071	Energy Decomposition Analysis of Protein-Ligand Interactions Using Molecules-in-Molecules Fragmentation-Based Method. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3474-3484.	2.5	35
10072	An azobenzene container showing a definite folding â€” synthesis and structural investigation. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 1534-1544.	1.3	5
10073	Functionalized pyrene-based AlEgens: synthesis, photophysical characterization and density functional theory studies. <i>Luminescence</i> , 2019, 34, 715-723.	1.5	5
10074	A facile synthesis of seven-membered N, O-ligands and their optical properties. <i>Journal of Molecular Structure</i> , 2019, 1197, 714-718.	1.8	4
10075	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17410-17422.	1.3	15
10076	Using Ultrafast X-ray Spectroscopy To Address Questions in Ligand-Field Theory: The Excited State Spin and Structure of [Fe(dcpp) ₂] ²⁺ . <i>Inorganic Chemistry</i> , 2019, 58, 9341-9350.	1.9	29
10077	Structures and Dissociation Products of Ce/Peptide Complexes: Competition between Coordination and Charge Delocalization. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5229-5237.	1.2	1
10078	Origin of Regiochemical Control in Rh(III)/Rh(V)-Catalyzed Reactions of Unsaturated Oximes and Alkenes to Form Pyridines. <i>ACS Catalysis</i> , 2019, 9, 7154-7165.	5.5	40
10079	Sâ€”H rotamerization <i>via</i> tunneling in a thiol form of thioacetamide. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17063-17071.	1.3	17
10080	A computational study on the identity of the active catalyst structure for Ru(II) carboxylate assisted Câ€”H activation in acetonitrile. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6678-6686.	1.5	3
10081	Liquid water structure from X-ray absorption and emission, NMR shielding and X-ray diffraction. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019, 62, 1.	2.0	5

#	ARTICLE	IF	CITATIONS
10082	Comparative DFT study on the platinum catalyzed $[3\pi+2\pi]$ and $[2\pi+2\pi]$ cycloaddition reactions between the derivatives of allene and alkene. Computational and Theoretical Chemistry, 2019, 1163, 112507.	1.1	2
10083	Facile Fluorescence Monitoring of Gut Microbial Metabolite Trimethylamine <i>N</i> -oxide via Molecular Recognition of Guanidinium-Modified Calixarene. Theranostics, 2019, 9, 4624-4632.	4.6	41
10084	Thermodynamic of solvation, solute π -Solvent electron transfer and ionization potential of BSCAPE molecule and its UV-vis spectra in aqueous solution. Journal of Molecular Graphics and Modelling, 2019, 92, 100-111.	1.3	5
10085	Second-Generation Synthesis of the Northern Fragment of Mandelalide A: Role of π -Stacking on Sharpless Dihydroxylation of <i>cis</i> -Enynes. Journal of Organic Chemistry, 2019, 84, 9196-9214.	1.7	6
10086	Scrutinizing the substituent effect on Mo-based electrocatalysts for molecular hydrogen release through axial-equatorial decomposition: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 16601-16614.	1.3	12
10087	Denitrogenative Hydrotrifluoromethylation of Benzaldehyde Hydrazones: Synthesis of (2,2,2-trifluoroethyl)arenes. Chemistry - A European Journal, 2019, 25, 11240-11245.	1.7	10
10088	First Direct Evidence of an <i>ortho</i> -Lithiated Aryloxetane: Solid and Solution Structure, and Dynamics. European Journal of Organic Chemistry, 2019, 2019, 5549-5556.	1.2	6
10089	Host-guest interactions between <i>p</i> -sulfonatocalix[4]arene and <i>p</i> -sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study. Beilstein Journal of Organic Chemistry, 2019, 15, 1321-1330.	1.3	8
10090	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. Journal of Physical Chemistry B, 2019, 123, 10073-10082.	1.2	18
10091	Flexibility in the Graphene Sheet: The Influence on Gas Adsorption from Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 28035-28047.	1.5	14
10092	Virtual Excited State Reference for the Discovery of Electronic Materials Database: An Open-Access Resource for Ground and Excited State Properties of Organic Molecules. Journal of Physical Chemistry Letters, 2019, 10, 6835-6841.	2.1	19
10093	A merged copper(I/II) cluster isolated from Glaser coupling. Nature Communications, 2019, 10, 4848.	5.8	36
10094	The ruthenium-ruthenium bonding in bridged ligand system: QTAIM study of $[\text{Ru}_3(\eta^4\text{-C}_6\text{H}_6)_2(\text{MelmCH})(\text{CO})_9]$ complex. AIP Conference Proceedings, 2019, , .	0.3	0
10095	Computational Exploration of Chiral Iron Porphyrin-Catalyzed Asymmetric Hydroxylation of Ethylbenzene Where Stereoselectivity Arises from π -Stacking Interaction. Journal of Organic Chemistry, 2019, 84, 13755-13763.	1.7	10
10096	Mechanisms for Hydrogen-Atom Abstraction by Mononuclear Copper(III) Cores: Hydrogen-Atom Transfer or Concerted Proton-Coupled Electron Transfer?. Journal of the American Chemical Society, 2019, 141, 17236-17244.	6.6	55
10097	Old Concepts, New Application π -Additive-Free Hydrogenation of Nitriles Catalyzed by an Air Stable Alkyl Mn(I) Complex. Advanced Synthesis and Catalysis, 2019, 361, 5412-5420.	2.1	41
10098	Blue LED Irradiation of Iodonium Ylides Gives Diradical Intermediates for Efficient Metal-Free Cyclopropanation with Alkenes. Angewandte Chemie, 2019, 131, 17115-17121.	1.6	10
10099	Blue LED Irradiation of Iodonium Ylides Gives Diradical Intermediates for Efficient Metal-Free Cyclopropanation with Alkenes. Angewandte Chemie - International Edition, 2019, 58, 16959-16965.	7.2	28

#	ARTICLE	IF	CITATIONS
10100	Coupling Constants, High Spin, and Broken Symmetry States of Organic Radicals: an Assessment of the Molecules-in-Molecules Fragmentation-Based Method. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5998-6009.	2.3	6
10101	New insights into differential aggregation of enantiomerically pure and racemic Al^{240} systems. <i>Peptide Science</i> , 2019, 111, e24139.	1.0	13
10102	Theoretical Quantum Control of Fluctuating Molecular Energy Levels in Complex Chemical Environments. <i>Advanced Quantum Technologies</i> , 2019, 2, 1800099.	1.8	1
10103	DFT and experimental study of triallylborane-mediated isomerization of $\hat{\pm}$ -allylated azaheterocycles. <i>Mendeleev Communications</i> , 2019, 29, 190-193.	0.6	4
10104	Accurate pK_a Evaluations for Complex Bio-Organic Molecules in Aqueous Media. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6025-6035.	2.3	31
10105	$\text{Ir/Thioether-Carbene}$, $\hat{\sim}$ Phosphinite, and $\hat{\sim}$ Phosphite Complexes for Asymmetric Hydrogenation. A Case for Comparison. <i>Organometallics</i> , 2019, 38, 4193-4205.	1.1	12
10106	Effectiveness of the bimetallic catalytic center over the monometallic one for catalyzing the rearrangement of cyclopropanated bicyclic derivatives. <i>Journal of Organometallic Chemistry</i> , 2019, 899, 120907.	0.8	1
10107	Computational Exploration of NO Single-Site Disproportionation on Fe-MOF-5. <i>Chemistry of Materials</i> , 2019, 31, 8875-8885.	3.2	20
10108	Ir-C^{N} Conjugation Enables Ultra-High Rate Capabilities and Cycling Stabilities in Phenothiazine Copolymers as Cathode-Active Battery Materials. <i>Advanced Functional Materials</i> , 2019, 29, 1906436.	7.8	88
10109	The Reliability of the Density-Functional Theory in Actinide Endohedral Systems. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900138.	1.3	8
10110	Mechanistic study of the solvent-controlled Pd(ii)-catalyzed chemoselective intermolecular 1,2-aminoxygenation and 1,2-oxyamination of conjugated dienes. <i>Organic Chemistry Frontiers</i> , 2019, 6, 486-492.	2.3	18
10111	Orbital angular momentum constraints in the variational optimization of the two-electron reduced-density matrix. <i>Physical Review A</i> , 2019, 100, .	1.0	9
10112	Star-Shaped Diketopyrrolopyrrole-Zinc Porphyrin that Delivers 900 nm Emission in Light-Emitting Electrochemical Cells. <i>Chemistry of Materials</i> , 2019, 31, 9721-9728.	3.2	34
10113	A theoretical investigation on the activation of small molecules by a disilenide: aDFT prediction. <i>Turkish Journal of Chemistry</i> , 2019, 43, 936-947.	0.5	0
10114	Influence of steric and electronic effect of carrier ligand on kinetics & mechanism of Pt(II) complexes with l-cysteine and its substituted derivatives: Their experimental and DFT-based theoretical study. <i>Inorganica Chimica Acta</i> , 2019, 498, 119117.	1.2	7
10115	Density Functional Computations for Co(I)-Catalyzed Intermolecular Hydroacylation of Benzaldehydes. <i>ChemistrySelect</i> , 2019, 4, 11315-11320.	0.7	1
10116	Tools for Prescreening the Most Active Sites on Ir and Rh Clusters toward C-H Bond Cleavage of Ethane: NBO Charges and Wiberg Bond Indexes. <i>ACS Omega</i> , 2019, 4, 18809-18819.	1.6	10
10117	Accurate and efficient DFT-based diabaticization for hole and electron transfer using absolutely localized molecular orbitals. <i>Journal of Chemical Physics</i> , 2019, 151, 164114.	1.2	17

#	ARTICLE	IF	CITATIONS
10118	Mechanomagnetics in Elastic Crystals: Insights from [Cu(acac) ₂]. <i>Angewandte Chemie</i> , 2019, 131, 15226-15232.	1.6	10
10119	Carboxylate Structural Effects on the Properties and Proton-Coupled Electron Transfer Reactivity of [CuO ₂ CR] ²⁺ Cores. <i>Inorganic Chemistry</i> , 2019, 58, 15872-15879.	1.9	16
10120	Thermalized Epoxide Formation in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10620-10630.	1.1	11
10121	Stacks of Metalloporphyrins: Comparison of Experimental and Computational Results. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10044-10060.	1.2	1
10122	Redetermination of the Structure of a Water-Soluble Hypervalent Iodine(V) Reagent AIBX and Its Synthetic Utility in the Oxidation of Alcohols and Synthesis of IsoxazolineN-Oxides. <i>Journal of Organic Chemistry</i> , 2019, 84, 14381-14393.	1.7	12
10123	External stimulus controlled recombination of hydrogen in photochromic dithienylethene frustrated lewis pairs. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 31141-31152.	3.8	11
10124	Doubly Charged Small Organic Fragments Derived from [Ce(tripeptide)(CH ₃ CN) _m] ³⁺ Complexes: Observation of the Elusive [bn + H] ²⁺ Ions. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10192-10201.	1.2	0
10125	Second-Order Perturbation Theory with Spin-Symmetry-Projected Hartree-Fock. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6688-6702.	2.3	10
10126	Palladium-Catalyzed C ₈ -Arylation of Naphthalenes through C [∞] H Activation: A Combined Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2019, 25, 14441-14446.	1.7	15
10127	Tetrapositive Hafnium-Diamide Complexes in the Gas Phase: Formation, Structure and Reaction. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 2623-2631.	1.2	5
10128	Investigating the Microstructure of Poly(cyclosilane) by ²⁹ Si Solid-State NMR Spectroscopy and DFT Calculations. <i>Chemistry of Materials</i> , 2019, 31, 9168-9178.	3.2	16
10129	Donor-Acceptor π -Conjugated Enamines: Functional Group-Compatible Synthesis from Amides and Their Photoabsorption and Photoluminescence Properties. <i>Journal of Organic Chemistry</i> , 2019, 84, 15236-15254.	1.7	13
10130	Rotational and vibrational fingerprints of the oxywater cation (H ₂ OO ⁺), a possible precursor to abiotic O ₂ . <i>Journal of Molecular Spectroscopy</i> , 2019, 364, 111183.	0.4	3
10131	Computational Study of the Oxidation of Guanine To Form 5-Carboxyamido-5-formamido-2-iminohydantoin (2lh). <i>Chemical Research in Toxicology</i> , 2019, 32, 2295-2304.	1.7	6
10132	High-Spin Mn(V)-Oxo Intermediate in Nonheme Manganese Complex-Catalyzed Alkane Hydroxylation Reaction: Experimental and Theoretical Approach. <i>Inorganic Chemistry</i> , 2019, 58, 14842-14852.	1.9	46
10133	Photostable Voltage-Sensitive Dyes Based on Simple, Solvatofluorochromic, Asymmetric Thiazolothiazoles. <i>Journal of the American Chemical Society</i> , 2019, 141, 18780-18790.	6.6	73
10134	The topological classification of the bonding in[(Cp [∞] Ru) ₂ (Cp [∞] Os)(η^3 -N) ₂ (η^4 -H) ₃] cluster. , 2019, , .		3
10135	The Fundamental Vibrational Frequencies and Spectroscopic Constants of the Dicyanoamine Anion, NCNCN ⁻ (C ₂ N ₃ ⁻): Quantum Chemical Analysis for Astrophysical and Planetary Environments. <i>Astrophysical Journal</i> , 2019, 883, 109.	1.6	5

#	ARTICLE	IF	CITATIONS
10136	Role of Graphitic Nitrogen and π -Conjugated Functional Groups in Selective Oxidation of Alcohols: A DFT based Mechanistic Elucidation. <i>Chemistry - an Asian Journal</i> , 2019, 14, 4798-4806.	1.7	2
10137	Mechanomagnetics in Elastic Crystals: Insights from $[\text{Cu}(\text{acac})_2]$. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 15082-15088.	7.2	36
10138	Covalent modification of phosphatidylethanolamine by 4-hydroxy-2-nonenal increases sodium permeability across phospholipid bilayer membranes. <i>Free Radical Biology and Medicine</i> , 2019, 143, 433-440.	1.3	13
10139	Strategies for Enhancing the Rate Constant of C-H Bond Cleavage by Concerted Proton-Coupled Electron Transfer. <i>Journal of the American Chemical Society</i> , 2019, 141, 15183-15189.	6.6	22
10140	Direct C-H Bond Imidation with Benzoyl Peroxide as a Mild Oxidant and a Reagent. <i>Journal of Organic Chemistry</i> , 2019, 84, 12992-13002.	1.7	22
10141	Synthesis, Characterization, and Photochromic Studies of Cyclometalated Iridium(III) Complexes Containing a Spiroanthoxazine Moiety. <i>Organometallics</i> , 2019, 38, 3542-3552.	1.1	14
10142	Improving Predicted Nuclear Magnetic Resonance Chemical Shifts Using the Quasi-Harmonic Approximation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5259-5274.	2.3	11
10143	Insight into the Origin of Competitive Emission of Copper(I) Complexes Bearing Diimine and Diphosphine Ligands. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 1684-1693.	2.0	12
10144	A comparison between $(\text{a}/\text{n-NHC})\text{PdX}_2(\text{pyridine})$ and $(\text{a}/\text{n-NHC})_2\text{PdX}_2$ ($\text{X} = \text{I}, \text{Cl}$) type complexes of abnormal fused-bicyclic imidazo[1,2-a]pyridine based N-heterocyclic carbene (a-NHC) and of normal imidazole based N-heterocyclic carbene (n-NHC) ligands in the Suzuki-Miyaura coupling reactions. <i>Inorganica Chimica Acta</i> , 2019, 498, 119090.	1.2	2
10145	Conducting poly(aniline blue)-gold nanoparticles composite modified fluorine-doped tin oxide electrode for sensitive and non-enzymatic electrochemical detection of glucose. <i>Journal of Electroanalytical Chemistry</i> , 2019, 850, 113394.	1.9	26
10146	DFT based engineering of N-heterocyclic carbenes to exacerbate its activity for SO_2 fixation and storage. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 93, 107437.	1.3	7
10147	Excited-state investigations of meso-mono-substituted-(amino-ferrocenyl)porphyrins: Experimental and theoretical approaches. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 384, 112048.	2.0	3
10148	A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. <i>Inorganic Chemistry</i> , 2019, 58, 12157-12166.	1.9	4
10149	Can the distinguishable cluster approximation be improved systematically by including connected triples?. <i>Journal of Chemical Physics</i> , 2019, 151, .	1.2	13
10150	Switchable second-order nonlinear optical response of platinum-sensitized dithienylethenes. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950022.	1.8	0
10151	Proton transfer in the benzimidazolone and benzimidazolthione tautomerism process catalyzed by polar protic solvents. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019, 44, 143-156.	1.1	4
10152	Computational Prediction of Ammonia-Borane Dehydrocoupling and Transfer Hydrogenation of Ketones and Imines Catalyzed by SCS Nickel Pincer Complexes. <i>Frontiers in Chemistry</i> , 2019, 7, 627.	1.8	8
10153	A trade-off for covalent and intercalation binding modes: a case study for Copper (II) ions and singly modified DNA nucleoside. <i>Scientific Reports</i> , 2019, 9, 12602.	1.6	2

#	ARTICLE	IF	CITATIONS
10154	Exploring the Excited-State Dynamics of Hydrocarbon Radicals, Biradicals, and Carbenes Using Time-Resolved Photoelectron Spectroscopy and Field-Induced Surface Hopping Simulations. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10643-10662.	1.1	11
10155	Chemical and Physical Viewpoints About the Bonding in Fullerene-Graphene Hybrid Materials: Interaction on Pristine and Fe-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 24209-24219.	1.5	13
10156	The Role for the Weak Interaction on the Stabilization of Copper-Containing Complex: DFT Investigation of Noncovalent Interactions in Ternary-Cu(II) (DA)(AA) Complexes (DA = Diamine and AA =) <i>Tj ETQq0 0.0 rgBT /Qverlock 10</i> 1874-1882.	2.0	7
10157	Further understanding of the Ru-centered [2+2] cycloreversion/cycloaddition involved into the interconversion of ruthenacyclobutane using the Grubbs catalysts from a reaction force analysis. <i>Journal of Molecular Modeling</i> , 2019, 25, 305.	0.8	4
10158	Computational characterization of the glutamate receptor antagonist perampanel and its close analogs: density functional exploration of conformational space and molecular docking study. <i>Journal of Molecular Modeling</i> , 2019, 25, 312.	0.8	7
10159	Probing the Partial Activation of Water by Open-Shell Interactions, $Cl(H_2O)_4$. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8657-8673.	1.1	9
10160	Theoretical Study on the C-H Activation of Methane by Liquid Metal Indium: Catalytic Activity of Small Indium Clusters. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8907-8912.	1.1	16
10161	Discriminatory Photoactivation of Diastereomeric RAFT Agents. <i>Macromolecules</i> , 2019, 52, 7157-7166.	2.2	14
10162	DFT Study of PNP-Mn-Catalyzed Acceptorless Dehydrogenative Coupling of Primary Alcohols with Hydrazine to Give Alkene or Azine. <i>Organometallics</i> , 2019, 38, 3590-3601.	1.1	6
10163	Synthesis, crystallographic studies, molecular modeling and in vitro biological studies of silver(I) complexes with aminoadamantane ligands. <i>Polyhedron</i> , 2019, 173, 114116.	1.0	11
10164	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 609.	1.8	3
10165	Mechanistic Insight into the Ring-Opening Polymerization of ϵ -Caprolactone and L-Lactide Using Ketimine-Ligated Aluminum Catalysts. <i>Polymers</i> , 2019, 11, 1530.	2.0	7
10166	Tracking Proton Transfer through Titratable Amino Acid Side Chains in Adaptive QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5794-5809.	2.3	18
10167	Machine Learning in Computational Chemistry: An Evaluation of Method Performance for Nudged Elastic Band Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6513-6523.	2.3	19
10168	Anti-inflammatory Chalcone-Isoflavone Dimers and Chalcone Dimers from <i>Caragana jubata</i> . <i>Journal of Natural Products</i> , 2019, 82, 2761-2767.	1.5	21
10169	Ab Initio/Transition-State Theory Study of the Reactions of H_5^+ Species of Relevance to 1,3-Pentadiene, Part I: Potential Energy Surfaces, Thermochemistry, and High-Pressure Limiting Rate Constants. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9019-9052.	1.1	19
10170	Chameleon-like Behavior of the Directing Group in the Rh(III)-Catalyzed Regioselective C-H Amidation of Indole: An Experimental and Computational Study. <i>ACS Catalysis</i> , 2019, 9, 10233-10244.	5.5	40
10171	Theoretical investigation of the reactivity of bispentamethylcyclopentadienyl uranium(IV) bistiolate complexes with the heteroallene molecules CS ₂ and CO ₂ . <i>Journal of Organometallic Chemistry</i> , 2019, 901, 120947.	0.8	5

#	ARTICLE	IF	CITATIONS
10172	Electronic and Geometric Effects on Chemical Reactivity of 3d-Transition-Metal-Doped Silver Cluster Cations toward Oxygen Molecules. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25890-25897.	1.5	12
10173	Atom-Based Bootstrap Embedding For Molecules. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6368-6374.	2.1	14
10174	Unravelling the Reaction Mechanism of Formic Acid Dehydrogenation by Cp*Rh(III) and Cp*Co(III) Catalysts with Proton-Responsive 4,4'- and 6,6'-Dihydroxy-2,2'-Bipyridine Ligands: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25061-25073.	1.5	12
10175	Proton Abstraction Mediates Interactions between the Super Photobase FR0-SB and Surrounding Alcohol Solvent. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8448-8456.	1.2	9
10176	Engineering of lysine cyclodeaminase conformational dynamics for relieving substrate and product inhibitions in the biosynthesis of <i>l</i> -proline. <i>Catalysis Science and Technology</i> , 2019, 9, 398-405.	2.1	11
10177	Discrete mononuclear and dinuclear compounds containing a MoO ₂ core and 4-aminobenzhydrazone ligands: synthesis, structure and organic-solvent-free epoxidation activity. <i>New Journal of Chemistry</i> , 2019, 43, 1791-1802.	1.4	26
10178	Understanding the <i>Z</i> -selectivity of the metal-free intermolecular aminoarylation of alkynes: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 125-133.	2.3	9
10179	Molecular design and synthesis of D-structured porphyrin dyes with various acceptor units for dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2019, 7, 2843-2852.	2.7	73
10180	Adaptive Partitioning QM/MM for Molecular Dynamics Simulations: 6. Proton Transport through a Biological Channel. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 892-905.	2.3	27
10181	Strategies towards rational design of gold(III) complexes for high-performance organic light-emitting devices. <i>Nature Photonics</i> , 2019, 13, 185-191.	15.6	118
10182	Probing enantioselectivity in rhodium-catalyzed Si-C bond cleavage to construct silicon-stereocenters: a theoretical study. <i>Catalysis Science and Technology</i> , 2019, 9, 646-651.	2.1	8
10183	Charge transport and glassy dynamics in polymeric ionic liquids as reflected by their inter- and intramolecular interactions. <i>Soft Matter</i> , 2019, 15, 1605-1618.	1.2	16
10184	A theoretical study of 5,6,7,8-tetrahydro-6-hydroxymethylpterin: insight into intrinsic photoreceptor properties of 6-substituted tetrahydropterins. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 516-523.	1.6	6
10185	Vertical Ionization Energies and Electron Affinities of Native and Damaged DNA Bases, Nucleotides, and Pairs from Density Functional Theory Calculations: Model Assessment and Implications for DNA Damage Recognition and Repair. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2042-2052.	2.3	19
10186	Curved Polar Dibenzocoronene Esters and Imides versus Their Planar Centrosymmetric Homologs: Photophysical and Optoelectronic Analysis. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4483-4492.	1.5	22
10187	Computational Insights into the Catalytic Mechanism of Bacterial Carboxylic Acid Reductase. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 832-841.	2.5	26
10188	Hole Hopping Across a Protein-Protein Interface. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1578-1591.	1.2	8
10189	Structural Changes of the Trinuclear Copper Center in Bilirubin Oxidase upon Reduction. <i>Molecules</i> , 2019, 24, 76.	1.7	3

#	ARTICLE	IF	CITATIONS
10190	A theoretical and experimental study: the influence of different standards on the determination of total phenol content in the Folin-Ciocalteu assay. <i>Journal of Food Measurement and Characterization</i> , 2019, 13, 1349-1356.	1.6	22
10191	Combined high resolution X-ray and DFT Bader analysis to reveal a proposed Ru-H π -Si interaction in Cp(IPr)Ru(H)2SiH(Ph)Cl. <i>Inorganica Chimica Acta</i> , 2019, 488, 292-298.	1.2	6
10192	Unimolecular Reactions of Peroxy Radicals Formed in the Oxidation of β -Pinene and γ -Pinene by Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1661-1674.	1.1	75
10193	Correlation between molecular acidity (pKa) and vibrational spectroscopy. <i>Journal of Molecular Modeling</i> , 2019, 25, 48.	0.8	8
10194	Computational evaluation of the chemical warfare agents capture performances of robust MOFs. <i>Microporous and Mesoporous Materials</i> , 2019, 280, 97-104.	2.2	19
10195	Constructing Molecular π -Orbital Active Spaces for Multireference Calculations of Conjugated Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1679-1689.	2.3	33
10196	Catalytic performance of bis(imino)pyridine Fe/Co complexes toward ethylene polymerization by 2D-QSPR modeling. <i>Journal of Computational Chemistry</i> , 2019, 40, 1374-1386.	1.5	14
10197	A Noncovalent Fluorescence Turn-On Strategy for Hypoxia Imaging. <i>Angewandte Chemie</i> , 2019, 131, 2399-2403.	1.6	24
10198	A Noncovalent Fluorescence Turn-On Strategy for Hypoxia Imaging. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2377-2381.	7.2	123
10199	Exploring the Mechanism of a Chiral <i>N</i> -Alkyl Imine-Based Light-Driven Molecular Rotary Motor at MS-CASPT2/CASSCF and MS-CASPT2/(TD) DFT Levels. <i>Chemistry - A European Journal</i> , 2019, 25, 4194-4201.	1.7	13
10200	Synthesis, crystal structure, self-assembly of C60 derivatives bearing rigid pyridine substituents. <i>RSC Advances</i> , 2019, 9, 3050-3055.	1.7	2
10201	A computational study on ligand assisted vs. ligand participation mechanisms for CO ₂ hydrogenation: importance of bifunctional ligand based catalysts. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3932-3941.	1.3	16
10202	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2966-2990.	1.1	76
10203	Atomic photoionization cross sections beyond the electric dipole approximation. <i>Journal of Chemical Physics</i> , 2019, 150, 044306.	1.2	5
10204	The ArNH^+ noble gas molecule: Stability, vibrational frequencies, and spectroscopic constants. <i>Journal of Molecular Spectroscopy</i> , 2019, 357, 4-8.	1.9	10
10205	Charge-transfer or excimeric state? Exploring the nature of the excited state in cofacially arrayed polyfluorene derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 374, 125-130.	2.0	2
10206	Forging Ru-C ^{sp2} Bonds in Paddlewheel Complexes Using the Lithium-Halogen Exchange Reaction. <i>Inorganic Chemistry</i> , 2019, 58, 2618-2626.	1.9	8
10207	Corrected Structure of Natural Hyacinthacine C ₁ via Total Synthesis. <i>Journal of Natural Products</i> , 2019, 82, 358-367.	1.5	10

#	ARTICLE	IF	CITATIONS
10208	The effect of 2-, 3- and 4-pyridyl substituents on photophysics of fac-[ReCl(CO) ₃ (n-pytpy- $\hat{\text{I}}^{\text{2N}}$)] complexes: Experimental and theoretical insights. <i>Journal of Luminescence</i> , 2019, 209, 346-356.	1.5	8
10209	Visible-light-responsive surface-modified TiO ₂ powder with 4-chlorophenol: A combined experimental and DFT study. <i>Optical Materials</i> , 2019, 89, 237-242.	1.7	20
10210	Quantum Chemical Study on the High-Pressure Effect for [4 + 4] Retrocycloaddition of Anthracene Cyclophane Photodimer. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4493-4501.	1.5	6
10211	Prediction on the origin of selectivities of NHC-catalyzed asymmetric dearomatization (CADA) reactions. <i>Catalysis Science and Technology</i> , 2019, 9, 465-476.	2.1	50
10212	A mechanistic investigation into N-heterocyclic carbene (NHC) catalyzed umpolung of ketones and benzonitriles: is the cyano group better than the classical carbonyl group for the addition of NHC?. <i>Organic Chemistry Frontiers</i> , 2019, 6, 523-531.	2.3	4
10213	Mega-stokes pyrene ceramide conjugates for STED imaging of lipid droplets in live cells. <i>Analyst</i> , The, 2019, 144, 1608-1621.	1.7	22
10214	Theoretical studies on the mechanism of Ru($\langle \text{sc} \rangle \text{ii} \langle / \text{sc} \rangle$)-catalyzed regioselective C-H allylation of indoles with allyl alcohols. <i>Dalton Transactions</i> , 2019, 48, 9181-9186.	1.6	3
10215	On the origins of stereoselectivity in the aminocatalytic remote alkylation of 5-alkylfurfurals. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6025-6031.	1.5	8
10216	Computational investigation of catalytic effects of CX ₃ COOH (X = F, Cl, H) on the three-component cyclocondensation reaction. <i>Journal of Molecular Modeling</i> , 2019, 25, 173.	0.8	6
10217	Synergistic Effect of i-C ₃ F ₇ CN/CO ₂ and i-C ₃ F ₇ CN/N ₂ Mixtures. <i>IEEE Access</i> , 2019, 7, 50159-50167.	2.6	8
10218	On the Design of Host-Guest Light-Emitting Electrochemical Cells: Should the Guest be Physically Blended or Chemically Incorporated into the Host for Efficient Emission?. <i>Advanced Optical Materials</i> , 2019, 7, 1900451.	3.6	19
10219	Silicanes Modified by Conjugated Substituents for Optoelectronic Devices. <i>Advanced Optical Materials</i> , 2019, 7, 1900696.	3.6	8
10220	P/N co-doped carbon derived from cellulose: A metal-free photothermal catalyst for transfer hydrogenation of nitroarenes. <i>Applied Surface Science</i> , 2019, 487, 616-624.	3.1	22
10221	Enantioselective separation of bupropion and its major metabolite hydroxybupropion: An experimental and theoretical study. <i>Chemical Physics Letters</i> , 2019, 730, 1-7.	1.2	4
10222	Molecularly imprinted conducting polymer for determination of a condensed lignin marker. <i>Sensors and Actuators B: Chemical</i> , 2019, 295, 186-193.	4.0	14
10223	In situ Investigations of a Proton Trap Material: A PEDOT-Based Copolymer with Hydroquinone and Pyridine Side Groups Having Robust Cyclability in Organic Electrolytes and Ionic Liquids. <i>ACS Applied Energy Materials</i> , 2019, 2, 4486-4495.	2.5	15
10224	Effect of acidity and porosity changes of dealuminated mordenite on n-pentane, n-hexane and light naphtha isomerization. <i>Microporous and Mesoporous Materials</i> , 2019, 287, 192-202.	2.2	25
10225	High Electron Mobility in [1]Benzothieno[3,2- <i>b</i>][1]benzothiophene-Based Field-Effect Transistors: Toward n-Type BTBTs. <i>Chemistry of Materials</i> , 2019, 31, 5254-5263.	3.2	55

#	ARTICLE	IF	CITATIONS
10226	Anti-corrosive properties of quercetin and its derivatives on Fe(111) surface: a quantum chemical approach. <i>SN Applied Sciences</i> , 2019, 1, 1.	1.5	5
10227	Stereochemistry of Dichlorocarbene Addition to Alkenes: A Collaborative, Discovery-Based Experiment for the Organic Chemistry Laboratory. <i>Journal of Chemical Education</i> , 2019, 96, 1727-1730.	1.1	3
10228	Synthesis of Fullerene-Fluorene Dyads through the Platinum-Catalyzed Reactions of [60]Fullerene with 9-Ethynyl-9H-fluoren-9-yl Carboxylates. <i>Journal of Organic Chemistry</i> , 2019, 84, 9025-9033.	1.7	7
10229	Photoexcitation of flavoenzymes enables a stereoselective radical cyclization. <i>Science</i> , 2019, 364, 1166-1169.	6.0	256
10230	Electronic factors determining the methane bond breaking process on small aluminum clusters. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26003.	1.0	1
10231	Direct Chemical Synthesis of Benzyl-Modified Silicane from Calcium Disilicide. <i>Chemistry of Materials</i> , 2019, 31, 4720-4725.	3.2	16
10232	Synthesis and Catalytic Reactivity of Bis(molybdenum-trihalide) Complexes Bridged by Ferrocene Skeleton toward Catalytic Nitrogen Fixation. <i>Organometallics</i> , 2019, 38, 2863-2872.	1.1	13
10233	Photophysical investigation of two emissive nucleosides exhibiting gigantic Stokes shifts. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1858-1865.	1.6	2
10234	Electric field-induced selective catalysis of single-molecule reaction. <i>Science Advances</i> , 2019, 5, eaaw3072.	4.7	161
10235	Molecular aggregation in liquid acetic acid: insight from molecular dynamics/quantum mechanics modelling of structural and NMR properties. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14811-14820.	1.3	12
10236	Molecular Dynamics of CH ₄ /N ₂ Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. <i>Frontiers in Chemistry</i> , 2019, 7, 386.	1.8	14
10237	Dynamic Behavior of C ₆₀ Fullerene in Carbon Nanopeapods: Tight Binding Molecular Dynamics Simulation. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 724-728.	1.0	5
10238	The deamination mechanism of 5,6-dihydrocytosine and 5,6-dihydro-5-methylcytosine under typical bisulfite condition. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3990.	0.9	0
10239	Peroxo-tungstate(VI) complexes: syntheses, characterization, reactivity, and DFT studies. <i>Monatshefte für Chemie</i> , 2019, 150, 1255-1266.	0.9	5
10240	Geometry, stability and aromaticity of $\hat{\text{I}}^2$ -diketiminato-coordinated alkaline-earth compounds. <i>Chinese Chemical Letters</i> , 2019, 30, 2249-2253.	4.8	10
10241	Dissociative electron attachment to 2-chlorotoluene: Unusual temperature effects for the formation of Cl $\dot{\text{A}}^{\cdot}$. <i>Chemical Physics Letters</i> , 2019, 730, 527-530.	1.2	2
10242	True Polymorphic Phase Transition or Dynamic Crystal Disorder? An Investigation into the Unusual Phase Behavior of Barbituric Acid Dihydrate. <i>Crystal Growth and Design</i> , 2019, 19, 4745-4753.	1.4	6
10243	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. <i>Nature Communications</i> , 2019, 10, 2570.	5.8	107

#	ARTICLE	IF	CITATIONS
10244	Synthesis of 2,6-Di- <i>t</i> -Bu and 2,6-Di- <i>i</i> -Pr Pyrimidine π -Systems Using Triorganoindium Reagents: Optical, Vibrational, and Electrochemical Studies. <i>Journal of Organic Chemistry</i> , 2019, 84, 8870-8885.	1.7	16
10245	Prediction of emission wavelengths of phosphorescent NHC based emitters for OLEDs. <i>Tetrahedron</i> , 2019, 75, 130431.	1.0	3
10246	Gold(I)-Catalyzed Chloroalkynylation of 1,1-Disubstituted Alkenes via 1,3-Chlorine Shift: A Combined Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 8210-8224.	1.7	23
10247	Tuning the fluorescence of calcium-discharged photoprotein obelin via mutating at the His22-Phe88-Trp92 triad – a QM/MM study. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1823-1832.	1.6	6
10248	Precious metal-free molecular machines for solar thermal energy storage. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 1096-1106.	1.3	5
10249	Adsorption mediated tandem acid catalyzed cellulose hydrolysis by ortho-substituted benzoic acids. <i>Molecular Catalysis</i> , 2019, 475, 110459.	1.0	6
10250	Mesoionic 1,2,3-Triazolo[1,5-a]pyridine-Cylydenes in Phosphorescent Platinum(II) Complexes. <i>ChemPhotoChem</i> , 2019, 3, 1000-1003.	1.5	6
10251	Flavonol biosynthesis by nonheme iron dioxygenases: A computational study into the structure and mechanism. <i>Journal of Inorganic Biochemistry</i> , 2019, 198, 110728.	1.5	17
10252	Tracking the origin of photostability in purine nucleobases: the photophysics of 2-oxopurine. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13467-13473.	1.3	9
10253	A review on non-relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25968.	1.0	45
10254	DFT Mechanistic Study of Methane Mono-Esterification by Hypervalent Iodine Alkane Oxidation Process. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15674-15684.	1.5	13
10255	Features of the Formation of the [(O)VIV(C2O4)(Phen)(H2O)] Complex in the Malic Acid Oxidation Process. <i>Russian Journal of General Chemistry</i> , 2019, 89, 741-746.	0.3	0
10256	Using Density Functional Theory Based Methods to Investigate the Photophysics of Polycyclic Aromatic Hydrocarbon Radical Cations: A Benchmark Study on Naphthalene, Pyrene and Perylene Cations. <i>ChemPhotoChem</i> , 2019, 3, 763-769.	1.5	6
10257	On the geometry dependence of tuned-range separated hybrid functionals. <i>Journal of Computational Chemistry</i> , 2019, 40, 2191-2199.	1.5	19
10258	Infrared spectral-shift induced by hydrogen bonding cooperativity in cyclic and prismatic water clusters. <i>Journal of Molecular Liquids</i> , 2019, 286, 110940.	2.3	5
10259	Spectroscopic diagnostic for the ring-size of carbohydrates in the gas phase: furanose and pyranose forms of GalNAc. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12460-12467.	1.3	13
10260	Identification of novel inhibitors of signal transducer and activator of transcription 3 over signal transducer and activator of transcription 1 for the treatment of breast cancer by in-silico and in-vitro approach. <i>Process Biochemistry</i> , 2019, 82, 153-166.	1.8	9
10261	Twelve Cadmium(II) Coordination Frameworks with Asymmetric Pyridinyl Triazole Carboxylate: Syntheses, Structures, and Fluorescence Properties. <i>Crystal Growth and Design</i> , 2019, 19, 3785-3806.	1.4	41

#	ARTICLE	IF	CITATIONS
10262	Mechanism of Cardiac Troponin C Calcium Sensitivity Modulation by Small Molecules Illuminated by Umbrella Sampling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2964-2972.	2.5	11
10263	Decomposition of Ferrocene on Pt(111) and Its Effect on Molecular Electronic Junctions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15569-15574.	1.5	8
10264	A theoretical research on intersystem crossing, radiative and nonradiative rates of cyclometalated platinum(II) complexes. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
10265	Computational Study of the Formation of C8, C5, and C4 Guanine:Lysine Adducts via Oxidation of Guanine by Sulfate Radical Anion. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5150-5163.	1.1	7
10266	Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 12184-12191.	1.3	8
10267	Chemoselective Reduction of Imines Catalyzed by Ruthenium(II) Half-Sandwich Complexes: A Mechanistic Study. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2947-2955.	1.0	2
10268	Synergy between Ionic Liquids and CuCl ₂ in Gas-Liquid Phase Reactions of Acetylene Hydrochlorination. <i>Catalysts</i> , 2019, 9, 504.	1.6	13
10269	Photophysics of proton transfer in hydrazides: a combined theoretical and experimental analysis towards OLED device application. <i>New Journal of Chemistry</i> , 2019, 43, 10413-10428.	1.4	16
10270	Prediction of Intramolecular Reorganization Energy Using Machine Learning. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7855-7863.	1.1	36
10271	Mechanistic Study on the Asymmetric Synthesis of the Wieland-Miescher Ketone and Analogs. <i>ChemCatChem</i> , 2019, 11, 4064-4071.	1.8	5
10272	Introduction of polar or nonpolar groups at the hydroquinone units can lead to the destruction of the columnar structure of Pillar[5]arenes. <i>Computational and Theoretical Chemistry</i> , 2019, 1161, 1-9.	1.1	11
10273	Structures of [GPGG ⁺ H ⁺ H ₂ O] ⁺ and [GPGG ⁺ H ⁺ H ₂ O NH ₂ CH ₂] ⁺ ions; evidence of rearrangement prior to dissociation. <i>International Journal of Mass Spectrometry</i> , 2019, 442, 51-57.	0.7	0
10274	Push-Pull Chromophores Based on the Naphthalene Scaffold: Potential Candidates for Optoelectronic Applications. <i>Materials</i> , 2019, 12, 1342.	1.3	29
10275	Interaction of trivalent arsenic on different topologies of Fe-doped graphene nanosheets at water environments: A computational study. <i>Journal of Molecular Liquids</i> , 2019, 289, 111137.	2.3	16
10276	2,3-(Dibenzimidazol-2-yl)quinoxalines: Unexpected Dynamical Effect on Steady-State Electronic Absorption Spectra. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5514-5523.	1.2	2
10277	DFT Study on the Effect of Aluminum Position in Zn-Exchanged MFI on Methane Activation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16164-16171.	1.5	12
10278	Suppressing the Shuttle Effect in Lithium-Sulfur Batteries by a UiO-66-Modified Polypropylene Separator. <i>ACS Omega</i> , 2019, 4, 10328-10335.	1.6	57
10279	Quantum Mechanical Modeling of the Vibrational Spectra of Minerals with a Focus on Clays. <i>Minerals (Basel, Switzerland)</i> , 2019, 9, 141.	0.8	18

#	ARTICLE	IF	CITATIONS
10280	Molecular inner-shell photoabsorption/photoionization cross sections at core-valence-separated coupled cluster level: Theory and examples. <i>Journal of Chemical Physics</i> , 2019, 150, 224104.	1.2	33
10281	An Improved Class of Phosphite-Oxazoline Ligands for Pd-Catalyzed Allylic Substitution Reactions. <i>ACS Catalysis</i> , 2019, 9, 6033-6048.	5.5	18
10282	Modulating absorption and charge transfer in bodipy-carbazole donor-acceptor dyads through molecular design. <i>Dalton Transactions</i> , 2019, 48, 8488-8501.	1.6	20
10283	Ammonia borane and hydrazine bis(borane) dehydrogenation mediated by an unsymmetrical (PNN) ruthenium pincer hydride: metal-ligand cooperation for hydrogen production. <i>Sustainable Energy and Fuels</i> , 2019, 3, 2583-2596.	2.5	11
10284	TriplatinNC and Biomolecules: Building Models Based on Non-covalent Interactions. <i>Frontiers in Chemistry</i> , 2019, 7, 307.	1.8	13
10285	Blue wine, a color obtained with synthetic blue dye addition: two case studies. <i>European Food Research and Technology</i> , 2019, 245, 1777-1782.	1.6	4
10286	Effect of chalcogen atoms on the electronic band gaps of donor-acceptor-donor type semiconducting polymers: a systematic DFT investigation. <i>Journal of Molecular Modeling</i> , 2019, 25, 167.	0.8	2
10287	Quantum chemical calculations for the norbadione A complexes with Cs ⁺ , K ⁺ , and Na ⁺ in gas and aqueous phases. <i>Chemical Physics Letters</i> , 2019, 730, 26-31.	1.2	2
10288	Insights into the mechanisms of Ag-catalyzed synthesis of CF ₃ -substituted heterocycles via [3+2]-cycloaddition from <i>l</i> -trifluoromethylated methyl isocyanides: effects of DBU and exploration of diastereoselectivity. <i>New Journal of Chemistry</i> , 2019, 43, 9265-9273.	1.4	3
10289	Cyclometalated Platinum(II) Complexes with Mesoionic Dibenzofuranyl-1,2,3-triazol-4-ylidene Ligands: Synthesis, Characterization and Photophysical Properties. <i>ChemPhotoChem</i> , 2019, 3, 554-558.	1.5	8
10290	Excited-State Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. <i>ChemPhotoChem</i> , 2019, 3, 619-629.	1.5	10
10291	The Selective <i>N</i> -Functionalization of Indoles via <i>aza</i> -Michael Addition in the Ligand Sphere of a Chiral Nickel(II) Complex: Asymmetric Synthesis of <i>S</i> - <i>H</i> -Indole-Alanine Derivatives. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 3699-3703.	1.2	19
10292	Structural correlation and computational quantum chemical explorations of two 1,2,3-triazolyl-methoxypyridine derivatives as CYP51 antifungal inhibitors. <i>Structural Chemistry</i> , 2019, 30, 2225-2243.	1.0	2
10293	Modulation of the conductance in platinum(<i>ii</i>) bis(acetylide) molecules through <i>ø</i> gating metal ions. <i>Journal of Materials Chemistry C</i> , 2019, 7, 7259-7266.	2.7	12
10294	Quantum interferences among Dexter energy transfer pathways. <i>Faraday Discussions</i> , 2019, 216, 301-318.	1.6	16
10295	Acid-Base Catalytic Effects on Reduction of Methanol in Hot Water. <i>Catalysts</i> , 2019, 9, 373.	1.6	2
10296	A Ru(II) polypyridyl complex bearing aldehyde functions as a versatile synthetic precursor for long-wavelength absorbing photodynamic therapy photosensitizers. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 2666-2675.	1.4	38
10297	Effects of Solvent Stabilization on Pharmaceutical Crystallization: Investigating Conformational Polymorphism of ProbucoL Using Combined Solid-State Density Functional Theory, Molecular Dynamics, and Terahertz Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6937-6947.	1.1	21

#	ARTICLE	IF	CITATIONS
10298	Aryl modification of diketopyrrolopyrrole-based quaternary ammonium salts and their applications in copper electrodeposition. <i>Dyes and Pigments</i> , 2019, 170, 107559.	2.0	21
10299	Spectral shifts of BODIPY derivatives: a simple continuous model. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1315-1323.	1.6	5
10300	Phosphine-catalyzed fixation of CO ₂ with β -hydroxyl alkynone under ambient temperature and pressure: kinetic resolution and further conversion. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2420-2429.	2.3	16
10301	Mechanisms and Activity of 1-Phenylethanol Dehydrogenation Catalyzed by Bifunctional NHC- π Complex. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 3929-3936.	1.2	4
10302	Selective Metal-Ion Detection and Activatable Photosensitization Properties of a Tetraphenylethylene-Based Salicylideneimine. <i>ChemistrySelect</i> , 2019, 4, 5707-5713.	0.7	3
10303	QM/MM study of the taxadiene synthase mechanism. <i>Journal of Computational Chemistry</i> , 2019, 40, 1902-1910.	1.5	17
10304	In vitro and computational studies showed that perezone inhibits PARP-1 and induces changes in the redox state of K562 cells. <i>Archives of Biochemistry and Biophysics</i> , 2019, 671, 225-234.	1.4	7
10305	Theoretical insight on the nanocomposite of tetraphenylporphyrin-graphene oxide quantum dot as a sensitizer of DSSC. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 379, 24-31.	2.0	15
10306	Polyacenes and diffuse interstellar bands. <i>Astronomy and Astrophysics</i> , 2019, 625, A41.	2.1	28
10307	Photophysical characterization of new and efficient synthetic sunscreens. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11376-11384.	1.3	18
10308	1,3-Dimethyl-2-phenyl-1,3-diazaphospholidine-2-oxide as ligand for the preparation of luminescent lanthanide complexes. <i>Journal of Coordination Chemistry</i> , 2019, 72, 1524-1536.	0.8	6
10309	Combining Benzotriazole and Benzodithiophene Host Units in Host-Guest Polymers for Efficient and Stable Near-Infrared Emission from Light-Emitting Electrochemical Cells. <i>Advanced Optical Materials</i> , 2019, 7, 1900280.	3.6	23
10310	Coexistence of structurally similar but electronically distinct isomers of delocalized cation radicals as a basis for the development of functional materials. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10738-10743.	1.3	1
10312	Magnetic iron oxide nanoparticles functionalized with C60 phosphonic acid derivative for catalytic reduction of 4-nitrophenol. <i>Journal of Environmental Chemical Engineering</i> , 2019, 7, 103147.	3.3	10
10313	High-K dielectric sulfur-selenium alloys. <i>Science Advances</i> , 2019, 5, eaau9785.	4.7	13
10314	Density functional calculations for Rh(I)-catalyzed C-C bond activation of siloxyvinylcyclopropanes and diazoesters. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4869.	1.7	2
10315	Preparation and crystal structure of the boranehydrazine complex [RuCl(η -1-NH ₂ NH ₂ BPh ₃){P(OEt) ₃ }] ₄ BPh ₄ . <i>Polyhedron</i> , 2019, 169, 78-83.	1.0	0
10316	Theoretical studies of capsular complexes of C _{2v} -symmetrical resorcin[4]arene tetraesters with tetramethylammonium cation. <i>Computational and Theoretical Chemistry</i> , 2019, 1159, 12-17.	1.1	2

#	ARTICLE	IF	CITATIONS
10317	Speed tunability of the excited-state intramolecular proton transfer process based on seven-membered ring pyrrole-indole H-bond systems. <i>Journal of Molecular Liquids</i> , 2019, 286, 110887.	2.3	17
10318	Quantum Chemical Rovibrational Characterization of CH ₂ ClH ⁺ , a Low-Energy Isomer of Ionized Chloromethane. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1296-1301.	1.2	1
10319	Exact subsystem time-dependent density-functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 181101.	1.2	30
10320	Addition of S-â€Heterocyclic Carbenes to Fullerenes: Formation and Characterization of Dithiomethano-â€Bridged Derivatives. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900064.	1.0	5
10321	Optimizing reaction paths for methanol synthesis from CO ₂ hydrogenation via metal-ligand cooperativity. <i>Nature Communications</i> , 2019, 10, 1885.	5.8	116
10322	Palladium-Catalyzed Direct Î±-C(sp ³) Heteroarylation of Ketones under Microwave Irradiation. <i>Journal of Organic Chemistry</i> , 2019, 84, 7652-7663.	1.7	9
10323	Perovskite Solar Cells Based on Oligotriarylamine Hexaarylbenzene as Hole-Transporting Materials. <i>Organic Letters</i> , 2019, 21, 3261-3264.	2.4	12
10324	Methodological Survey of Simplified TD-DFT Methods for Fast and Accurate Interpretation of UV-Vis-NIR Spectra of Phthalocyanines. <i>ACS Omega</i> , 2019, 4, 7265-7284.	1.6	86
10325	Insight into conformationally-dependent binding of 1- <i>n</i> -alkyl-3-methylimidazolium cations to porphyrin molecules using quantum mechanical calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10095-10104.	1.3	4
10326	Unravelling the Origins of Hydroboration Chemoselectivity Inversion Using an N,O-Chelated Ir(I) Complex: A Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 6709-6718.	1.7	10
10327	Anthracene-based azo dyes for photo-induced proton-coupled electron transfer. <i>Chemical Communications</i> , 2019, 55, 5874-5877.	2.2	11
10328	Catalytic upgrading of ethanol to <i>n</i> -butanol using an aliphatic Mn-â€PNP complex: theoretical insights into reaction mechanisms and product selectivity. <i>Catalysis Science and Technology</i> , 2019, 9, 2794-2805.	2.1	19
10329	DFT Mechanistic Study on the Complete Oxidation of Ethylene by the Silica-Supported Pt Catalyst: C-â€C Activation via the Ethylene Dioxide Intermediate. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12706-12715.	1.5	19
10330	CO ₂ reduction by a Mn electrocatalyst in the presence of a Lewis acid: a DFT study on the reaction mechanism. <i>Sustainable Energy and Fuels</i> , 2019, 3, 1730-1738.	2.5	11
10331	Direct Access to IMes ^F and IMes ^F ₂ by Electrophilic Fluorination of Abnormal N-Heterocyclic Carbenes. <i>Organometallics</i> , 2019, 38, 2330-2337.	1.1	19
10332	<i>t</i> -Butyl peroxy radical: ground and first excited state energetics and fundamental frequencies. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9747-9758.	1.3	7
10333	An EXAFS study for characterizing the time-dependent adsorption of cesium on bentonite. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 930-937.	1.7	4
10334	Molecular Dynamics Simulations on Relaxed Reduced-Dimensional Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2019, 123, 4543-4554.	1.1	5

#	ARTICLE	IF	CITATIONS
10335	Mechanism of Catalytic O ₂ Reduction by Iron Tetraphenylporphyrin. <i>Journal of the American Chemical Society</i> , 2019, 141, 8315-8326.	6.6	99
10336	Catalytic enantioselective synthesis of perfluoroalkyl-substituted $\hat{\text{I}}^2$ -lactones <i>via</i> a concerted asynchronous [2 + 2] cycloaddition: a synthetic and computational study. <i>Chemical Science</i> , 2019, 10, 6162-6173.	3.7	40
10337	Mechanistic insights and computational design of half-sandwich iridium and rhodium complexes for hydrogenation of quinoline. <i>New Journal of Chemistry</i> , 2019, 43, 8459-8464.	1.4	2
10338	Gate-Efficient Simulation of Molecular Eigenstates on a Quantum Computer. <i>Physical Review Applied</i> , 2019, 11, .	1.5	104
10339	Unravelling the Mechanism and Selectivity of the NHC-catalyzed Three-Membered Ring-Opening/Fluorination of Epoxy Enals: A DFT Study. <i>ChemCatChem</i> , 2019, 11, 2919-2925.	1.8	20
10340	Calculated relative populations for the Eu@C ₈₂ isomers. <i>Chemical Physics Letters</i> , 2019, 726, 29-33.	1.2	13
10341	The photochemical ring-opening of 1,3-cyclohexadiene imaged by ultrafast electron diffraction. <i>Nature Chemistry</i> , 2019, 11, 504-509.	6.6	157
10342	Reversible temperature-induced polymorphic phase transitions of [Y(OAr) ₃] and [Ce(OAr) ₃] (Ar =) <i>Tj ETQq1 1 0.784314 rgBT /Overlo</i> <i>Chemical Science</i> , 2019, 10, 2884-2892.	1.3	4
10343	Determination of the best functional and basis sets for optimization of the structure of hypervalent iodines and calculation of their first and second bond dissociation enthalpies. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3961.	0.9	26
10344	Application of density functional theory and optical spectroscopy for the prediction of the photophysical properties of δ -pyridylphospholanes. <i>Russian Chemical Bulletin</i> , 2019, 68, 254-261.	0.4	3
10345	How cyclic chain topology can reduce the crystallization rate of poly(3-hexylthiophene) and promote the formation of liquid crystalline phases in comparison with linear analogue chains. <i>Journal of Materials Chemistry C</i> , 2019, 7, 6548-6558.	2.7	9
10346	Catalytically Active Species in Copper/DiPPAM-catalyzed 1,6-Asymmetric Conjugate Addition of Dialkylzinc to Dienones: A Computational Overview. <i>ChemCatChem</i> , 2019, 11, 4108-4115.	1.8	6
10347	Hydrogenation of CO ₂ to Methanol Catalyzed by Cp*Co Complexes: Mechanistic Insights and Ligand Design. <i>Inorganic Chemistry</i> , 2019, 58, 5494-5502.	1.9	16
10348	Highly regioselective complexation of tungsten with Eu@C ₈₂ /Eu@C ₈₄ : interplay between endohedral and exohedral metallic units induced by electron transfer. <i>Chemical Science</i> , 2019, 10, 4945-4950.	3.7	19
10349	Mass spectrometry evidence for self-rigidification of $\hat{\text{I}}^{\text{E}}$ -conjugated oligomers containing 3,4-ethylenedioxythiophene groups using RRKM theory and internal energy calibration. <i>European Journal of Mass Spectrometry</i> , 2019, 25, 239-250.	0.5	0
10350	Determination of Two-Photon-Absorption Cross Sections Using Time-Dependent Density Functional Theory Tight Binding: Application to Fluorescent Protein Chromophores. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3153-3161.	2.3	6
10351	Ligand Effects on the Linear Response Hubbard U: The Case of Transition Metal Phthalocyanines. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3214-3222.	1.1	6
10352	Nonadiabatic Investigation of the Electronic Spectroscopy of <i>trans</i> -1,3-Butadiene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3255-3271.	1.1	8

#	ARTICLE	IF	CITATIONS
10353	Grafting of a new bis-silylamido aluminum species on silica: insight from solid-state NMR into interactions with the surface. <i>Dalton Transactions</i> , 2019, 48, 5243-5252.	1.6	6
10354	Theoretical insight into the photophysical properties of long-lifetime Ir(III) and Rh(III) complexes for two-photon photodynamic therapy. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8394-8401.	1.3	4
10355	Evaluation of attractive interactions in the second coordination sphere of iron complexes containing pendant amines. <i>Dalton Transactions</i> , 2019, 48, 4867-4878.	1.6	12
10356	Understanding Color Tuning and Reversible Oxidation of Conjugated Azomethines. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2687-2693.	1.1	6
10357	Ni _m Mo _n (m + n = 5) Clusters for Hydrogen Electric Reduction: Synergistic Effect of Ni and Mo on the Adsorption and OH Breaking of H ₂ O. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9247-9254.	1.5	6
10358	Highly Sensitive Detection of Carbendazim and Its Electrochemical Oxidation Mechanism at a Nanohybrid Sensor. <i>Journal of the Electrochemical Society</i> , 2019, 166, B322-B327.	1.3	47
10359	Metal-ligand bifunctional based Mn-catalysts for CO ₂ hydrogenation reaction. <i>Molecular Catalysis</i> , 2019, 468, 109-116.	1.0	15
10360	A Combined Spin-Flip and IP/EA Approach for Handling Spin and Spatial Degeneracies: Application to Double Exchange Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2278-2290.	2.3	7
10361	Unraveling Excitonic Effects for the First Hyperpolarizabilities of Chromophore Aggregates. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13818-13836.	1.5	8
10362	Molecular design principles towards exo-exclusive Diels-Alder reactions. <i>RSC Advances</i> , 2019, 9, 7246-7250.	1.7	3
10363	Dinuclear NHC Gold(I) Allenyl and Propargyl Complexes: An Experimental and Theoretical Study. <i>Organometallics</i> , 2019, 38, 1524-1533.	1.1	11
10364	Formation of Cyclophane Macrocycles in Carbazole-Based Biradicaloids: Impact of the Dicyanomethylene Substitution Position. <i>ACS Omega</i> , 2019, 4, 4761-4769.	1.6	23
10365	Assessing structure and stability of polymer/lithium-metal interfaces from first-principles calculations. <i>Journal of Materials Chemistry A</i> , 2019, 7, 8394-8404.	5.2	77
10366	Carbene-Catalyzed Enantioselective Decarboxylative Annulations to Access Dihydrobenzoxazinones and Quinolones. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5941-5945.	7.2	46
10367	Evaluation of the antioxidant potential of myricetin 3-O-β-L-rhamnopyranoside and myricetin 4-O-β-L-rhamnopyranoside through a computational study. <i>Journal of Molecular Modeling</i> , 2019, 25, 89.	0.8	37
10368	Diselenide Bonds as an Alternative to Outperform the Efficiency of Disulfides in Self-Healing Materials. <i>Journal of Organic Chemistry</i> , 2019, 84, 4200-4210.	1.7	32
10369	Chromo-Fluorogenic Detection of Soman and Its Simulant by Thiourea-Based Rhodamine Probe. <i>Molecules</i> , 2019, 24, 827.	1.7	11
10370	Excited state tracking during the relaxation of coordination compounds. <i>Journal of Computational Chemistry</i> , 2019, 40, 1420-1428.	1.5	12

#	ARTICLE	IF	CITATIONS
10371	Adsorption of Ethene-1,2-Dione on Materials Based on Graphene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6316-6325.	1.5	1
10372	Aggregation behavior and non-covalent functionalization of borofullerenes B ₂₈ , B ₃₈ , and B ₄₀ : A density functional theory investigation. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25921.	1.0	4
10373	Following local light-induced structure changes and dynamics of the photoreceptor PYP with the thiocyanate IR label. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6622-6634.	1.3	15
10374	The importance of diffuse functions in basis sets to produce reliable 3D pictures of dual descriptor. <i>Chemical Physics Letters</i> , 2019, 724, 29-34.	1.2	5
10375	Coordination Structures of the Uranyl(VI)-Diamide Complexes: A Combined Mass Spectrometric, EXAFS Spectroscopic, and Theoretical Study. <i>Inorganic Chemistry</i> , 2019, 58, 5695-5702.	1.9	13
10376	Computational Study on the Mechanism and Origin of the Regioselectivity and Stereospecificity in Pd/SIPr-Catalyzed Ring-Opening Cross-Coupling of 2-Arylaziridines with Arylboronic Acids. <i>ACS Catalysis</i> , 2019, 9, 4582-4592.	5.5	12
10377	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. <i>Journal of the American Chemical Society</i> , 2019, 141, 6234-6246.	6.6	42
10378	Metal-free dehydropolymerisation of phosphine-boranes using cyclic (alkyl)(amino)carbenes as hydrogen acceptors. <i>Nature Communications</i> , 2019, 10, 1370.	5.8	29
10379	Improvement of the electrochemical and singlet fission properties of anthraquinones by modification of the diradical character. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7941-7952.	1.3	8
10380	Influence of metal ions on glyphosate detection by FMOCl. <i>Environmental Monitoring and Assessment</i> , 2019, 191, 244.	1.3	16
10381	Novel aluminum complexes bearing 2-(aminomethylene)malonate ligands with high efficiency and controllability in ring-opening polymerization of μ -caprolactone. <i>European Polymer Journal</i> , 2019, 115, 399-408.	2.6	11
10382	Reductive Debromination of Polybrominated Diphenyl Ethers: Dependence on Br Number of the Br-Rich Phenyl Ring. <i>Environmental Science & Technology</i> , 2019, 53, 4433-4439.	4.6	28
10383	Robust Triplatinum Redox-Chromophore for a Post-Synthetic Color-Tunable Electrochromic System. <i>Chemistry - A European Journal</i> , 2019, 25, 7669-7678.	1.7	9
10384	A computational mechanistic insight into H ₂ activation and CO ₂ reduction over η^2 -Diketiminato-ligated group 13 metal complexes. <i>Journal of Catalysis</i> , 2019, 373, 1-12.	3.1	6
10385	Structure elucidation of cyclohexene (9Z)-octadec-9-enyl ethers isolated from the leaves of <i>Uvaria cherreensis</i> (Annonaceae). <i>Tetrahedron</i> , 2019, 75, 2336-2342.	1.0	5
10386	Ultrafast electron-transfer in a fully conjugated coumarin-ferrocene donor-acceptor dyads. <i>Journal of Organometallic Chemistry</i> , 2019, 887, 86-97.	0.8	4
10387	Trifluoromethylation for affecting the structural, electronic and redox properties of cobalt corroles. <i>Dalton Transactions</i> , 2019, 48, 4798-4810.	1.6	28
10388	A new palladium(II) complex with ibuprofen: Spectroscopic characterization, DFT studies, antibacterial activities and interaction with biomolecules. <i>Journal of Molecular Structure</i> , 2019, 1186, 144-154.	1.8	17

#	ARTICLE	IF	CITATIONS
10389	Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping solute "solvent bands. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	0
10390	Atomic basis functions for molecular electronic structure calculations. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	53
10391	Quantitative Solvent-Free Thermal Synthesis of Luminescent Cu(I) Coordination Polymers. <i>Inorganic Chemistry</i> , 2019, 58, 4456-4464.	1.9	29
10392	Theoretical Study on the Transition-Metal-Catalyzed Cycloadditions of <i>2-H-Azirines</i> with Alkynes: Implication of Carbenoid Intermediates. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 619-628.	2.0	3
10393	Water Network Dynamics Next to the Oxygen-Evolving Complex of Photosystem II. <i>Inorganics</i> , 2019, 7, 39.	1.2	15
10394	Molecular dynamics of carbon nanohorns and their complexes with cisplatin in aqueous solution. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 167-177.	1.3	16
10395	A highly selective and sensitive dual-mode sensor for colorimetric and turn-on fluorescent detection of cyanide in water, agro-products and living cells. <i>Analytica Chimica Acta</i> , 2019, 1065, 113-123.	2.6	53
10396	Theoretical insights into CO ₂ hydrogenation to methanol by a Mn "PNP complex. <i>Catalysis Science and Technology</i> , 2019, 9, 1867-1878.	2.1	30
10397	Photoprotection assessment of olive (<i>Olea europaea</i> L.) leaves extract standardized to oleuropein: In vitro and in silico approach for improved sunscreens. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2019, 193, 162-171.	1.7	43
10398	Molybdenum(ν) complexes of hemilabile aroylhydrazone ligands as efficient catalysts for greener cyclooctene epoxidation: an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2019, 43, 5531-5542.	1.4	29
10399	Role of Alkaline-Earth Metal-Catalyst: A Theoretical Study of Pyridines Hydroboration. <i>Frontiers in Chemistry</i> , 2019, 7, 149.	1.8	5
10400	Carbene-Catalyzed Enantioselective Decarboxylative Annulations to Access Dihydrobenzoxazinones and Quinolones. <i>Angewandte Chemie</i> , 2019, 131, 6002-6006.	1.6	17
10401	Transfer Hydrogenation of Carbonyl Groups, Imines and <i>N-Heterocycles</i> Catalyzed by Simple, Bipyridine-Based Mn ^I Complexes. <i>ChemCatChem</i> , 2019, 11, 3844-3852.	1.8	44
10402	Supramolecular Coordination of Pb ²⁺ Defects in Hybrid Lead Halide Perovskite Films Using Truxene Derivatives as Lewis Base Interlayers. <i>ChemPhysChem</i> , 2019, 20, 2702-2711.	1.0	10
10403	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3802-3808.	1.1	26
10404	Synthesis and Characterization of Cyclometalated NHC Platinum Complexes with Chelating Carboxylate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2284-2290.	1.0	9
10405	DFT study on selective autocatalyzed α -alkylation of ketones with alcohols. <i>Journal of Catalysis</i> , 2019, 373, 126-138.	3.1	6
10406	Effect of fluorosubstitution and central metals on the molecular structure and vibrational spectra of metal phthalocyanines. <i>Journal of Molecular Structure</i> , 2019, 1189, 73-80.	1.8	23

#	ARTICLE	IF	CITATIONS
10407	Photochemical Synthesis and Catalytic Applications of Gold Nanoplates Fabricated Using Quercetin Diphosphate Macromolecules. ACS Omega, 2019, 4, 6511-6520.	1.6	12
10408	Chain rigidity modification to promote the electrochemical performance of polymeric battery electrode materials. Journal of Materials Chemistry A, 2019, 7, 10581-10588.	5.2	33
10409	Thermodynamic and kinetic aspects of glycine and its radical cation under interstellar medium conditions. Monthly Notices of the Royal Astronomical Society, 2019, 486, 2153-2164.	1.6	9
10410	Concerted proton-electron transfer reactions in the Marcus inverted region. Science, 2019, 364, 471-475.	6.0	104
10411	A Small Molecule with PAH Vibrational Properties and a Detectable Rotational Spectrum: $c\text{-}(C)C_3H_2$, Cyclopropenylidene Carbene. Astrophysical Journal, 2019, 871, 236.	1.6	37
10412	Reaction mechanism of non-enzymatic stereoselective formation of wine lactone. Chemical Physics Letters, 2019, 725, 114-118.	1.2	0
10413	Formation of an N^2 -Diimine from Isocyanide Coupling Using Thorium(IV) and Uranium(IV) Phosphido-Methyl Complexes. Organometallics, 2019, 38, 1733-1740.	1.1	11
10414	Oxidatively-mediated in silico epimerization of a highly amyloidogenic segment in the human calcitonin hormone (hCT15-19). Computational Biology and Chemistry, 2019, 80, 259-269.	1.1	2
10415	Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts. Journal of Physical Chemistry Letters, 2019, 10, 2051-2057.	2.1	11
10416	Symplectic integration and physical interpretation of time-dependent coupled-cluster theory. Journal of Chemical Physics, 2019, 150, 144106.	1.2	57
10417	Isomerization Dynamics of Electronically Coupled but Thermodynamically Decoupled Bisazobenzenes. ChemPhotoChem, 2019, 3, 411-417.	1.5	6
10418	Theoretical study of chloro- $\text{N}^2, \text{N}^2, \text{N}^3, \text{N}^3$ -tetraphenylporphyrinato cobalt(III) dimer reaction: A reaction path to form N^2 cation radicals. Chemical Physics, 2019, 523, 28-33.	0.9	1
10419	Photoemission spectroscopy of rubrene thin films doped with heavy alkali metal: A first-principles investigation. Journal of Physics and Chemistry of Solids, 2019, 132, 1-9.	1.9	1
10420	Structure-Property Relationship in an Organic Semiconductor: Insights from Energy Frameworks, Charge Density Analysis, and Diode Devices. Crystal Growth and Design, 2019, 19, 3019-3029.	1.4	6
10421	A rational design of manganese electrocatalysts for Lewis acid-assisted carbon dioxide reduction. Physical Chemistry Chemical Physics, 2019, 21, 8849-8855.	1.3	12
10422	The mechanism of the gold-catalyzed intramolecular [3 + 2]-cycloaddition of 1,6-diyne: a DFT study. Dalton Transactions, 2019, 48, 5698-5704.	1.6	4
10423	1,3- O^2 -Transposition or Trisubstituted Z^2 -Enol Ester? A Comparative Study of Reactions of Yrones. Chemistry - an Asian Journal, 2019, 14, 1941-1944.	1.7	0
10424	Small binary iron-carbon clusters with persistent high magnetic moments. A theoretical characterization. International Journal of Quantum Chemistry, 2019, 119, e25932.	1.0	11

#	ARTICLE	IF	CITATIONS
10425	A dual-mode highly selective and sensitive Schiff base chemosensor for fluorescent colorimetric detection of Ni ²⁺ and colorimetric detection of Cu ²⁺ . Photochemical and Photobiological Sciences, 2019, 18, 1512-1525.	1.6	43
10426	Finite-temperature-based linear-scaling divide-and-conquer self-consistent field method for static electron correlation systems. Chemical Physics Letters, 2019, 725, 18-23.	1.2	13
10427	Towards developing efficient aminopyridine-based electrochemical catalysts for CO ₂ reduction. A density functional theory study. Journal of Catalysis, 2019, 373, 75-80.	3.1	10
10428	Nanoscrolls Formed from Two-Dimensional Covalent Organic Frameworks. Chemistry of Materials, 2019, 31, 3265-3273.	3.2	12
10429	How does Mo-dependent perchlorate reductase work in the decomposition of oxyanions?. Dalton Transactions, 2019, 48, 5683-5691.	1.6	11
10430	Encapsulation of anticancer drug doxorubicin inside dendritic macromolecular cavities: First-principles benchmarks. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 217, 278-287.	2.0	4
10431	Characterization of Rh-Al Bond in Rh(PAIP) (PAIP = Pincer-type Diphosphino-Alumanyl Ligand) in Comparison with Rh(L)(PMe ₃) ₂ (L = AlMe ₂), Tj ETQqO 0 0 rgBT /Overlock 10 Tf 50 502-Td (Al(NM	1.9	27
10432	Aromaticity and Antiaromaticity in the Excited States of Porphyrin Nanorings. Journal of Physical Chemistry Letters, 2019, 10, 2017-2022.	2.1	39
10433	Study on the structure, stability and tautomerisms of meta-benziporphodimethene and N-Confused isomers containing ¹³ C-lactam ring. Journal of Molecular Structure, 2019, 1187, 138-150.	1.8	12
10434	Electrochemical sensing of ecstasy with electropolymerized molecularly imprinted poly(o-phenylenediamine) polymer on the surface of disposable screen-printed carbon electrodes. Sensors and Actuators B: Chemical, 2019, 290, 378-386.	4.0	77
10435	Franck-Condon Blockade and Aggregation-Modulated Conductance in Molecular Devices Using Aggregation-Induced Emission-Active Molecules. Angewandte Chemie, 2019, 131, 6012-6016.	1.6	6
10436	The deamination mechanism of the 5,6-dihydro-6-hydroxy-6-hydroxylcytosine and 5,6-dihydro-5-methyl-6-hydroxylcytosine under typical bisulfite conditions. Molecular Physics, 2019, 117, 759-767.	0.8	0
10437	Water-Involved Hydrogen Bonds in Dimeric Supramolecular Structures of Magnesium and Zinc Phthalocyaninato Complexes. ACS Omega, 2019, 4, 3673-3683.	1.6	10
10438	Prediction of upper flammability limits for fuel mixtures using quantitative structure-property relationship models. Chemical Engineering Communications, 2019, 206, 247-253.	1.5	18
10439	CO ₂ Adsorption on the B ₁₂ N ₁₂ Nanocage Encapsulated with Alkali Metals: A Density Functional Study. Nano, 2019, 14, 1950034.	0.5	5
10440	4-aminoazobenzene modified natural glucomannan as a green eco-friendly inhibitor for the mild steel in 0.5 M HCl solution. Corrosion Science, 2019, 151, 132-142.	3.0	128
10441	Spectroscopic and quantum chemical study of difluoroboron ¹² -diketonate luminophores: Isomeric acetylnaphtholate chelates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 67-78.	2.0	6
10442	Distinguishing artificial and essential symmetry breaking in a single determinant: approach and application to the C ₆₀ , C ₃₆ , and C ₂₀ fullerenes. Physical Chemistry Chemical Physics, 2019, 21, 4763-4778.	1.3	40

#	ARTICLE	IF	CITATIONS
10443	Effects of Lewis Acidic Metal Ions (M) on Oxygen-Atom Transfer Reactivity of Heterometallic Mn ₃ MO ₄ Cubane and Fe ₃ MO(OH) and Mn ₃ MO(OH) Clusters. <i>Inorganic Chemistry</i> , 2019, 58, 2336-2345.	1.9	21
10444	Theoretical Rationalization of the Dual Photophysical Behavior of C ₆₀ . <i>Journal of Physical Chemistry A</i> , 2019, 123, 1824-1829.	1.1	7
10445	Inclusion vs. micellization in the cethylpyridine chloride / β -cyclodextrin system: A structural and thermodynamic approach. <i>Journal of Molecular Structure</i> , 2019, 1184, 289-297.	1.8	16
10446	Assessing the Conformational Equilibrium of Carboxylic Acid via Quantum Mechanical and Molecular Dynamics Studies on Acetic Acid. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1957-1964.	2.5	14
10447	Investigation of main group promoted carbon dioxide reduction. <i>Tetrahedron</i> , 2019, 75, 2099-2105.	1.0	6
10448	Quantitative descriptors of electronic structure in the framework of molecular orbital theory. <i>Advances in Inorganic Chemistry</i> , 2019, 73, 191-219.	0.4	1
10449	Formaldehyde Generation in Photooxidation of Isoprene on Iron Oxide Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5120-5127.	1.5	10
10450	Theoretical investigation on the mechanism of Cu(II)-catalyzed synthesis of 4-quinolones: effects of additives HOTf vs. HOTs. <i>New Journal of Chemistry</i> , 2019, 43, 4291-4305.	1.4	5
10451	Computational Design of SCS Nickel Pincer Complexes for the Asymmetric Transfer Hydrogenation of 1-Acetonaphthone. <i>Catalysts</i> , 2019, 9, 101.	1.6	8
10452	Copolymerization of (meth)acrylates with vinyl aromatic macromonomers: understanding the mechanism of retardation on the kinetics with acrylates. <i>Polymer Chemistry</i> , 2019, 10, 1769-1779.	1.9	8
10453	Effect of Ligands on the Lewis Acidity of the Metal and the Binding of N-Bases to Iridium Pincer Complexes. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1389-1397.	1.0	5
10454	Spiral Graphene Nanoribbons with Azulene Defects as Potential Nonlinear Optical Materials. <i>ACS Applied Nano Materials</i> , 2019, 2, 1648-1654.	2.4	26
10455	Dimerization of substituted 4-aryl-1,3-diacetylenes – quantum chemical calculations and kinetic studies. <i>Organic Chemistry Frontiers</i> , 2019, 6, 1010-1021.	2.3	9
10456	A DFT-Assisted Topological Analysis of Four Polymorphic, β -Shaped β -2 Fibril Structures. <i>ChemBioChem</i> , 2019, 20, 1722-1724.	1.3	5
10457	Tuning the Product Spectrum of a Glycoside Hydrolase Enzyme by a Combination of Site-Directed Mutagenesis and Tyrosine-Specific Chemical Modification. <i>Chemistry - A European Journal</i> , 2019, 25, 6533-6541.	1.7	13
10458	Enantioselective Synthesis of Homochiral Au ₁₃ Nanoclusters and Their Chiroptical Activities. <i>Inorganic Chemistry</i> , 2019, 58, 3670-3675.	1.9	40
10459	Effect of the exchange-correlation functional on the synchronicity/nonsynchronicity in bond formation in Diels-Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428.	1.3	31
10460	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. <i>Australian Journal of Chemistry</i> , 2019, 72, 563.	0.5	115

#	ARTICLE	IF	CITATIONS
10461	Carbon-centered radical initiators for polymerization of unsaturated monomers: Modeling and reactivity studies. <i>Polymer Engineering and Science</i> , 2019, 59, E52.	1.5	4
10462	In Situ Measure of Intrinsic Bond Strength in Crystalline Structures: Local Vibrational Mode Theory for Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1761-1776.	2.3	32
10463	Structures of Rhodium Oxide Cluster Cations $Rh_7O_m^{+n}$ ($m = 4-7, 12, 14$) Revealed by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5964-5971.	1.5	7
10464	Orbital-dependent redox potential regulation of quinone derivatives for electrical energy storage. <i>RSC Advances</i> , 2019, 9, 5164-5173.	1.7	12
10465	Circularly polarized luminescence of S_m (III) and E_u (III) complexes with chiral ligand (R / S)-BINAPO. <i>Chirality</i> , 2019, 31, 301-311.	1.3	16
10466	Three-Component Cascade Synthesis of Carbazoles through [1s,6s] Sigmatropic Shift under Metal-Free Conditions. <i>Journal of Organic Chemistry</i> , 2019, 84, 3121-3131.	1.7	21
10467	Franck-Condon Blockade and Aggregation-Modulated Conductance in Molecular Devices Using Aggregation-Induced Emission-Active Molecules. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5951-5955.	7.2	36
10468	Heats of Adsorption of N_2 , CO, Ar, and CH_4 versus Coverage on the Zr-Based MOF NU-1000: Measurements and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6586-6591.	1.5	8
10469	Exploring the mechanism of alkene hydrogenation catalyzed by defined iron complex from DFT computation. <i>Journal of Molecular Modeling</i> , 2019, 25, 61.	0.8	3
10470	Ultrafast electronic relaxations from the S_3 state of pyrene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14111-14125.	1.3	8
10471	Phosphorylation of pyridoxal azomethines. Synthesis of phosphorus containing azomethines and furopyridines. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2019, 194, 120-126.	0.8	1
10472	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. <i>Chemistry of Materials</i> , 2019, 31, 1507-1519.	3.2	29
10473	Both Reactivity and Accessibility Are Important in Cytochrome P450 Metabolism: A Combined DFT and MD Study of Fenamic Acids in BM3 Mutants. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 743-753.	2.5	13
10474	Effect of Chemical Structure on the Electrochemical Cleavage of Alkoxyamines. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5273-5281.	1.5	31
10475	Catalytic H_2 Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2134-2139.	1.0	14
10476	A Quantum Mechanical Approach for Accurate Rate Parameters of Free-Radical Polymerization Reactions. , 2019, , 17-46.		1
10477	Chemical Insight on Decreased Sensitivity of CL-20/TNT Cocrystal Revealed by ReaxFF MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2079-2092.	2.5	30
10478	Unimolecular Decomposition Reactions of Propylamine and Protonated Propylamine. <i>ACS Omega</i> , 2019, 4, 3306-3313.	1.6	15

#	ARTICLE	IF	CITATIONS
10479	Iterative multireference configuration interaction. Chinese Journal of Chemical Physics, 2019, 32, 701-707.	0.6	2
10480	Computational Modeling of the Ce@C ₈₂ Metallofullerene Isomeric Composition. ECS Journal of Solid State Science and Technology, 2019, 8, M118-M121.	0.9	9
10481	Effect of Solvent Polarity on Bromobutyl Rubber Isomerization. Russian Journal of Physical Chemistry A, 2019, 93, 2687-2693.	0.1	1
10482	A Computational Insight into Reaction Between Different Amino Acids with Reactive Aldehydes 4-hydroxy-2-nonenal and 4-oxo-2-nonenal. Croatica Chemica Acta, 2019, 92, 229-239.	0.1	0
10483	Absorption-emission symmetry breaking and the different origins of vibrational structures of the 1Qy and 1Qx electronic transitions of pheophytin <i>a</i> . Journal of Chemical Physics, 2019, 151, 165102.	1.2	17
10484	Rovibrational Spectral Analysis of CO ₃ and C ₂ O ₃ : Potential Sources for O ₂ Observed in Comet 67P/Churyumovâ€™Gerasimenko. Astrophysical Journal Letters, 2019, 886, L10.	3.0	10
10485	Coordination Ring-Opening Polymerization of Cyclic Esters: A Critical Overview of DFT Modeling and Visualization of the Reaction Mechanisms. Molecules, 2019, 24, 4117.	1.7	45
10486	Chemical and Structural Parameter Connecting Cavity Architecture, Confined Hydrocarbon Pool Species, and MTO Product Selectivity in Small-Pore Cage-Based Zeolites. ACS Catalysis, 2019, 9, 11542-11551.	5.5	51
10487	Catalytic Hydrolysis Mechanism of Cocaine by Human Carboxylesterase 1: An Orthoester Intermediate Slows Down the Reaction. Molecules, 2019, 24, 4057.	1.7	3
10488	Cation Solvation and Physicochemical Properties of Ca Battery Electrolytes. Journal of Physical Chemistry C, 2019, 123, 29524-29532.	1.5	57
10489	Singlet-Triplet Energy Gaps in Binuclear Copper Complexes and Organic Diradicals by Approximate Spin Projected Spin-unrestricted Coupled Cluster Method. Chemistry Letters, 2019, 48, 1441-1444.	0.7	3
10490	The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. Catalysis Science and Technology, 2019, 9, 6482-6491.	2.1	7
10491	Synthesis, characterization, and cytotoxic and antimicrobial activities of mixed-ligand hydrazone complexes of variable valence VO _{z+} (<i>z</i> = 2, 3). New Journal of Chemistry, 2019, 43, 16714-16729.	1.4	4
10492	Molecular Dynamics model of peptide-protein conjugation: case study of covalent complex between Sos1 peptide and N-terminal SH3 domain from Grb2. Scientific Reports, 2019, 9, 20219.	1.6	3
10493	DNA and RNA binding studies on a novel bromo-bridged dimeric copper(II) complex stabilized from a Schiff base ligand. Journal of Coordination Chemistry, 2019, 72, 3625-3644.	0.8	8
10494	A new dibenzothiophene-based dual-channel chemosensor for cyanide with aggregation induced emission. Analytical Methods, 2019, 11, 5553-5561.	1.3	22
10495	¹³ Câ€™ ¹³ C spin-coupling constants in crystalline ¹³ C-labeled saccharides: conformational effects interrogated by solid-state ¹³ C NMR spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 23576-23588.	1.3	9
10496	Structural peculiarities of keto-carotenoids in water-soluble proteins revealed by simulation of linear absorption. Physical Chemistry Chemical Physics, 2019, 21, 25707-25719.	1.3	18

#	ARTICLE	IF	CITATIONS
10497	Selective conformational control by excitation of NH imino vibrational antennas. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24935-24949.	1.3	13
10498	The diverse mechanisms for the oxidative addition of C–Br bonds to Pd(PR ₃) ₃ and Pd(PR ₃) ₂ complexes. <i>Dalton Transactions</i> , 2019, 48, 16242-16248.	1.6	21
10499	Proton-assisted air oxidation mechanisms of iron(ii) bis-thiosemicarbazone complexes at physiological pH: a kinetic-mechanistic study. <i>Dalton Transactions</i> , 2019, 48, 16578-16587.	1.6	4
10500	Solvent basicity controlled deformylation for the formation of furfural from glucose and fructose. <i>Green Chemistry</i> , 2019, 21, 6146-6153.	4.6	39
10501	Insights into the mechanisms of Cu(i)-catalyzed heterocyclization of α -acyl- β -alkynyl ketene dithioacetals to form 3-cyanofurans: the roles of NH ₄ OAc. <i>New Journal of Chemistry</i> , 2019, 43, 19149-19158.	1.4	4
10502	Systematic characterisation of the structure and radical scavenging potency of Pu'Er tea () polyphenol theaflavin. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 9942-9950.	1.5	11
10503	Combined Experimental and Theoretical Study of Cobalt Corroles as Catalysts for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30129-30136.	1.5	26
10504	Atoms in Generalized Orbital Configurations: Towards Atom-Dedicated Density Functionals. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5943.	1.8	4
10505	α -Cyclization of α -Propargyl Mandelic Acid Amides towards 2,5-Dihydrofurans. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 7656-7665.	1.2	5
10506	Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics. <i>Journal of the American Chemical Society</i> , 2019, 141, 20470-20479.	6.6	33
10507	Quantifying Inter-Residue Contacts through Interaction Energies. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5034-5044.	2.5	10
10508	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. <i>Molecules</i> , 2019, 24, 3810.	1.7	14
10509	A First Principle Model of Differential Ion Mobility: the Effect of Ion-Solvent Clustering. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 2711-2725.	1.2	25
10510	Hydration of Closely Related Manganese and Magnesium Porphyrins in Aqueous Solutions: Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10769-10779.	1.2	3
10511	Interrogating the Structure of Molecular Cavity Polaritons with Resonance Raman Scattering: An Experimentally Motivated Theoretical Description. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30551-30561.	1.5	12
10512	Formation of Oligo-Nuclear Carboxylate Nickel(II) Complexes with Nitrogen-Containing Ligands. Quantum-Chemical Simulation. <i>Russian Journal of General Chemistry</i> , 2019, 89, 2264-2272.	0.3	2
10513	Synthesis and Antimicrobial Activity of N-(Indolyl)trifluoroacetamides. <i>Moscow University Chemistry Bulletin</i> , 2019, 74, 236-240.	0.2	4
10514	Chemosensor Based on Hydrazinyl Pyridine for Selective Detection of F ⁻ , Ion in Organic Media and CO ₃ ²⁻ Ions in Aqueous Media: Design, Synthesis, Characterization and Practical Application. <i>ChemistrySelect</i> , 2019, 4, 14120-14131.	0.7	9

#	ARTICLE	IF	CITATIONS
10515	Intra-residue methyl-methyl correlations for valine and leucine residues in large proteins from a 3D-HMBC-HMQC experiment. <i>Journal of Biomolecular NMR</i> , 2019, 73, 749-757.	1.6	14
10516	Predicting Stability Constants for Terbium(III) Complexes with Dipicolinic Acid and 4-Substituted Dipicolinic Acid Analogues using Density Functional Theory. <i>ACS Omega</i> , 2019, 4, 20665-20671.	1.6	19
10517	Excess electron solvation in ammonia clusters. <i>Journal of Chemical Physics</i> , 2019, 151, 204304.	1.2	13
10518	Self-trapped holes (small polarons) in ferroelectric KH ₂ PO ₄ crystals. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 505503.	0.7	5
10519	Guanidinocalix[5]arene for sensitive fluorescence detection and magnetic removal of perfluorinated pollutants. <i>Nature Communications</i> , 2019, 10, 5762.	5.8	116
10520	DFT Modeling of Organocatalytic Ring-Opening Polymerization of Cyclic Esters: A Crucial Role of Proton Exchange and Hydrogen Bonding. <i>Polymers</i> , 2019, 11, 2078.	2.0	23
10521	Controllable catalytic difluorocarbene transfer enables access to diversified fluoroalkylated arenes. <i>Nature Chemistry</i> , 2019, 11, 948-956.	6.6	125
10522	Cr(II) and Cr(I) PCP Pincer Complexes: Synthesis, Structure, and Catalytic Reactivity. <i>Organometallics</i> , 2019, 38, 4669-4678.	1.1	17
10523	Adsorption of nitrogen-containing compounds on hydroxylated α -quartz surfaces. <i>RSC Advances</i> , 2019, 9, 36066-36074.	1.7	0
10524	Mechanistic insights into artificial metalloenzymes towards imine reduction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23408-23417.	1.3	2
10525	Metadynamics for automatic sampling of quantum property manifolds: exploration of molecular biradicality landscapes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24716-24722.	1.3	2
10526	Reactivity patterns of vanadium(IV)-oxo complexes with olefins in the presence of peroxides: a computational study. <i>Dalton Transactions</i> , 2019, 48, 16899-16910.	1.6	12
10527	Highly selective hydrogenation of amides catalysed by a molybdenum pincer complex: scope and mechanism. <i>Chemical Science</i> , 2019, 10, 10566-10576.	3.7	41
10528	Trapping an unprecedented Ti ₃ C ₃ unit inside the icosahedral C ₈₀ fullerene: a crystallographic survey. <i>Chemical Science</i> , 2019, 10, 10925-10930.	3.7	33
10529	Synthesis, photoluminescence and electroluminescence of triphenylphosphine functionalized cyclometalated iridium(III) complexes. <i>Dyes and Pigments</i> , 2019, 160, 717-725.	2.0	8
10530	Synthesis, characterization, DFT calculations, and biological activity of copper(II) complexes with 1,1,1-trifluoro-4-(2-methoxyphenyl)butan-2,4-dione. <i>Journal of Molecular Structure</i> , 2019, 1176, 515-528.	1.8	6
10531	Response properties of embedded molecules through the polarizable embedding model. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25717.	1.0	37
10532	Superatom-assembly induced transition from insulator to semiconductor: A theoretical study. <i>Science China Materials</i> , 2019, 62, 416-422.	3.5	10

#	ARTICLE	IF	CITATIONS
10533	Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 439-447.	1.2	23
10534	Modulation of Electronic Communication between Two Equivalent Ferrocenyl Groups Mediated Through Tricarbonylcyclobutadieneiron. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 668-675.	1.0	4
10535	Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 949-960.	2.3	19
10536	Selective colorimetric chemosensor for the detection of Hg ²⁺ and arsenite ions using Isatin based Schiff's bases; DFT Studies and Applications in test strips. <i>Sensors and Actuators B: Chemical</i> , 2019, 284, 271-280.	4.0	43
10537	Selective Carbanion-Pyridine Coordination of a Reactive P,N Ligand to Rh I. <i>Chemistry - A European Journal</i> , 2019, 25, 3875-3883.	1.7	8
10538	Simultaneous Prediction of the Energies of σ and π Bands and Intramolecular Charge-Transfer Transitions in Benzoannulated and Non-Peripherally Substituted Metal-Free Phthalocyanines and Their Analogues: No Standard TDDFT Silver Bullet Yet. <i>Journal of Physical Chemistry A</i> , 2019, 123, 132-152.	1.1	22
10539	Molecular and NLO Properties of Red Fluorescent Coumarins - DFT Computations Using Long-Range Separated and Conventional Functionals. <i>Journal of Fluorescence</i> , 2019, 29, 241-253.	1.3	10
10540	Intramolecular Hydrogen Shift Chemistry of Hydroperoxy-Substituted Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2019, 123, 590-600.	1.1	31
10541	Nickel-catalyzed carboxylation of aryl zinc reagent with CO ₂ : A theoretical and experimental study. <i>Journal of CO₂ Utilization</i> , 2019, 29, 262-270.	3.3	3
10542	Adsorption and encapsulation of the drug doxorubicin on covalent functionalized carbon nanotubes: A scrutinized study by using molecular dynamics simulation and quantum mechanics calculation. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 88, 11-22.	1.3	50
10543	Computational Study of the pH-Dependent Competition between Carbonate and Thymine Addition to the Guanine Radical. <i>Chemical Research in Toxicology</i> , 2019, 32, 195-210.	1.7	9
10544	Reactions between N-Heterocyclic Carbene and Lutetium-Metallofullerenes: High Regioselectivity Directed by Electronic Effect in Addition to Steric Hindrance. <i>Journal of Organic Chemistry</i> , 2019, 84, 606-612.	1.7	12
10545	Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry. <i>Journal of Organic Chemistry</i> , 2019, 84, 613-621.	1.7	5
10546	Kinetic Resolution of Alkylidene Norcamphors via a Ligand-Controlled Umpolung-Type 1,3-Dipolar Cycloaddition. <i>IScience</i> , 2019, 11, 146-159.	1.9	25
10547	Borane Incorporation in a Non-Fullerene Acceptor To Tune Steric and Electronic Properties and Improve Organic Solar Cell Performance. <i>ACS Applied Energy Materials</i> , 2019, 2, 1229-1240.	2.5	43
10548	Cucurbit[7]uril-Carbazole Two-Photon Photoinitiators for the Fabrication of Biocompatible Three-Dimensional Hydrogel Scaffolds by Laser Direct Writing in Aqueous Solutions. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 1782-1789.	4.0	52
10549	One-Electron Reduction of 2-Mono(2,6-diisopropylphenylimino)acenaphthene-1-one (dpp ⁺ mian). <i>Chemistry - A European Journal</i> , 2019, 25, 3858-3866.	1.7	13
10550	A density functional theory study on mechanism and substituent effects of a base-free and catalyst-free synthesis of functionalized dihydrobenzoxazoles. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25836.	1.0	7

#	ARTICLE	IF	CITATIONS
10551	Collision-induced mass spectrometric fragmentation of protonated dimethoate and omethoate generated by electrospray ionization. <i>Rapid Communications in Mass Spectrometry</i> , 2019, 33, 259-271.	0.7	1
10552	Actinia-like multifunctional nano-coagulant for single-step removal of water contaminants. <i>Nature Nanotechnology</i> , 2019, 14, 64-71.	15.6	89
10553	The possibility of CNH^+ within Titan's atmosphere: Rovibrational analysis of CNH^+ and CCH_2^+ and CCH_2 . <i>Icarus</i> , 2019, 321, 1-10.	1.1	1
10554	Dissociation of $[\text{H}^+]$ ions composed of one β -methyltryptophan and four alanine residues: The effect of the β -methyl group. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 52-58.	0.7	0
10555	Phenothiazine-based small molecules for bulk heterojunction organic solar cells; variation of side-chain polarity and length of conjugated system. <i>Organic Electronics</i> , 2019, 65, 232-242.	1.4	19
10556	Novel fluorescent probes for relay detection copper/citrate ion and application in cell imaging. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 211, 9-17.	2.0	21
10557	Routes for the gas-phase total synthesis of dihydroxy magnesium carboxylate anions, $[(\text{RCO}_2)\text{Mg}(\text{OH})_2]^+$ ($\text{R} = \text{CH}_3$ and CH_2CH_3). <i>International Journal of Mass Spectrometry</i> , 2019, 436, 91-100.	0.7	0
10558	Helical Multi-coordination Anion-binding Catalysts for the Highly Enantioselective Dearomatization of Pyrylium Derivatives. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3217-3221.	7.2	42
10559	On the silicon-silicon bonds σ -coordinated to group 10 transition metals. <i>Inorganica Chimica Acta</i> , 2019, 486, 449-457.	1.2	1
10560	Proline autocatalysis in the origin of biological enantioenriched chirality. <i>Chirality</i> , 2019, 31, 5-10.	1.3	4
10561	A family of solution processable ligands and their Re(I) complexes towards light emitting applications. <i>Dyes and Pigments</i> , 2019, 163, 86-101.	2.0	22
10562	Photophysical and photocatalytic properties of corophyll and chlorophyll. <i>Computational Materials Science</i> , 2019, 158, 228-234.	1.4	15
10563	Diverse Reactivity of Dienes with Pentaphenylborole and 1-Phenyl-2,3,4,5-tetramethylborole Dimer. <i>Chemistry - A European Journal</i> , 2019, 25, 1581-1587.	1.7	22
10564	A Density Functional Theory Study on Nonlinear Optical Properties of Double Cage Excess Electron Compounds: Theoretically Design $\text{M}[\text{Cu}(\text{Ag})@(\text{NH}_3)_n]$ ($\text{M} = \text{Be, Mg and Ca}$; $n = 1-3$). <i>Journal of Computational Chemistry</i> , 2019, 40, 971-979.	1.5	18
10565	GARLEEK: Adding an extra flavor to ONIOM. <i>Journal of Computational Chemistry</i> , 2019, 40, 381-386.	1.5	6
10566	Complexes between core-modified porphyrins $\text{ZnP}(X)_4$ ($X = \text{P and S}$) and small semiconductor nanoparticle ZnS : are they possible?. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	3
10567	Incremental Introduction of Organocatalytic Activity into Conformationally Engineered Porphyrins. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2448-2452.	1.2	19
10568	Multiply Wrapped Porphyrin Dyes with a Phenothiazine Donor: A High Efficiency of 11.7% Achieved through a Synergetic Coadsorption and Cosensitization Approach. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 5046-5054.	4.0	83

#	ARTICLE	IF	CITATIONS
10569	A colorimetric and fluorometric oligothiophene-indenedione-based sensor for rapid and highly sensitive detection of cyanide in real samples and bioimaging in living cells. <i>Dyes and Pigments</i> , 2019, 163, 667-674.	2.0	50
10570	Tuning the physicochemical properties of the single-walled boron nitride nanotube by covalent grafting of triazolium-based [MTZ] ⁺ [X] ⁻ (X ⁻ = NTf ₂ ⁻ , TfO ⁻ and BF ₄ ⁻) ionic liquids in the gas phase and solvent media: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2019, 277, 726-737.	2.3	2
10571	How boron is adsorbed by -glucamine: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2019, 1150, 85-90.	1.1	13
10572	Use of Circular Statistics To Model β -Man-(1 \rightarrow 2)- β -Man and β -Man-(1 \rightarrow 3)- β - β Man <i>O</i> -Glycosidic Linkage Conformation in ¹³ C-Labeled Disaccharides and High-Mannose Oligosaccharides. <i>Biochemistry</i> , 2019, 58, 546-560.	1.2	29
10573	Role of Oleylamine Revisited: An Original Disproportionation Route to Monodispersed Cobalt and Nickel Nanocrystals. <i>Chemistry of Materials</i> , 2019, 31, 960-968.	3.2	21
10574	Synthesis and <i>O</i> -Glycosidic Linkage Conformational Analysis of ¹³ C-Labeled Oligosaccharide Fragments of an Antifreeze Glycolipid. <i>Journal of Organic Chemistry</i> , 2019, 84, 1706-1724.	1.7	15
10575	The Importance of Peroxy Radical Hydrogen-Shift Reactions in Atmospheric Isoprene Oxidation. <i>Journal of Physical Chemistry A</i> , 2019, 123, 920-932.	1.1	66
10576	Ionization and Electron Attachment for Nucleobases in Water. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1237-1247.	1.2	24
10577	Dehydrogenation of formic acid catalysed by M-embedded nitrogen-doped graphene (M = Fe, Ru, Os): a DFT study. <i>New Journal of Chemistry</i> , 2019, 43, 1440-1448.	1.4	15
10578	Accurate Ionization Potentials, Electron Affinities and Electronegativities of Single-Walled Carbon Nanotubes by State-of-the-Art Local Coupled-Cluster Theory. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 170-174.	2.0	3
10579	Spin-spin coupling constants in linear substituted HCN clusters. <i>Molecular Physics</i> , 2019, 117, 693-704.	0.8	3
10580	Shogaol but not gingerol has a neuroprotective effect on hemorrhagic brain injury: Contribution of the α , β -unsaturated carbonyl to heme oxygenase-1 expression. <i>European Journal of Pharmacology</i> , 2019, 842, 33-39.	1.7	11
10581	Cross-strand disulfides in the hydrogen bonding site of antiparallel β -sheet (α CSDhs): Forbidden disulfides that are highly strained, easily broken. <i>Protein Science</i> , 2019, 28, 239-256.	3.1	4
10582	DFT and AIMD prediction of a SNS manganese pincer complex for hydrogenation of acetophenone. <i>Chemical Physics Letters</i> , 2019, 714, 37-44.	1.2	11
10583	Reaction mechanism of NO with hydrolysates of NAMI-A: an MD simulation by combining the QM/MM(ABEEM) with the MD-FEP method. <i>Journal of Computational Chemistry</i> , 2019, 40, 1141-1150.	1.5	7
10584	Deep eutectic solvents formed by quaternary ammonium salts and aprotic organic compound succinonitrile. <i>Journal of Molecular Liquids</i> , 2019, 274, 414-417.	2.3	23
10585	Orthopalladated 1,4-iminonaphthoquinone derivative: Syntheses, redox series, molecular and electronic structures. <i>Inorganica Chimica Acta</i> , 2019, 487, 240-246.	1.2	1
10586	Mechanism study on rhodium(III)-catalyzed C-H functionalization of <i>o</i> -vinylphenols with alkynes: Regioselectivity and chemoselectivity. <i>Computational and Theoretical Chemistry</i> , 2019, 1147, 40-50.	1.1	1

#	ARTICLE	IF	CITATIONS
10587	Optoelectrical characterization of different fabricated donor substituted benzothiazole based sensitizers for efficient DSSCs. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 372, 35-41.	2.0	13
10588	Investigation of tyrosinase inhibition by some 1,2,4 triazole derivative compounds: in vitro and in silico mechanisms. <i>Turkish Journal of Biochemistry</i> , 2019, 44, 473-481.	0.3	5
10589	Experimental and density functional theory insights into the effect of withdrawing ligands on the fluorescence yield of Ru(II)-based complexes. <i>Applied Organometallic Chemistry</i> , 2019, 33, e4677.	1.7	9
10590	Helikale Multi-Koordinations-Anionenbindungskatalysatoren ermöglichen hoch enantioselektive Dearomatisierung von Pyryliumderivaten. <i>Angewandte Chemie</i> , 2019, 131, 3250-3255.	1.6	23
10591	Revisited Mechanism of Reaction between a Model Lysine Amino Acid Side Chain and 4-Hydroxynonenal in Different Solvent Environments. <i>Journal of Organic Chemistry</i> , 2019, 84, 526-535.	1.7	14
10592	A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. <i>Journal of Computational Chemistry</i> , 2019, 40, 532-542.	1.5	2
10593	Ratiometric Monitoring of Thorium Contamination in Natural Water Using a Dual-Emission Luminescent Europium Organic Framework. <i>Environmental Science & Technology</i> , 2019, 53, 332-341.	4.6	90
10594	Half-sandwich ruthenium(II)-arene complexes: synthesis, spectroscopic studies, biological properties, and molecular modeling. <i>Journal of Coordination Chemistry</i> , 2019, 72, 148-163.	0.8	4
10595	Concerted bond switching mechanism coupled with one-electron transfer for the oxygen-oxygen bond formation in the oxygen-evolving complex of photosystem II. <i>Chemical Physics Letters</i> , 2019, 714, 219-226.	1.2	17
10596	Probing Basis Set Requirements for Calculating Core Ionization and Core Excitation Spectroscopy by the $\tilde{\rho}^n$ Self-Consistent-Field Approach. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 325-337.	2.3	58
10597	Hydrogen atom transfer in the radical cations of tryptophan-containing peptides AW and WA studied by mass spectrometry, infrared multiple-photon dissociation spectroscopy, and theoretical calculations. <i>European Journal of Mass Spectrometry</i> , 2019, 25, 112-121.	0.5	6
10598	Carvedilol-Imprinted Polymer: Rational design and selectivity studies. <i>Journal of Molecular Structure</i> , 2019, 1177, 101-106.	1.8	24
10599	Maximal orbital analysis of molecular wavefunctions. <i>Journal of Computational Chemistry</i> , 2019, 40, 39-50.	1.5	3
10600	Robust metal-pentagon interactions in the Th-based endohedral metallofullerenes revealed by DFT calculations. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25826.	1.0	8
10601	NHC-Stabilized Radicals in the Formal Hydroacylation Reaction of Alkynes. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 557-561.	1.2	7
10602	Metal-catalyzed alkyne oxidation/C-H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. <i>Journal of Computational Chemistry</i> , 2019, 40, 1038-1044.	1.5	2
10603	Novel fluorescent probes for sequential detection of Cu ²⁺ and citrate anion and application in living cell imaging. <i>Dyes and Pigments</i> , 2019, 161, 331-340.	2.0	47
10604	Structural insight into antisense gapmer-RNA oligomer duplexes through molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2823-2836.	2.0	7

#	ARTICLE	IF	CITATIONS
10605	The structure design of biotransformed unsymmetrical nitro-contained 1,5-diaryl-3-oxo-1,4-pentadienyls for the anti-parasitic activities. <i>Arabian Journal of Chemistry</i> , 2019, 12, 4006-4016.	2.3	7
10606	Quantum Calculations on Plant Cell Wall Component Interactions. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2019, 11, 485-495.	2.2	10
10607	Convergence Study of Different Approaches of Solving the Hartree-Fock Equation on the Potential Curve of the Hydrogen Fluoride. <i>Lecture Notes in Electrical Engineering</i> , 2020, , 461-471.	0.3	0
10608	Development of a semiacenaphthenofluorescein-based optical and fluorescent sensor for imaging cysteine in cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 386, 112090.	2.0	6
10609	Design and synthesis new colorimetric receptors for naked-eye detection of biologically important fluoride and acetate anions in organic and arsenite in aqueous medium based on ICT mechanism: DFT study and test strip application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 225, 117522.	2.0	14
10610	Amphiphilic hyper-crosslinked porous cyclodextrin polymer with high specific surface area for rapid removal of organic micropollutants. <i>Chemical Engineering Journal</i> , 2020, 382, 123015.	6.6	62
10611	Structure and activity of activated carbon functionalized with maleic anhydride by diels-alder reaction. <i>Catalysis Today</i> , 2020, 357, 409-415.	2.2	5
10612	Triazole derived azo-azomethine dye as a new colorimetric anion chemosensor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 226, 117566.	2.0	11
10613	Ion spectroscopy of heterogeneous mixtures: IRMPD and DFT analysis of anomers and conformers of monosaccharides. <i>International Journal of Mass Spectrometry</i> , 2020, 447, 116235.	0.7	14
10614	Peracetic acid: Structural elucidation for applications in wastewater treatment. <i>Water Research</i> , 2020, 168, 115143.	5.3	76
10615	Intra- and Intermolecular Fluorescence Quenching of Alkylthio-Substituted Phthalimides by Photoinduced Electron Transfer: Distance, Position and Conformational Dependence. <i>ChemPhotoChem</i> , 2020, 4, 89-97.	1.5	2
10616	The theoretical study of dehydrogenation mechanism from Sr(NH ₂ BH ₃) ₂ . <i>Structural Chemistry</i> , 2020, 31, 339-350.	1.0	4
10617	Spectroscopic and structural investigations on modafinil by FT-IR, FT-Raman, NMR, UV-Vis and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117449.	2.0	22
10618	Development and validation of an experimental and theoretical method for the chiral discrimination of dinotefuran. <i>Chirality</i> , 2020, 32, 53-63.	1.3	4
10619	Hemicyanine based naked-eye ratiometric fluorescent probe for monitoring lysosomal pH and its application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 227, 117767.	2.0	19
10620	Electronic spectroscopic characterization of the formation of iron(III) metal complexes: The 8-HydroxyQuinoline as ligand case study. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110864.	1.5	11
10621	Exploring DNA binding ability of two novel β -N-heterocyclic thiosemicarbazone palladium(II) complexes. <i>Journal of Inorganic Biochemistry</i> , 2020, 203, 110875.	1.5	15
10622	Cobalt phthalocyanine is a suitable scaffold for lithium polysulfide (Li ₂ S _n , n = 2-8). <i>Chemical Physics Letters</i> , 2020, 739, 136942.	1.2	20

#	ARTICLE	IF	CITATIONS
10623	Perylene-diimide-based n-type semiconductors with enhanced air and temperature stable photoconductor and transistor properties. <i>Dyes and Pigments</i> , 2020, 174, 108014.	2.0	15
10624	Ether based flexible bis Schiff base fluorescent colorimetric chemosensors for selective and sensitive detection of HF ₂ ^{âˆ’} ion. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 389, 112179.	2.0	5
10625	One-electron oxidation and redox potential of nucleobases and deoxyribonucleosides computed by QM/MM simulations. <i>Chemical Physics Letters</i> , 2020, 739, 136948.	1.2	10
10626	Can a Mononuclear Iron(III)â€•Superoxo Active Site Catalyze the Decarboxylation of Dodecanoic Acid in UndA to Produce Biofuels?. <i>Chemistry - A European Journal</i> , 2020, 26, 2233-2242.	1.7	24
10627	Unconventional Reactivity of Ethynylbenziodoxolone Reagents and Thiols: Scope and Mechanism. <i>Chemistry - A European Journal</i> , 2020, 26, 2386-2394.	1.7	28
10628	Baseâ€•Initiated Formation of Fe I â€•PNP Pincer Complexes. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1101-1105.	1.0	4
10629	Endohedral Metallofullerene M ₂ @C ₈₀ : A New Class of Magnetic Superhalogen. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2131-2136.	1.5	16
10630	A Computational Study of Solvent and Electric Field Effects on Propylene Oxide Ringâ€•Opening Reaction. <i>ChemistrySelect</i> , 2020, 5, 384-391.	0.7	0
10631	Catalytic Dehydrogenation of Amineâ€•Boranes using Geminal Phosphinoâ€•Boranes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 586-592.	0.6	12
10632	Exploring the mechanism of olfactory recognition in the initial stage by modeling the emission spectrum of electron transfer. <i>PLoS ONE</i> , 2020, 15, e0217665.	1.1	2
10633	Bioinspired Synthesis of (âˆ’)-â€•PFâ€•1018. <i>Angewandte Chemie</i> , 2020, 132, 5301-5305.	1.6	6
10634	Paramagnetic bioactives encapsulated in poly(D,L-lactide) microparticules: Spatial distribution and in vitro release kinetics. <i>Journal of Supercritical Fluids</i> , 2020, 158, 104748.	1.6	10
10635	Quantum Mechanics/Molecular Mechanics Density Functional Theory Simulations of the Optical Properties Fingerprinting the Ligand-Binding of Pentameric Formyl Thiophene Acetic Acid in Amyloid-Î²(1â€•42). <i>Journal of Physical Chemistry A</i> , 2020, 124, 875-888.	1.1	11
10636	Influence of Electrolyte Composition on Ultrafast Interfacial Electron Transfer in Fe-Sensitized TiO ₂ -Based Solar Cells. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1794-1811.	1.5	19
10637	Time-Domain Terahertz Spectroscopy and Solid-State Density Functional Theory Analysis of p-Nitrophenol Polymorphs. <i>Journal of Infrared, Millimeter, and Terahertz Waves</i> , 2020, 41, 1337-1354.	1.2	2
10638	Mechanism and stereoselectivity of benzylic Câ€•H hydroxylation by Ruâ€•porphyrin: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 346-352.	1.5	8
10639	Dinuclear copper(II) complex with a benzimidazole derivative: Crystal structure, theoretical calculations, and cytotoxic activity. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5425.	1.7	7
10640	Theoretical insight into the redox-switchable activity of group 4 metal complexes for the ring-opening polymerization of Î¼-caprolactone. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 961-971.	3.0	23

#	ARTICLE	IF	CITATIONS
10641	Theoretical Studies on Rh-Catalyzed Cycloisomerization of Homopropargylallene-Alkynes through C(sp ³)-C(sp) Bond Activation. <i>ACS Catalysis</i> , 2020, 10, 1828-1837.	5.5	13
10642	Syntheses and electronic, electrochemical, and theoretical studies of a series of 1/4-oxo-triruthenium carboxylates bearing orthometalated phenazines. <i>Dalton Transactions</i> , 2020, 49, 1688-1698.	1.6	3
10643	Tuning the excited-state intramolecular proton transfer (ESIPT) process of indole-pyrrole systems by π -conjugation and substitution effects: experimental and computational studies. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1409-1415.	1.3	16
10644	Rapid and accurate molecular deprotonation energies from quantum alchemy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10519-10525.	1.3	19
10645	DFT study of trialkylborohydride-catalysed hydrosilylation of alkenes – the mechanism and its implications. <i>Catalysis Science and Technology</i> , 2020, 10, 1066-1072.	2.1	14
10646	3-Amino-1-propanol and <i>N</i> -methylaminoethanol: coordination to zinc(II) vs. decomposition to ammonia. <i>New Journal of Chemistry</i> , 2020, 44, 387-400.	1.4	7
10647	A BPt4S4 cluster: a planar tetracoordinate boron system with three charges all at their global energy minima. <i>New Journal of Chemistry</i> , 2020, 44, 767-772.	1.4	8
10648	Diversity-oriented approach to functional thiophene dyes by Suzuki coupling-lithiation one-pot sequences. <i>Organic Chemistry Frontiers</i> , 2020, 7, 329-339.	2.3	8
10649	Carbon based Y-type molecules for application in nonlinear optics. <i>Journal of Materials Chemistry C</i> , 2020, 8, 1879-1886.	2.7	10
10650	Efficient Electronic Structure to Stabilize N ₂ -Bridged Dinuclear Complexes Intended for N ₂ Activation: Iminophosphorane Iron(I) and Cobalt(I). <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1411-1417.	1.0	5
10651	Effect of 1-ethyl-3-methylimidazolium acetate on the oxidation of caffeic acid benzyl ester: An electrochemical and theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4044.	0.9	3
10652	A theoretical investigation on the encapsulation process of mepivacaine into β -cyclodextrin. <i>Chemical Physics Letters</i> , 2020, 740, 137060.	1.2	15
10653	Synthesis, structures, thermal behavior and vapour pressures of new strontium and barium β -diketonate complexes [M(t-BuCOCHCOCF ₃) ₂ (18-crown-6)] and [M(t-BuCOCHCOCF ₇) ₂ (18-crown-6)] (M = Sr, Ba). <i>Polyhedron</i> , 2020, 177, 114263.	1.0	7
10654	Synthesis and Reactivity of Re(III) and Re(V) Fischer Carbenes. <i>Organometallics</i> , 2020, 39, 388-396.	1.1	5
10655	Visible Light- and Heat-Promoted C [^] O Coupling Reaction of Phenols and Aryl Halides. <i>Asian Journal of Organic Chemistry</i> , 2020, 9, 116-120.	1.3	24
10656	Bipyridyl/carbazolate silver(I) and gold(I) π -heterocyclic carbene complexes: A systematic study of geometric constraints and electronic properties. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5335.	1.7	6
10657	Molecular Basis for Metabolic Regioselectivity and Mechanism of Cytochrome P450s toward Carcinogenic 4-(Methylnitrosamino)-(3-pyridyl)-1-butanone. <i>Chemical Research in Toxicology</i> , 2020, 33, 436-447.	1.7	10
10658	Boosting Photoelectric Conductivity in Porphyrin-Based MOFs Incorporating C ₆₀ . <i>Journal of Physical Chemistry C</i> , 2020, 124, 1878-1887.	1.5	27

#	ARTICLE	IF	CITATIONS
10659	The vinylogous aldol reaction of N-Sulfinyl metallodienamines. <i>Tetrahedron</i> , 2020, 76, 130901.	1.0	5
10660	Controlling Coordination Number of Rhodium(III) Complex by Ligand-Based Redox for Catalytic C-H Amination. <i>Bulletin of the Chemical Society of Japan</i> , 2020, 93, 279-286.	2.0	15
10661	Hierarchy of Intermolecular Interactions and Selective Topochemical Reactivity in Different Polymorphs of Fused-Ring Heteroaromatics. <i>Crystal Growth and Design</i> , 2020, 20, 1229-1236.	1.4	13
10662	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1162-1174.	2.3	12
10663	Synthesis and Photophysical Behavior of a Highly Fluorescent Family of Unsymmetrical Organoboron Complexes Containing 5-(Pyridin-2-ylmethylene)imidazolidine-2,4-dione Moieties. <i>Journal of Organic Chemistry</i> , 2020, 85, 441-448.	1.7	6
10664	Do Carbon Nanoions Behave as Nanoscopic Faraday Cages? A Comparison of the Reactivity of C ₆₀ , C ₂₄₀ , C ₆₀ @C ₂₄₀ , Li ⁺ @C ₆₀ , Li ⁺ @C ₂₄₀ , and Li ⁺ @C ₆₀ @C ₂₄₀ . <i>Chemistry - A European Journal</i> , 2020, 26, 804-808.	1.7	12
10665	Rational design, synthesis and biological profiling of new KDM4C inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115128.	1.4	9
10666	Mechanistic Study on Catalytic Disproportionation of Hydrazine by a Protic Pincer-Type Iron Complex through Proton-Coupled Electron Transfer. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1472-1482.	1.0	8
10667	Insights into the role of D _{3h} type proaromatic organic dyes with thieno[3,4-b]pyrazine as A acceptor group into dye-sensitized solar cells. A TDFT/periodic DFT study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26108.	1.0	6
10668	A DFT study on mechanisms of CO ₂ coupling with propargylic alcohols using alkali carbonates. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26150.	1.0	2
10669	Copper-based redox shuttles supported by preorganized tetradentate ligands for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2020, 49, 343-355.	1.6	19
10670	Software to obtain spatially localized functions from different radial functions. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 267-280.	1.3	1
10671	Engineering aromatic heterocycle strategy: Improving copper electrodeposition performance via tuning the bandgap of diketopyrrolopyrrole-based leveler. <i>Tetrahedron</i> , 2020, 76, 130882.	1.0	6
10672	Coordination properties of diethylenetriamine in relation to zinc phthalocyanine. <i>Polyhedron</i> , 2020, 178, 114313.	1.0	12
10673	Atomistic Simulations of COSAN: Amphiphiles without a Head and Tail Design Display Head and Tail Surfactant Behavior. <i>Angewandte Chemie</i> , 2020, 132, 3112-3116.	1.6	8
10674	Atomistic Simulations of COSAN: Amphiphiles without a Head and Tail Design Display Head and Tail Surfactant Behavior. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 3088-3092.	7.2	43
10675	Nitrogen Fixation Catalyzed by Dinitrogen-Bridged Dimolybdenum Complexes Bearing PCP- and PNP-Type Pincer Ligands: A Shortcut Pathway Deduced from Free Energy Profiles. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1490-1498.	1.0	17
10676	Keteniminium Salts: Reactivity and Propensity toward Electrocyclization Reactions. <i>Journal of Organic Chemistry</i> , 2020, 85, 449-463.	1.7	7

#	ARTICLE	IF	CITATIONS
10677	The Importance of Metal–Ligand Cooperativity in the Phosphorus–Nitrogen P ₃ P Platform: A Computational Study on Mn-Catalyzed Pyrrole Synthesis. <i>Organometallics</i> , 2020, 39, 18-24.	1.1	9
10678	Base-Controlled Directed Synthesis of Metal–Methyleneimidazoline (Mlz) and Metal–Mesoionic Carbene (MIC) Compounds. <i>Organometallics</i> , 2020, 39, 189-200.	1.1	5
10679	Discovering Biomolecules with Huisgenase Activity: Designed Repeat Proteins as Biocatalysts for (3 + 2) Cycloadditions. <i>Journal of the American Chemical Society</i> , 2020, 142, 762-776.	6.6	8
10680	Substituent Effects on Photochemistry of Anthracene–Phenol–Pyridine Triads Revealed by Multireference Calculations. <i>Journal of the American Chemical Society</i> , 2020, 142, 487-494.	6.6	8
10681	Dopant-Free, Donor–Acceptor-Type Polymeric Hole-Transporting Materials for the Perovskite Solar Cells with Power Conversion Efficiencies over 20%. <i>Advanced Energy Materials</i> , 2020, 10, 1903146.	10.2	74
10682	New β -unsubstituted isoxazolones as potent human neutrophil elastase inhibitors: Synthesis and molecular dynamic simulation. <i>Drug Development Research</i> , 2020, 81, 338-349.	1.4	11
10683	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 249-258.	2.5	12
10684	Symmetrical and Unsymmetrical 4,7-Bis(arylvinyl)benzo[2,1,3]chalcogenodiazoles: Synthesis, Photophysical and Electrochemical Properties and Biomolecular Interaction Studies. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 348-361.	1.2	8
10685	Synthesis, characterization and biological evaluation of <i>N</i> -substituted triazinane-2-thiones and theoretical–experimental mechanism of condensation reaction. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5329.	1.7	8
10686	Naked diazaborepin dyes: Synthesis, photophysical properties, substituent effects and theoretical calculations on ESIPT process. <i>Dyes and Pigments</i> , 2020, 175, 108128.	2.0	7
10687	Syntheses, Characterizations, and Crystal Structures of Dinitrogen–Divanadium Complexes Bearing Triamidoamine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1456-1464.	1.0	12
10688	Interfacial charge-transfer transitions between TiO ₂ and indole. <i>Chemical Physics Letters</i> , 2020, 739, 136974.	1.2	19
10689	Theoretical study on cyclophane amide molecular receptors and its complexation behavior with TCNQ. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2020, 203, 111735.	1.7	11
10690	Atomic-Level Alloying of Sulfur and Selenium for Advanced Lithium Batteries. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 1005-1013.	4.0	14
10691	Organocatalytic Access to a <i>cis</i> -Cyclopentyl- β -amino Acid: An Intriguing Model of Selectivity and Formation of a Stable 10/12-Helix from the Corresponding β -Peptide. <i>Journal of the American Chemical Society</i> , 2020, 142, 1382-1393.	6.6	11
10692	Enstatite (MgSiO ₃) and forsterite (Mg ₂ SiO ₄) monomers and dimers: highly detectable infrared and radioastronomical molecular building blocks. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 492, 276-282.	1.6	18
10693	Preferential Formation of Mono-Metallofullerenes Governed by the Encapsulation Energy of the Metal Elements: A Case Study on Eu@C _{2n} (2n=74–84) Revealing a General Rule. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 5259-5262.	7.2	27
10694	Density Functional Extension to Excited-State Mean-Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 164-178.	2.3	22

#	ARTICLE	IF	CITATIONS
10695	Bioinspired Synthesis of (â)â€PFâ€1018. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 5263-5267.	7.2	18
10696	Origin of Regioâ€and Stereoselectivity in the NHCâ€catalyzed Reaction of Alkyl Pyridinium with Aliphatic Enal. <i>ChemCatChem</i> , 2020, 12, 1068-1074.	1.8	27
10697	Chemically Modified Carbon Nanohorns as Nanovectors of the Cisplatin Drug: A Molecular Dynamics Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 500-512.	2.5	16
10698	Designing new donor materials based on functionalized DCCnT with different electronâ€donating groups: A density functional theory (DFT) and time dependent density functional theory (TDDFT)â€based study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26112.	1.0	5
10699	Gold(I)â€Catalysed Hydroarylation of Lactamâ€Derived Enynes as an Entry to Tetrahydrobenzo[<i>g</i>]quinolines. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 646-653.	1.2	6
10700	Chemical pathways for the formation of benzofuran and dibenzofuran in combustion. <i>Combustion and Flame</i> , 2020, 212, 216-233.	2.8	17
10701	Ligandâ€Mediated Regioselective Rhodiumâ€Catalyzed Benzotriazoleâ€Allene Coupling: Mechanistic Exploration and Quantum Chemical Analysis. <i>Chemistry - A European Journal</i> , 2020, 26, 2342-2348.	1.7	16
10702	First-principles study of the reaction mechanism governing the S _N Ar of the dimethylamine on 2-methoxy-5-nitrothiophenes. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	5
10703	Coordination Chemistry of Ru(II) Complexes of an Asymmetric Bipyridine Analogue: Synergistic Effects of Supporting Ligand and Coordination Geometry on Reactivities. <i>Molecules</i> , 2020, 25, 27.	1.7	8
10704	Structural Dynamics and Stereoselectivity of Chiral Benzylideneamine N,Câ€Chelate Borane Photoâ€Thermal Isomerization. <i>Chemistry - A European Journal</i> , 2020, 26, 2276-2284.	1.7	4
10705	Chalcogenborines and Derivatives: Probing the Origin of Relative Thermodynamic Stabilities. <i>ChemistrySelect</i> , 2020, 5, 83-90.	0.7	1
10706	Elucidating the Role of Catalyst Steric and Electronic Effects in Controlling the Synthesis of Î€-Conjugated Polymers. <i>Macromolecules</i> , 2020, 53, 138-148.	2.2	15
10707	Probing the Aromaticity and Stability of Metallatricycles by DFT Calculations: Toward Clar Structure in Organometallic Chemistry. <i>Organometallics</i> , 2020, 39, 80-86.	1.1	7
10708	Electroactivated alkylation of amines with alcohols <i>via</i> both direct and indirect borrowing hydrogen mechanisms. <i>Green Chemistry</i> , 2020, 22, 860-869.	4.6	8
10709	Hole Transfer in Open Carbynes. <i>Materials</i> , 2020, 13, 3979.	1.3	3
10710	Is It Conjugated or Not? The Theoretical and Experimental Electron Density Map of Bonding in p-CH ₃ CH ₂ COC ₆ H ₄ -Câ€Câ€C-p-C ₆ H ₄ COCH ₃ CH ₂ . <i>Molecules</i> , 2020, 25, 4388.	1.7	1
10711	Acetonyl Peroxy and Hydro Peroxy Self- and Cross-Reactions: Kinetics, Mechanism, and Chaperone Enhancement from the Perspective of the Hydroxyl Radical Product. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8128-8143.	1.1	7
10712	Propene Hydroformylation Reaction Catalyzed by HRh(CO)(BISBI): A Thermodynamic and Kinetic Analysis of the Full Catalytic Cycle. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3907-3916.	1.0	9

#	ARTICLE	IF	CITATIONS
10713	Excited state structures projected onto two dimensions: correlations with luminescent behavior. <i>Journal of Mathematical Chemistry</i> , 2020, 58, 2254-2272.	0.7	2
10714	Impact of the Novel Z-Acceptor Ligand Bis(<i>ortho</i> -diphenylphosphino)phenyl}zinc (ZnPhos) on the Formation and Reactivity of Low-Coordinate Ru(0) Centers. <i>Inorganic Chemistry</i> , 2020, 59, 15606-15619.	1.9	9
10715	Unraveling the Reaction Mechanism and Active Sites of Metal-Organic Frameworks for Glucose Transformations in Water: Experimental and Theoretical Studies. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 16143-16155.	3.2	19
10716	Substituted glycolides from natural sources: preparation, alcoholysis and polymerization. <i>Polymer Chemistry</i> , 2020, 11, 6890-6902.	1.9	5
10717	Element table of TM-substituted polyoxotungstates for direct electrocatalytic reduction of nitric oxide to ammonia: a DFT guideline for experiments. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 4507-4516.	3.0	19
10718	Synthesis, physicochemical properties and computational study of donor-acceptor polymer for optical limiting application. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	2
10719	Machine Learning Predicts Degree of Aromaticity from Structural Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4560-4568.	2.5	3
10720	PyVibMS: a PyMOL plugin for visualizing vibrations in molecules and solids. <i>Journal of Molecular Modeling</i> , 2020, 26, 290.	0.8	14
10721	Synthesis and properties of 6,7-dihydroxybenzopyrylium perchlorate halogen derivatives: X-ray, spectroscopic and theoretical studies. <i>Tetrahedron</i> , 2020, 76, 131514.	1.0	10
10722	Asymmetric α -Clip-Cycle-Synthesis of Pyrrolidines and Spiropyrrolidines. <i>Organic Letters</i> , 2020, 22, 8116-8121.	2.4	18
10723	An enzymatic Alder-ene reaction. <i>Nature</i> , 2020, 586, 64-69.	13.7	41
10724	Heuristic Global Optimization in Chemical Compound Space. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9044-9060.	1.1	7
10725	A pyridinic Fe-N ₄ macrocycle models the active sites in Fe/N-doped carbon electrocatalysts. <i>Nature Communications</i> , 2020, 11, 5283.	5.8	286
10726	Production of Long-Lived Benzene Dications from Electron Impact in the 20-2000 eV Energy Range Combined with the Search for Global Minimum Structures. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9261-9271.	1.1	11
10727	Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Protein-Inhibitor Complexes in Relevance to Developing Parkinson's Therapeutics. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7648.	1.8	9
10728	Theoretical Study of the Mechanism of Palladium(0)-Catalyzed Intramolecular [2+2+2] Cycloaddition of Ester-Substituted Alkynes. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 7455-7465.	1.2	3
10729	Twisted-Planar-Twisted expanded porphyrinoid dimer as a rudimentary reaction-based methanol indicator. <i>Nature Communications</i> , 2020, 11, 5289.	5.8	20
10730	The adsorption of chlorofluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QAIM study. <i>Molecular Simulation</i> , 2020, 46, 1405-1416.	0.9	33

#	ARTICLE	IF	CITATIONS
10731	The adsorption of chlorofluoromethane on pristine, and Al- and Ga-doped boron nitride nanosheets: a DFT, NBO, and QTAIM study. <i>Journal of Molecular Modeling</i> , 2020, 26, 287.	0.8	35
10732	Understanding the solubilization of Ca acetylide with a new computational model for ionic pairs. <i>Chemical Science</i> , 2020, 11, 13102-13112.	3.7	12
10733	Formation of an unusual glutamine tautomer in a blue light using flavin photocycle characterizes the light-adapted state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 26626-26632.	3.3	34
10734	Photoluminescence, photophysics, and photochemistry of the $V\langle B \rangle$ defect in hexagonal boron nitride. <i>Physical Review B</i> , 2020, 102.	1.1	60
10735	Coordination Flexibility of the Rh(PXP) Complex to NH_3 , CO, and C_2H_4 (PXP = Diphosphine-Based Pincer Ligand; X = B, Al, and Ga): Theoretical Insight. <i>Inorganic Chemistry</i> , 2020, 59, 15862-15876.	1.9	9
10736	Solvation of HeH ⁺ in neon atoms: Proton-bound complexes of mixed He and Ne. <i>Chemical Physics</i> , 2020, 539, 110927.	0.9	3
10737	Exploring the optical and nonlinear optical features of heteroleptic complexes with BODIPY and amido-BODIPY substitutions; A comparative theoretical study. <i>Inorganic Chemistry Communication</i> , 2020, 121, 108234.	1.8	2
10738	Synthesis, Characterization, Catalytic Activity, and DFT Calculations of Zn(II) Hydrazone Complexes. <i>Molecules</i> , 2020, 25, 4043.	1.7	47
10739	Combined MD/QTAIM techniques to evaluate ligand-receptor interactions. Scope and limitations. <i>European Journal of Medicinal Chemistry</i> , 2020, 208, 112792.	2.6	19
10740	Unveiling the Mechanism, Origin of Stereoselectivity, and Ligand-Dependent Reactivity in the Pd(II)-Catalyzed Unbiased Methylene $C(sp^3)H$ Alkenylation/Aza-Wacker Cyclization Reaction. <i>Journal of Organic Chemistry</i> , 2020, 85, 13191-13203.	1.7	7
10741	N-Activated 1,3-Benzoxazine Monomer as a Key Agent in Polybenzoxazine Synthesis. <i>Macromolecules</i> , 2020, 53, 8202-8215.	2.2	10
10742	Highly Stable Supramolecular Donor-Acceptor Complexes Involving a Bis(18-Crown-6)azobenzene as Weak Donor: Structure-Property Relationships. <i>ACS Omega</i> , 2020, 5, 25993-26004.	1.6	4
10743	Borataalkene or boratabenzene? Understanding the aromaticity of 9-borataphenanthrene anions and its central ring. <i>New Journal of Chemistry</i> , 2020, 44, 18069-18073.	1.4	13
10744	Relativistic two-component projection-based quantum embedding for open-shell systems. <i>Journal of Chemical Physics</i> , 2020, 153, 094113.	1.2	10
10745	PyDISH: database and analysis tools for heme porphyrin distortion in heme proteins. <i>Database: the Journal of Biological Databases and Curation</i> , 2023, 2023, .	1.4	12
10746	Tracking the ultraviolet-induced photochemistry of thiophenone during and after ultrafast ring opening. <i>Nature Chemistry</i> , 2020, 12, 795-800.	6.6	44
10747	Computational study of the unimolecular and bimolecular decomposition mechanisms of propylamine. <i>Scientific Reports</i> , 2020, 10, 11698.	1.6	11
10748	Palladium-catalyzed carbonylative synthesis and theoretical study of elongated tubular cavitands. <i>Journal of Organometallic Chemistry</i> , 2020, 923, 121387.	0.8	3

#	ARTICLE	IF	CITATIONS
10749	Macrocyclic Ligands with an Unprecedented Size-Selectivity Pattern for the Lanthanide Ions. <i>Journal of the American Chemical Society</i> , 2020, 142, 13500-13506.	6.6	37
10750	Thermoelasticity in organic semiconductors determined with terahertz spectroscopy and quantum quasi-harmonic simulations. <i>Journal of Materials Chemistry C</i> , 2020, 8, 10917-10925.	2.7	20
10751	Holeâ€“hole Tammâ€“Dancoff-approximated density functional theory: A highly efficient electronic structure method incorporating dynamic and static correlation. <i>Journal of Chemical Physics</i> , 2020, 153, 024110.	1.2	34
10752	Microextraction by packed molecularly imprinted polymer to selectively determine caffeine in soft and energy drinks. <i>Microchemical Journal</i> , 2020, 158, 105252.	2.3	19
10753	Theoretical study of closo-borate derivatives of general type [BnHn-1COR]2â€“ (n=6, 10, 12; R=H, CH3). <i>Tj ETQo0 0 0 rgBT /Overlo</i>	1.0	15
10754	2-Amino-3-methylpyridinium, 2-amino-4-methylbenzothiazolium and 2-amino-5-chloropyridinium salts. Experimental and theoretical findings. <i>Journal of Molecular Structure</i> , 2020, 1222, 128914.	1.8	13
10755	Determination of the pKa values of trans-Resveratrol, a Triphenolic Stilbene, by Singular Value Decomposition. Comparison with Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6294-6302.	1.1	11
10756	Single-Step Replacement of an Unreactive C-H Bond by a C-S Bond Using Polysulfide as the Direct Sulfur Source in the Anaerobic Ergothioneine Biosynthesis. <i>ACS Catalysis</i> , 2020, 10, 8981-8994.	5.5	15
10757	Enzymatic control of product distribution in terpene synthases: insights from multiscale simulations. <i>Current Opinion in Biotechnology</i> , 2020, 65, 248-258.	3.3	26
10758	Effect of substitutions on the geometry and intramolecular hydrogen bond strength in meta-benzoporphodimethenes: A new porphyrin analogue. <i>Journal of Molecular Structure</i> , 2020, 1220, 128773.	1.8	16
10759	Elucidating the effect of the ionic liquid type and alkyl chain length on the stability of ionic liquidâ€“iron porphyrin complexes. <i>Journal of Chemical Physics</i> , 2020, 153, 034306.	1.2	6
10760	Intramolecular Electrostatic Effects on O ₂ , CO ₂ , and Acetate Binding to a Cationic Iron Porphyrin. <i>Inorganic Chemistry</i> , 2020, 59, 17402-17414.	1.9	20
10761	Carbon Monoxide Activation on Small Iron Magnetic Cluster Surfaces, Fe _n CO, n = 1â€“20. A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9951-9962.	1.1	8
10762	Probing the tautomerization of disilenes and disilabenzenes with their isomeric silylenes: significant substituent, aromaticity and base effects. <i>Dalton Transactions</i> , 2020, 49, 17341-17349.	1.6	2
10763	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 26852-26864.	1.3	12
10764	Surface Hopping Dynamics for Azobenzene Photoisomerization: Effects of Packing Density on Surfaces, Fluorination, and Excitation Wavelength. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26287-26295.	1.5	7
10765	PySurf: A Framework for Database Accelerated Direct Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7681-7689.	2.3	12
10766	Oxidation of isoprene by titanium oxide cluster cations in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27357-27363.	1.3	4

#	ARTICLE	IF	CITATIONS
10767	Examining the Spin State and Redox Chemistry of Ni(Diimine) Catalysts during the Synthesis of π -Conjugated Polymers. <i>Macromolecular Chemistry and Physics</i> , 2020, 221, 2000321.	1.1	5
10768	Observation of π -Backbonding in a Boronyl-Coordinated Transition Metal Complex TaBO ⁺ . <i>Journal of Physical Chemistry A</i> , 2020, 124, 10001-10007.	1.1	0
10769	A Computational and Experimental Investigation of the Origin of Selectivity in the Chiral Phosphoric Acid Catalyzed Enantioselective Minisci Reaction. <i>Journal of the American Chemical Society</i> , 2020, 142, 21091-21101.	6.6	38
10770	Asymmetry in the Qy Fluorescence and Absorption Spectra of Chlorophyll a Pertaining to Exciton Dynamics. <i>Frontiers in Chemistry</i> , 2020, 8, 588289.	1.8	5
10771	Royleanone Derivatives From <i>Plectranthus</i> spp. as a Novel Class of P-Glycoprotein Inhibitors. <i>Frontiers in Pharmacology</i> , 2020, 11, 557789.	1.6	9
10772	Stereochemistry of Vanadium Peroxido Complexes: The Case of the Quinoline-2-carboxylato Ligand. <i>Inorganic Chemistry</i> , 2020, 59, 17162-17170.	1.9	3
10773	SCC-DFTB Parameters for Fe π -C Interactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9674-9682.	1.1	3
10774	Polarization consistent basis sets using the projector augmented wave method: a renovation brought by PAW into Gaussian basis sets. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27037-27052.	1.3	2
10775	Michler's hydrolytic blue elucidates structural differences in prion strains. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 29677-29683.	3.3	2
10776	Effect of the nature of lanthanide on intramolecular C-F π -Ln dative interactions in hexafluoroisopropoxide complexes. <i>Russian Chemical Bulletin</i> , 2020, 69, 2082-2090.	0.4	2
10777	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9729-9737.	1.1	4
10778	Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis. <i>Frontiers in Chemistry</i> , 2020, 8, 587084.	1.8	6
10779	CHARMM-DYES: Parameterization of Fluorescent Dyes for Use with the CHARMM Force Field. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7817-7824.	2.3	6
10780	Calculating the distance from an electronic wave function to the manifold of Slater determinants through the geometry of Grassmannians. <i>Physical Review A</i> , 2020, 102, .	1.0	7
10781	What Does the Brønsted Slope Measure in the Phosphoryl Transfer Transition State?. <i>ACS Catalysis</i> , 2020, 10, 13932-13945.	5.5	3
10782	Low-Dose X-ray-Responsive Diselenide Nanocarriers for Effective Delivery of Anticancer Agents. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 43398-43407.	4.0	27
10783	On the relations between backbone thiophene functionalization and charge carrier mobility of π -type small molecules. <i>New Journal of Chemistry</i> , 2020, 44, 15177-15185.	1.4	6
10784	Effect of Metal-Ligand Coordination Complexes on Molecular Dynamics and Structure of Cross-Linked Poly(dimethylsiloxane). <i>Polymers</i> , 2020, 12, 1680.	2.0	6

#	ARTICLE	IF	CITATIONS
10785	Pyrolyzed pencil graphite coated cellulose paper as an interlayer: An effective approach for high-performance lithium-sulfur battery. <i>Applied Surface Science</i> , 2020, 533, 147483.	3.1	30
10786	Molecular Features of Reline and Homologous Deep Eutectic Solvents Contributing to Nonideal Mixing Behavior. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7586-7597.	1.2	15
10787	Ab Initio Molecular Dynamics Simulations of Solvated Electrons in Ammonia Clusters. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7205-7216.	1.2	7
10788	Excited State Molecular Dynamics of Photoinduced Proton-Coupled Electron Transfer in Anthracene-Phenol-Pyridine Triads. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7109-7115.	2.1	6
10789	A hemicyanine-based σ -turn-on fluorescent probe for the selective detection of Cu ²⁺ ions and imaging in living cells. <i>Analytical Methods</i> , 2020, 12, 4181-4184.	1.3	17
10790	Electrosynthesis of a Baurone by Controlled Dimerization of Flavone: Mechanistic Insight and Large-Scale Application. <i>Journal of Organic Chemistry</i> , 2020, 85, 10658-10669.	1.7	3
10791	Energetics of Hybrid Structures between Cycloparaphenylene and Carbon Nanotubes: A Dispersion-Corrected Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17836-17847.	1.5	7
10792	Structure, Stability, and Spectroscopic Properties of Small Acetonitrile Cation Clusters. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6845-6855.	1.1	6
10793	Role of MLCT States in the Franck-Condon Region of Neutral, Heteroleptic Cu(I)-H-imidazolate Complexes: A Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6607-6616.	1.1	13
10794	Rationale Strategy to Tune the Optical Properties of Gold Catenane Nanoclusters by Doping with Silver Atoms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 19368-19374.	1.5	7
10795	σ -Bond Migration Assisted Decarboxylative Activation of Vinylene Carbonate in Rh-Catalyzed 4 + 2 Annulation: A Theoretical Study. <i>Organometallics</i> , 2020, 39, 2813-2819.	1.1	19
10796	Mechanism and origins of selectivity in the enantioselective oxa-Pictet-Spengler reaction: a cooperative catalytic complex from a hydrogen bond donor and chiral phosphoric acid. <i>Chemical Science</i> , 2020, 11, 8736-8743.	3.7	9
10797	Desymmetrization of Perylene diimide Bay Regions Using Selective Suzuki-Miyaura Reactions from Dinitro Substituted Derivatives. <i>Chemistry - A European Journal</i> , 2020, 26, 15881-15891.	1.7	8
10798	Modeling of Hydrogen Storage Utilizing Silsesquioxane Cages: Adsorption and Quasi-Dynamic Simulations of Encapsulation of H ₂ Molecule into Silsesquioxane Cages. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6344-6351.	1.1	3
10799	The effect of additives (pyrazine, pyrazole and their derivatives) in the oxidation of 2-butanol with FeCl ₃ ·H ₂ O ₂ in aqueous solutions. <i>Catalysis Today</i> , 2021, 381, 163-170.	2.2	5
10800	Electrochemical and spectroelectrochemical investigations of perylene peri-tetracarboxyl species. <i>Dyes and Pigments</i> , 2020, 183, 108735.	2.0	4
10801	The origin of the high reactivity of triazolinediones (TADs) in Diels-Alder reactions from a theoretical perspective. <i>Tetrahedron</i> , 2020, 76, 131459.	1.0	4
10802	Photophysics and ultrafast processes in rhenium(σ) diimine dicarbonyls. <i>Dalton Transactions</i> , 2020, 49, 11565-11576.	1.6	12

#	ARTICLE	IF	CITATIONS
10803	Evaluation of the Lewis acidity of metal complexes using ESI mass spectrometry. <i>European Journal of Mass Spectrometry</i> , 2020, 26, 332-340.	0.5	4
10804	An experimental and theoretical study of $\text{LuNC@C}_{76,82}$ revealing a cage-cluster selection rule. <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 4563-4571.	3.0	14
10805	Unexpected Findings in a Simple Metathesis Reaction of Europium and Ytterbium Diiodides with Perfluorinated Mercaptobenzothiazolates of Alkali Metals. <i>Organometallics</i> , 2020, 39, 2972-2983.	1.1	6
10806	Reversible Silane complexes as frustrated Lewis pairs for catalytic hydrosilylation. <i>Dalton Transactions</i> , 2020, 49, 11403-11411.	1.6	7
10807	Quantum chemical prediction of the spectroscopic properties and ionic composition of the molten NaF-AlF ₃ salts. <i>Journal of Molecular Liquids</i> , 2020, 317, 113937.	2.3	12
10808	Enhanced Sulfur Dioxide Adsorption in UiO-66 Through Crystal Engineering and Chalcogen Bonding. <i>Crystal Growth and Design</i> , 2020, 20, 6139-6146.	1.4	18
10809	DFT Studies on Copper-Catalyzed Dearomatization of Pyridine. <i>ACS Catalysis</i> , 2020, 10, 9585-9593.	5.5	12
10810	Dielectric Properties of $\text{CF}_3\text{SO}_2\text{F/N}_2$ and $\text{CF}_3\text{SO}_2\text{F/CO}_2$ Mixtures as a Substitute to SF_6 . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 15796-15804.	1.8	15
10811	Understanding the Electrochemical Stability Window of Polymer Electrolytes in Solid-State Batteries from Atomic-Scale Modeling: The Role of Li-Ion Salts. <i>Chemistry of Materials</i> , 2020, 32, 7237-7246.	3.2	101
10812	AMBER force field parameters for the Zn (II) ions of the tunneling-fold enzymes GTP cyclohydrolase I and 6- π -pyruvoyl tetrahydropterin synthase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 5843-5860.	2.0	13
10813	Chain-growth polycondensation via the substituent effect: Investigation of the monomer structure on synthesis of poly(N -octylbenzamide). <i>Journal of Polymer Science</i> , 2020, 58, 2389-2406.	2.0	5
10814	Synthesis, Spectroscopic, and Structural Characterization of Organyl Disulfanides and a Tetrasulfanide. <i>Inorganic Chemistry</i> , 2020, 59, 12322-12336.	1.9	10
10815	Infrared spectra of PEHA molecule and its resistance to oxidation in water and methanol media at 298.15 K: solvent cluster size dependency. <i>Journal of Molecular Modeling</i> , 2020, 26, 323.	0.8	3
10816	Mechanistic insights of selective syngas conversion over Zn grafted on ZSM-5 zeolite. <i>Catalysis Science and Technology</i> , 2020, 10, 8173-8181.	2.1	6
10817	Photoinduced charge transfer in Zn(II) and Au(III)-ligated symmetric and asymmetric bacteriochlorin dyads: A computational study. <i>Journal of Chemical Physics</i> , 2020, 153, 134111.	1.2	13
10818	The Non-innocent Role of Spin Traps in Monitoring Radical Formation in Copper-Catalyzed Reactions. <i>Applied Magnetic Resonance</i> , 2020, 51, 1529-1542.	0.6	3
10819	Exploring ground and low-lying excited states for diquat, paraquat, and dipyrindyl isomers. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 402, 112817.	2.0	9
10820	New Insights into the Radical Chemistry and Product Distribution in the OH-Initiated Oxidation of Benzene. <i>Environmental Science & Technology</i> , 2020, 54, 13467-13477.	4.6	32

#	ARTICLE	IF	CITATIONS
10821	Catalytic Mechanism of Liquid-Metal Indium for Direct Dehydrogenative Conversion of Methane to Higher Hydrocarbons. <i>ACS Omega</i> , 2020, 5, 28158-28167.	1.6	15
10822	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coronene—a DFT study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2316-2326.	2.0	10
10823	High level <i>ab initio</i> investigation of the catalytic effect of water on formic acid decomposition and isomerization. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25638-25651.	1.3	8
10824	Anisotropic Triplet Exciton Diffusion in Crystalline Functionalized Pentacene. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23541-23550.	1.5	13
10825	Stepwise construction of silica-supported tantalum/iridium heteropolymetallic catalysts using surface organometallic chemistry. <i>Journal of Catalysis</i> , 2020, 392, 287-301.	3.1	11
10826	A mechanochemical model for the simulation of molecules and molecular crystals under hydrostatic pressure. <i>Journal of Chemical Physics</i> , 2020, 153, 134503.	1.2	16
10827	Synthesis and redox properties of cyclometallated iridium (III) complexes modified with arylamino groups. <i>Journal of Organometallic Chemistry</i> , 2020, 930, 121580.	0.8	1
10828	Exceptionally High O—H Bond Dissociation Free Energy of a Dicopper(II) μ_4 -Hydroxo Complex and Insights into the Geometric and Electronic Structure Origins Thereof. <i>Journal of the American Chemical Society</i> , 2020, 142, 16292-16312.	6.6	10
10829	Detection of <i>Pseudomonas aeruginosa</i> quorum sensing molecules at an electrified liquid liquid micro-interface through facilitated proton transfer. <i>Analyst</i> , 2020, 145, 7000-7008.	1.7	12
10830	N-Substituted Phenothiazines as Environmentally Friendly Hole-Transporting Materials for Low-Cost and Highly Stable Halide Perovskite Solar Cells. <i>ACS Omega</i> , 2020, 5, 23334-23342.	1.6	9
10831	Metal coordination of phosphoniocarbynes. <i>Dalton Transactions</i> , 2020, 49, 12731-12741.	1.6	8
10832	Complexation of Ln ³⁺ with Pyridine-2,6-dicarboxamide: Formation of the 1:2 Complexes in Solution and Gas Phase. <i>Inorganic Chemistry</i> , 2020, 59, 14486-14492.	1.9	7
10833	Li-Metal Anode in Dilute Electrolyte LiFSI/TMP: Electrochemical Stability Using <i>Ab Initio</i> Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21919-21934.	1.5	19
10834	Triangulenium dyes: the comprehensive photo-absorption and emission story of a versatile family of chromophores. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20673-20684.	1.3	5
10835	5-(N-Trifluoromethylcarboxy)aminouracil as a Potential DNA Radiosensitizer and Its Radiochemical Conversion into N-Uracil-5-yloxamic Acid. <i>International Journal of Molecular Sciences</i> , 2020, 21, 6352.	1.8	5
10836	Charge-Transfer Excitation Energies Expressed as Orbital Energies of Kohn—Sham Density Functional Theory with Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8079-8087.	1.1	14
10837	ReaxFF Reactive Molecular Dynamics Simulations of Mechano-Chemical Decomposition of Perfluoropolyether Lubricants in Heat-Assisted Magnetic Recording. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22496-22505.	1.5	17
10838	Origin of stereoselectivity in an isothiourea catalyzed Michael addition reaction of aryl ester with vinyl disulfone. <i>New Journal of Chemistry</i> , 2020, 44, 17906-17911.	1.4	1

#	ARTICLE	IF	CITATIONS
10839	Convergence of Defect Energetics Calculations. <i>Journal of Physical Chemistry C</i> , 2020, 124, 21178-21183.	1.5	12
10840	Ladder-type bithiophene imide-based organic semiconductors: understanding charge transport mechanisms in organic field effect transistors. <i>Journal of Materials Chemistry C</i> , 2020, 8, 15759-15770.	2.7	6
10841	Impact of Aaronsohnia pubescens Essential Oil to Prevent Against the Corrosion of Mild Steel in 1.0 M HCl: Experimental and Computational Modeling Studies. <i>Journal of Failure Analysis and Prevention</i> , 2020, 20, 1939-1953.	0.5	8
10842	Reactivity of Iron Hydride Anions FeH_2 with Carbon Dioxide. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8414-8420.	1.1	7
10843	Theoretical investigation on the nature of 4-substituted Hantzsch esters as alkylation agents. <i>RSC Advances</i> , 2020, 10, 31425-31434.	1.7	12
10844	Self-Assembly of Hollow Organic Nanotubes Driven by Arene Regioisomerism. <i>ChemPlusChem</i> , 2020, 85, 2372-2375.	1.3	4
10845	Metalated Ir(III) CNP Complexes Containing Imidazolinylidene and Imidazolidinylidene Donors: Synthesis, Structure, Luminescence, and Metal-Ligand Cooperative Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3944-3953.	1.0	6
10846	Chiral Metal-BODIPY-Based Iridium(III) Complexes: Synthesis and Luminescence Properties. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4045-4053.	1.0	7
10847	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. <i>Communications Physics</i> , 2020, 3, .	2.0	28
10848	Theoretical Study of VX Hydrolysis Mechanism Catalyzed by Phosphotriesterase Mutant H254R. <i>ChemistrySelect</i> , 2020, 5, 8986-8991.	0.7	2
10849	Sigmoidally hydrochromic molecular porous crystal with rotatable dendrons. <i>Communications Chemistry</i> , 2020, 3, .	2.0	14
10850	Block deformation analysis: Density matrix blocks as intramolecular deformation density. <i>Journal of Computational Chemistry</i> , 2020, 41, 2446-2458.	1.5	2
10851	Electronic Properties of Cyano Ionic Liquids: a Valence Band Photoemission Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7909-7917.	1.2	5
10852	Naphthalene imides as novel p-type sensitizers for NiO-based p-type dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2020, 44, 15526-15537.	1.4	6
10853	Visible-Light-Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23020-23024.	7.2	29
10854	Visible-Light-Mediated Heterocycle Functionalization via Geometrically Interrupted [2+2] Cycloaddition. <i>Angewandte Chemie</i> , 2020, 132, 23220-23224.	1.6	5
10855	Color Differences Highlight Concomitant Polymorphism of Chalcones. <i>Crystal Growth and Design</i> , 2020, 20, 6346-6355.	1.4	9
10856	Toward universal substituent constants: Model chemistry sensitivity of descriptors from the quantum theory of atoms in molecules. <i>Journal of Computational Chemistry</i> , 2020, 41, 2485-2503.	1.5	4

#	ARTICLE	IF	CITATIONS
10857	Heteroatom-Rich Porous Carbons Derived from Nontoxic Green Organic Crystals for High-Performance Symmetric and Asymmetric Supercapacitors with Aqueous/Gel Electrolyte. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 13634-13647.	3.2	13
10858	Functionalized pyridine in pycen-based iron(Fe^{III}) complexes: evaluation of fundamental properties. <i>RSC Advances</i> , 2020, 10, 31165-31170.	1.7	9
10859	Theoretical study of the adsorption of amantadine on pristine, Al-, Ga-, P-, and As-doped boron nitride nanosheets: a PBC-DFT, NBO, and QTAIM study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	18
10860	Do weak interactions affect the biological behavior of DNA? A DFT study of CpG island-like chains. <i>Journal of Molecular Modeling</i> , 2020, 26, 266.	0.8	3
10861	Nonequilibrium Dynamics of Proton-Coupled Electron Transfer in Proton Wires: Concerted but Asynchronous Mechanisms. <i>ACS Central Science</i> , 2020, 6, 1594-1601.	5.3	20
10862	Comparing Reaction Routes for RO_2 Intermediates Formed in Peroxy Radical Self- and Cross-Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8305-8320.	1.1	24
10863	Single or Paired? Structure and Reactivity of PNP-Chromium(II) Hydrides. <i>Inorganic Chemistry</i> , 2020, 59, 14526-14535.	1.9	9
10864	Single Fe Site on the Surface of Al_2O_3 : Insights from Density Functional Theory Periodic Boundary Approach. <i>Journal of Physical Chemistry C</i> , 2020, 124, 20931-20941.	1.5	7
10865	Chain-growth polycondensation via the substituent effect: Investigation in to the role of initiator and base on the synthesis of poly(<i>N</i> -octyl benzamide). <i>Journal of Polymer Science</i> , 2020, 58, 2407-2422.	2.0	3
10866	Electronic Asymmetry of an Annelated Pyridyl-Mesoionic Carbene Scaffold: Application in Pd(II)-Catalyzed Wacker-Type Oxidation of Olefins. <i>ACS Catalysis</i> , 2020, 10, 11385-11393.	5.5	21
10867	Reactions of Schiff Base-Substituted Diselenides and Tellurides with Ni(II), Pd(II) and Pt(II) Phosphine Complexes. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 4303-4312.	1.0	2
10868	Fluorescence and Metal-Binding Properties of the Highly Preorganized Tetradentate Ligand 2,2'-Bi-1,10-phenanthroline and Its Remarkable Affinity for Cadmium(II). <i>Inorganic Chemistry</i> , 2020, 59, 13117-13127.	1.9	13
10869	Local and macrocyclic (anti)aromaticity of porphyrinoids revealed by the topology of the induced magnetic field. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 21267-21274.	1.3	8
10870	$\text{Pincer-Pyridine-Dicarbene-Iridium}$ and Ruthenium Complexes and Derivatives Thereof. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3359-3369.	1.0	5
10871	Molecular dynamics simulation of non-covalent interactions between polynuclear platinum(II) complexes and DNA. <i>Journal of Biological Inorganic Chemistry</i> , 2020, 25, 963-978.	1.1	6
10872	Understanding the <i>g</i> -tensors of perchlorotriphenylmethyl and Finland-type trityl radicals. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20792-20800.	1.3	9
10873	Selective active site placement in Lewis acid zeolites and implications for catalysis of oxygenated compounds. <i>Chemical Science</i> , 2020, 11, 10225-10235.	3.7	23
10874	Phenothiazine versus Phenoxazine: Structural Effects on the Photophysical Properties of NIR-II AIE Fluorophores. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 43466-43473.	4.0	26

#	ARTICLE	IF	CITATIONS
10875	Probing structural properties and antioxidant activity mechanisms for eleocarpanthraquinone. <i>Journal of Molecular Modeling</i> , 2020, 26, 233.	0.8	29
10876	A New Basis Set for the Calculation of ¹³ C NMR Chemical Shifts within a Non-empirical Correlated Framework. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7322-7330.	1.1	4
10877	Effect on the aromaticity of heterocyclic ligands by coordination with ruthenium electron-withdrawing metal centers. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26412.	1.0	0
10878	A TDDFT investigation of the Photosystem II reaction center: Insights into the precursors to charge separation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 19705-19712.	3.3	9
10879	Atmospheric Autoxidation of Amines. <i>Environmental Science & Technology</i> , 2020, 54, 11087-11099.	4.6	33
10880	Molecular engineering of pyrene carbazole dyes with a single bond and double bond as the mode of linkage. <i>New Journal of Chemistry</i> , 2020, 44, 16511-16525.	1.4	11
10881	¹³ C CPMAS NMR as a Tool for Full Structural Description of 2-Phenyl Substituted Imidazoles That Overcomes the Effects of Fast Tautomerization. <i>Molecules</i> , 2020, 25, 3770.	1.7	4
10882	Disentangling the Contributions to the Proton Magnetic Shielding in Carbon Nanohoops and Nanobelts: Evidence for a Paratropic Belt-Current. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7489-7494.	2.1	7
10883	Highly Chemoselective Esterification from <i>i>O</i>-Aminoallylation of Carboxylic Acids: Metal- and Reagent-Free Hydrocarboxylation of Allenamides. <i>Chemistry - A European Journal</i>, 2020, 26, 13826-13831.</i>	1.7	10
10884	Computation of Dipole Moments: A Recommendation on the Choice of the Basis Set and the Level of Theory. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7538-7548.	1.1	25
10885	Effects of Chemically-Modified Polypyridyl Ligands on the Structural and Redox Properties of Tricarbonylmanganese(I) Complexes. <i>Molecules</i> , 2020, 25, 5921.	1.7	3
10886	Mean-field density matrix decompositions. <i>Journal of Chemical Physics</i> , 2020, 153, 214109.	1.2	10
10887	Solvated State of Ethylenediamine in Nonaqueous Solvents, According to Quantum Chemical Data. <i>Russian Journal of Physical Chemistry A</i> , 2020, 94, 2051-2054.	0.1	0
10888	Rational Design of an Ion-Imprinted Polymer for Aqueous Methylmercury Sorption. <i>Nanomaterials</i> , 2020, 10, 2541.	1.9	18
10889	Differences in the Nature of the Phosphoryl Transfer Transition State in Protein Phosphatase 1 and Alkaline Phosphatase: Insights from QM Cluster Models. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9371-9384.	1.2	4
10890	Attempted characterisation of phenanthrene-4,5-quinone and electrochemical synthesis of violanthrone-16,17-quinone. How does the stability of bay quinones correlate with structural and electronic parameters?. <i>RSC Advances</i> , 2020, 10, 38004-38012.	1.7	2
10891	Electrochemical performance and storage mechanism study of conjugate donor-acceptor organic polymers as anode materials of lithium-ion battery. <i>Energy Reports</i> , 2020, 6, 2094-2105.	2.5	21
10892	Intermolecular interaction between anthraquinone dyes and TEMPO mediator in dye-sensitized photocatalytic systems. <i>Journal of Photochemistry and Photobiology</i> , 2020, 2, 100003.	1.1	0

#	ARTICLE	IF	CITATIONS
10893	Systematic Study of the Properties of CdS Clusters with Carboxylate Ligands Using a Deep Neural Network Potential Developed with Data from Density Functional Theory Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10472-10481.	1.1	9
10894	Core-Level Excitation Energies of Nucleic Acid Bases Expressed as Orbital Energies of the Kohn-Sham Density Functional Theory with Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10482-10494.	1.1	9
10895	How external perturbations affect the chemoselectivity of substrate activation by cytochrome P450 OleT _{JE} . <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27178-27190.	1.3	13
10896	Spectroscopic evidence of chirality in tetranuclear Cu(II)-Schiff base complexes, catalytic potential for oxidative kinetic resolution of racemic benzoin. <i>Inorganic and Nano-Metal Chemistry</i> , 2021, 51, 1714-1724.	0.9	2
10897	Probing the Effect of Side Alkyl Chain Length on the Structural and Dynamical Micro-heterogeneities in Dicationic Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11446-11462.	1.2	5
10898	Fluorophore-Appendant 5,5'-Bicalixarene Scaffolds for Host-Guest Sensing of Nitric Oxide. <i>Organic Letters</i> , 2020, 22, 9706-9711.	2.4	4
10899	Novel electrosynthesis of CdS/FeS nanocomposite-modified poly(o-phenylenediamine) with views to their use as a biosensor for <i>Escherichia coli</i> . <i>Arabian Journal of Chemistry</i> , 2020, 13, 8758-8767.	2.3	4
10900	Transferable MP2-Based Machine Learning for Accurate Coupled-Cluster Energies. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7453-7461.	2.3	14
10901	Unraveling the Structure and Binding Energy of Adsorbed CO ₂ /H ₂ O on Amine Sorbents. <i>Journal of Physical Chemistry C</i> , 2020, 124, 24677-24689.	1.5	24
10902	Infrared spectroscopy and anharmonic theory of H ₃ +Ar _{2,3} complexes: The role of symmetry in solvation. <i>Journal of Chemical Physics</i> , 2020, 153, 134305.	1.2	3
10903	Design of Novel 4-Aminobenzofuroxans and Evaluation of Their Antimicrobial and Anticancer Activity. <i>International Journal of Molecular Sciences</i> , 2020, 21, 8292.	1.8	5
10904	Microsolvation of myrtanal studied by microwave spectroscopy highlights the role of quasi-hydrogen bonds in the stabilization of its hydrates. <i>Journal of Chemical Physics</i> , 2020, 153, 104304.	1.2	12
10905	On the Structure of Intermediates in Enyne Gold(I)-Catalyzed Cyclizations: Formation of <i>trans</i> -Fused Bicyclo[5.1.0]octanes as a Case Study. <i>Chemistry - A European Journal</i> , 2020, 26, 15738-15745.	1.7	12
10906	Effect of Lewis acid on catalytic dehydration of a chitin-derived sugar alcohol. <i>Molecular Catalysis</i> , 2020, 498, 111282.	1.0	6
10907	Porphyrin-based systems containing polyaromatic fragments: decoupling the synergistic effects in aromatic-porphyrin-fullerene systems. <i>RSC Advances</i> , 2020, 10, 36164-36173.	1.7	7
10908	Computational and experimental characterization of novel ultraviolet filters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25390-25395.	1.3	8
10909	Evaluating Classical Force Fields against Experimental Cross-Solvation Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7556-7580.	2.3	28
10910	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. <i>ACS Catalysis</i> , 2020, 10, 13455-13467.	5.5	13

#	ARTICLE	IF	CITATIONS
10911	Chemical reactivity from the vibrational ground-state level. The role of the tunneling path in the tautomerization of urea and derivatives. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24951-24963.	1.3	4
10912	Comparative Study of the Biphasic Behavior of Cyanex301 and Its Two Analogs by Molecular Dynamics Simulations. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900242.	1.3	1
10913	Reagent addition sequence and equivalent in $N\text{-heterocyclic carbene}$ -catalyzed nonpolar inversion enable conversion from aldimine to benzoxazole. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26249.	1.0	2
10914	Tetranuclear molybdenum(vi) hydrazone oxoepoxidation (pre)catalysts: Is water always the best choice?. <i>Catalysis Communications</i> , 2020, 142, 106027.	1.6	9
10915	Synthesis, crystal structure, spectroscopic and hirshfeld surface analysis, NCI-RDG, DFT computations and antibacterial activity of new asymmetrical azines. <i>Journal of Molecular Structure</i> , 2020, 1217, 128376.	1.8	23
10916	Theoretical Modeling of Electronic Structures of Polyiodide Species Included in β -Cyclodextrin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4089-4096.	1.2	13
10917	Use of Ligand Steric Properties to Control the Thermodynamics and Kinetics of Oxidative Addition and Reductive Elimination with Pincer-Ligated Rh Complexes. <i>Organometallics</i> , 2020, 39, 1917-1933.	1.1	15
10918	Discrete and polymeric ensembles based on dinuclear molybdenum(vi) building blocks with adaptive carbohydrazide ligands: from the design to catalytic epoxidation. <i>New Journal of Chemistry</i> , 2020, 44, 8085-8097.	1.4	9
10919	From cyclic amines and acetonitrile to amidine zinc(ii) complexes. <i>RSC Advances</i> , 2020, 10, 18200-18221.	1.7	9
10920	Measuring the distribution and concentration of cysteine by fluorescent sensor for the visual study of paracetamol-induced pro-sarcopenic effect. <i>Sensors and Actuators B: Chemical</i> , 2020, 318, 128258.	4.0	13
10921	Theoretical investigation on the Cu(i)-catalyzed N -carboxamidation of indoles with isocyanates to form indole-1-carboxamides: effects of solvents. <i>New Journal of Chemistry</i> , 2020, 44, 9878-9887.	1.4	2
10922	A vibrational spectroscopic and computational study of gaseous protonated and alkali metal cationized $G\text{-C}$ base pairs. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11546-11557.	1.3	11
10923	Highly Oxidized States of Phthalocyaninato Terbium(III) Multiple-Decker Complexes Showing Structural Deformations, Biradical Properties and Decreases in Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2020, 26, 8621-8630.	1.7	19
10924	$Co(II)$ Pincer Complexes: Paramagnetic NMR Spectroscopy in Solution and Application as Hydrosilylation Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2335-2342.	1.0	16
10925	A potential bio-antioxidant for mineral oil from cashew nutshell liquid: an experimental and theoretical approach. <i>Brazilian Journal of Chemical Engineering</i> , 2020, 37, 369-381.	0.7	10
10926	Beyond the electric-dipole approximation in simulations of x-ray absorption spectroscopy: Lessons from relativistic theory. <i>Journal of Chemical Physics</i> , 2020, 152, 184110.	1.2	17
10927	Cyclization from Higher Excited States of Diarylethenes Having a Substituted Azulene Ring. <i>Chemistry - A European Journal</i> , 2020, 26, 11441-11450.	1.7	3
10928	Double addition of phenylacetylene onto the mixed bridge phosphinito-phosphanido Pt(i) complex $[(\text{PhC}\equiv\text{C})_2\text{Pt}(\text{P}(\text{O})(\text{C}_6\text{H}_5)_2)_2\text{Pt}(\text{P}(\text{O})(\text{C}_6\text{H}_5)_2)_2\text{Pt}(\text{P}(\text{O})(\text{C}_6\text{H}_5)_2)_2]$. <i>Dalton Transactions</i> , 2020, 49, 6776-6789.	1.6	16

#	ARTICLE	IF	CITATIONS
10929	Quinonoid <i>vs.</i> aromatic structures of heteroconjugated polymers from oligomer calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11431-11439.	1.3	5
10930	Smart Colorimetric Chemosensors for Multi-Analyte Signaling: Recognition of Heavy Metal Ions in an Aqueous Medium and DFT Studies. <i>ChemistrySelect</i> , 2020, 5, 5289-5299.	0.7	6
10931	Outer-sphere effects on ligand-field excited-state dynamics: solvent dependence of high-spin to low-spin conversion in [Fe(bpy) ₃] ²⁺ . <i>Chemical Science</i> , 2020, 11, 5191-5204.	3.7	11
10932	Mechanistic Study on Palladium-Catalyzed Regioselective Oxidative Amination: Roles of Ammonium Salts. <i>Journal of Organic Chemistry</i> , 2020, 85, 6981-6991.	1.7	8
10933	Formation of bis-benzimidazole and bis-benzoxazole through organocatalytic depolymerization of poly(ethylene terephthalate) and its mechanism. <i>Polymer Chemistry</i> , 2020, 11, 4904-4913.	1.9	13
10934	The Mechanism of the Intramolecular Hydrocarbyl Metathesis within a Planar Triruthenium Cluster: Combining Core Flexibility with Hydride Mobility. <i>Chemistry - A European Journal</i> , 2020, 26, 13880-13889.	1.7	1
10935	Computational Investigation into Ligand Effects on Correlated Geared Dynamics in Dirhodium Supramolecular Gears—Insights Beyond the NMR Experimental Window. <i>Journal of Organic Chemistry</i> , 2020, 85, 8695-8701.	1.7	3
10936	Heterobimetallic η^2 -carbido complexes of platinum and tungsten. <i>Dalton Transactions</i> , 2020, 49, 8143-8161.	1.6	12
10937	A promising class of luminescent derivatives of Silver(I) and Gold(I)—heterocyclic carbene. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5673.	1.7	8
10938	Novel thiazoline-phenothiazine based "push-pull" molecules as fluorescent probes for volatile acids detection. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2020, 397, 112509.	2.0	13
10939	Using Polypeptide Bearing Furan Side Chains as a General Platform to Achieve Highly Effective Preparation of Smart Glycopolypeptide Analogue-Based Nano-Prodrugs for Cancer Treatment. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020, 194, 111165.	2.5	5
10940	Mechanistic study of Selectfluor-mediated digold-catalyzed Csp ³ -Csp ² coupling reaction. <i>Chemical Physics Letters</i> , 2020, 754, 137668.	1.2	1
10941	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3566-3576.	2.5	13
10942	Probing Sulfur Chemical and Electronic Structure with Experimental Observation and Quantitative Theoretical Prediction of K _L and Valence-to-Core K _L ² X-ray Emission Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5415-5434.	1.1	30
10943	Two-dimensional two-photon absorptions and third-order nonlinear optical properties of <i>h</i> fullerenes and fullerene anions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14225-14235.	1.3	16
10944	Accelerating role of deaggregation agents in lithium-catalysed hydrosilylation of carbonyl compounds. <i>Dalton Transactions</i> , 2020, 49, 7932-7937.	1.6	8
10945	Photorelaxation Pathways of 4-(N,N-Dimethylamino)-4'-nitrostilbene Upon S ₁ Excitation Revealed by Conical Intersection and Intersystem Crossing Networks. <i>Molecules</i> , 2020, 25, 2230.	1.7	2
10946	Magnetic molecularly imprinted conducting polymer for determination of praziquantel enantiomers in milk. <i>Analyst</i> , 2020, 145, 4245-4253.	1.7	19

#	ARTICLE	IF	CITATIONS
10947	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	1.2	616
10948	QSAR modeling, docking, ADME and reactivity of indazole derivatives as antagonizes of estrogen receptor alpha (ER- α) positive in breast cancer. <i>Journal of Molecular Structure</i> , 2020, 1217, 128442.	1.8	14
10949	Quantum Mechanical Investigation of Three-Dimensional Activity Cliffs Using the Molecules-in-Molecules Fragmentation-Based Method. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2924-2938.	2.5	9
10950	A General Hypoxia-Responsive Molecular Container for Tumor-Targeted Therapy. <i>Advanced Materials</i> , 2020, 32, e1908435.	11.1	81
10951	A Fullerene-Based Molecular Torsion Balance for Investigating Noncovalent Interactions at the C 60 Surface. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16133-16140.	7.2	10
10952	Existence of π - π mangostin conformers and effects of aprotic and protic solvents on their equilibria, UV-Vis spectra, and chemical descriptors: Density functional theory and time-dependent density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4080.	0.9	0
10953	Improved Basis-Set Incompleteness Potentials for Accurate Density-Functional Theory Calculations in Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4176-4191.	2.3	15
10954	Theoretical Study of Formation of Methanol under Hydrothermal Conditions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4496-4505.	1.1	0
10955	Active-Space Pair Two-Electron Reduced Density Matrix Theory for Strong Correlation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4848-4854.	1.1	7
10956	A Two Carrier Families Spectral Profile Model for Anomalous Microwave Emission. <i>Astrophysical Journal</i> , 2020, 892, 69.	1.6	1
10957	Construction of frustrated Lewis pair from nitride and phosphine for the activation and cleavage of molecular hydrogen. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5811.	1.7	0
10958	Achieving Site-Selectivity for C-H Activation Processes Based on Distance and Geometry: A Carpenter's Approach. <i>Journal of the American Chemical Society</i> , 2020, 142, 10571-10591.	6.6	236
10959	Luminescence Activity Decreases When <i>v</i> -coelenterazine Replaces Coelenterazine in Calcium-Regulated Photoprotein-A Theoretical and Experimental Study. <i>Photochemistry and Photobiology</i> , 2020, 96, 1047-1060.	1.3	10
10960	Nanoscale Organization of a Platinum(II) Acetylide Cholesteric Liquid Crystal Molecular Glass for Photonics Applications. <i>Advanced Functional Materials</i> , 2020, 30, 1910562.	7.8	7
10961	A Fullerene-Based Molecular Torsion Balance for Investigating Noncovalent Interactions at the C 60 Surface. <i>Angewandte Chemie</i> , 2020, 132, 16267-16274.	1.6	5
10962	Reversal of Clar's Aromatic Sextet Rule in Ultrashort Single-Capped [5,5] Carbon Nanotubes. <i>ChemistryOpen</i> , 2020, 9, 616-622.	0.9	4
10963	Structural and energetic investigation on the host/guest inclusion process of benzyl isothiocyanate into β -cyclodextrin using dispersion-corrected DFT calculations. <i>Carbohydrate Research</i> , 2020, 491, 107980.	1.1	18
10964	Hole Transfer in Cumulenic and Polyynic Carbynes. <i>Journal of Physical Chemistry C</i> , 2020, 124, 12834-12849.	1.5	4

#	ARTICLE	IF	CITATIONS
10965	Entangled Electrons Drive a Non-superexchange Mechanism in a Cobalt Quinoid Dimer Complex. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4584-4590.	2.1	18
10966	Comparative Insertion Reactivity of CO, CO ₂ , tBuCN, and tBuNC into Thorium ^{IV} and Uranium ^{IV} Phosphorus Bonds. <i>Organometallics</i> , 2020, 39, 2152-2161.	1.1	19
10967	Unveiling the Chemo- and Stereoselectivities of NHC-Catalyzed Reactions of an Aliphatic Ester with Aminochalcone. <i>Journal of Organic Chemistry</i> , 2020, 85, 8437-8446.	1.7	26
10968	Microwave-Assisted Synthesis of Zirconium Phosphate Nanoplatelet-Supported Ru-Anadem Nanostructures and Their Catalytic Study for the Hydrogenation of Acetophenone. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 30670-30679.	4.0	10
10969	Two-Photon Absorption Cross-Sections in Fluorescent Proteins Containing Non-canonical Chromophores Using Polarizable QM/MM. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 111.	1.6	6
10970	Rate coefficients and product branching ratios for (<i>E</i>)-2-butenal + H reactions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14246-14254.	1.3	4
10971	Synthetic flavonoid derivatives targeting the glycogen phosphorylase inhibitor site: QM/MM-PBSA motivated synthesis of substituted 5,7-dihydroxyflavones, crystallography, in vitro kinetics and ex-vivo cellular experiments reveal novel potent inhibitors. <i>Bioorganic Chemistry</i> , 2020, 102, 104003.	2.0	13
10972	Heavy-Atom Tunneling Processes during Denitrogenation of 2,3-Diazabicyclo[2.2.1]hept-2-ene and Ring Closure of Cyclopentane-1,3-diyl Diradical. Stereoselectivity in Tunneling and Matrix Effect. <i>Journal of Organic Chemistry</i> , 2020, 85, 8881-8892.	1.7	11
10973	Oxidative Amidation of Amines in Tandem with Transamidation: A Route to Amides Using Visible-Light Energy. <i>Journal of Organic Chemistry</i> , 2020, 85, 9219-9229.	1.7	28
10974	Efficient Construction of Excited-State Hessian Matrices with Machine Learning Accelerated Multilayer Energy-Based Fragment Method. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5684-5695.	1.1	27
10975	Uracil-5-yl O-Sulfamate: An Illusive Radiosensitizer. Pitfalls in Modeling the Radiosensitizing Derivatives of Nucleobases. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5600-5613.	1.2	13
10976	Electron-Rich Gold Clusters Stabilized by Poly(vinylpyridines) as Robust and Active Oxidation Catalysts. <i>Langmuir</i> , 2020, 36, 7844-7849.	1.6	13
10977	Quantum-Based Modeling of Dephosphorylation in the Catalytic Site of Serine/Threonine Protein Phosphatase-5 (PPP5C). <i>Catalysts</i> , 2020, 10, 674.	1.6	3
10978	Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO ₂ to CO with Ruthenium CNC Pincer Complexes. <i>ChemCatChem</i> , 2020, 12, 4879-4885.	1.8	7
10979	Effects on the aromaticity and on the biradicaloid nature of acenes by the inclusion of a cyclobutadiene linkage. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	5
10980	Boron-based metallocene-like molecules and nanowires: A computational study. <i>Chemical Physics Letters</i> , 2020, 747, 137336.	1.2	2
10981	The Nanostructure of HMT-PMBI, a Sterically Hindered Ionene. <i>Macromolecules</i> , 2020, 53, 4908-4916.	2.2	4
10982	Reversible and efficient SO ₂ capture by a chemically stable MOF CAU-10: experiments and simulations. <i>Dalton Transactions</i> , 2020, 49, 9203-9207.	1.6	21

#	ARTICLE	IF	CITATIONS
10983	Palladium-catalyzed synthesis of β -hydroxy compounds <i>via</i> a strained 6,4-palladacycle from directed C-H activation of anilines and C-O insertion of epoxides. <i>Chemical Science</i> , 2020, 11, 7260-7265.	3.7	14
10984	Primary Vinyl Ethers as Acetylene Surrogate: A Flexible Tool for Deuterium-Labeled Pyrazole Synthesis. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 4571-4580.	1.2	14
10985	Asymmetric effects of anions in magnetic ionic liquids. <i>Chemical Physics Letters</i> , 2020, 748, 137389.	1.2	5
10986	Amorphous and crystalline thioacetamide ice: Infrared spectra as a probe for temperature and structure. <i>Journal of Molecular Structure</i> , 2020, 1220, 128719.	1.8	6
10987	Designing Novel Zn-Decorated Inorganic B ₁₂ P ₁₂ Nanoclusters with Promising Electronic Properties: A Step Forward toward Efficient CO ₂ Sensing Materials. <i>ACS Omega</i> , 2020, 5, 15547-15556.	1.6	71
10988	Covalent vs Charge-Shift Nature of the Metal-Metal Bond in Transition Metal Complexes: A Unified Understanding. <i>Journal of the American Chemical Society</i> , 2020, 142, 12277-12287.	6.6	37
10989	Structural and Electronic Characterization of a Photoresponsive Lanthanum(III) Complex Incorporated into Electrospun Fibers for Phosphate Ester Catalysis. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 28607-28615.	4.0	8
10990	Asymmetric deformation density analysis in carbon nanotubes. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26277.	1.0	1
10991	Proton trap effect on catechol-pyridine redox polymer nanoparticles as organic electrodes for lithium batteries. <i>Sustainable Energy and Fuels</i> , 2020, 4, 3934-3942.	2.5	16
10992	Reactivity and Product Analysis of a Pair of Cumyloxyl and <i>tert</i> -Butoxyl Radicals Generated in Photolysis of <i>tert</i> -Butyl Cumyl Peroxide. <i>Journal of Organic Chemistry</i> , 2020, 85, 8627-8638.	1.7	13
10993	Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2709-2717.	1.0	10
10994	Vibrational Sum-Frequency Generation Spectroscopy in the Energy Representation from Dual-Level Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5675-5683.	1.1	1
10995	Electronegativity and location of anionic ligands drive yttrium NMR for molecular, surface and solid-state structures. <i>Chemical Science</i> , 2020, 11, 6724-6735.	3.7	15
10996	Computational and Crystallographic Examination of Naphthoquinone Based Diarylethene Photochromes. <i>Molecules</i> , 2020, 25, 2630.	1.7	2
10997	Deciphering the mechanism of oxygen atom transfer by non-heme Mn ^{IV} -oxo species: an <i>ab initio</i> and DFT exploration. <i>Dalton Transactions</i> , 2020, 49, 10380-10393.	1.6	9
10998	5,8-Disubstituted crown-naphthalonitriles as a platform for highly soluble naphthalocyanines. <i>Dyes and Pigments</i> , 2020, 180, 108484.	2.0	5
10999	The rupture mechanism of rubredoxin is more complex than previously thought. <i>Chemical Science</i> , 2020, 11, 6036-6044.	3.7	1
11000	Computational Study on O-O Bond Formation on a Mononuclear Non-Heme Iron Center. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2573-2581.	1.0	2

#	ARTICLE	IF	CITATIONS
11001	Conformational and electronic study of dopamine interacting with the D_2 dopamine receptor. <i>Journal of Computational Chemistry</i> , 2020, 41, 1898-1911.	1.5	9
11002	Multireference Ground and Excited State Electronic Structures of Free- versus Iron Porphyrin-Carbenes. <i>Inorganic Chemistry</i> , 2020, 59, 8707-8715.	1.9	9
11003	Effect of Cycling Ion and Solvent on the Redox Chemistry of Substituted Quinones and Solvent-Induced Breakdown of the Correlation between Redox Potential and Electron-Withdrawing Power of Substituents. <i>Journal of Physical Chemistry C</i> , 2020, 124, 13609-13617.	1.5	22
11004	Probing the Origin of Adaptive Aromaticity in 16-Valence Electron Metallapentalenes. <i>Chemistry - A European Journal</i> , 2020, 26, 12964-12971.	1.7	28
11005	Assessing the Performance of Density Functional Theory Methods on the Prediction of Low-Frequency Vibrational Spectra. <i>Journal of Infrared, Millimeter, and Terahertz Waves</i> , 2020, 41, 1411-1429.	1.2	12
11006	Hole Hopping through Cytochrome P450. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3065-3073.	1.2	5
11007	Quantitative Analysis of Infrared Spectra of Binary Alcohol + Cyclohexane Solutions with Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3077-3089.	1.1	15
11008	Electride-Sponsored Radical-Controlled CO ₂ Reduction to Organic Acids: A Computational Design. <i>Chemistry - A European Journal</i> , 2020, 26, 6234-6239.	1.7	3
11009	Opening up the Valence Shell: A σ -Shaped Iron(I) Metalloradical and Its Potential for Atom Abstraction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9448-9452.	7.2	21
11010	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO) ₃ (Dmp)(His124)(Trp122)] ⁺ in <i>Pseudomonas aeruginosa</i> azurin: a nonadiabatic dynamics study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 65.	0.5	17
11011	Octapodal Corannulene Porphyrin-Based Assemblies: Allosteric Behavior in Fullerene Hosting. <i>Journal of Organic Chemistry</i> , 2020, 85, 4918-4926.	1.7	14
11012	Atomistic Molecular Dynamics Simulations of Surfactant-Induced Wettability Alteration in Crevices of Calcite Nanopores. <i>Energy & Fuels</i> , 2020, 34, 3135-3143.	2.5	20
11013	Intermetallic Nanocatalysts from Heterobimetallic Group 10-14 Pyridine-2-thiolate Precursors. <i>Organometallics</i> , 2020, 39, 1092-1104.	1.1	11
11014	A Porous Aromatic Framework Functionalized with Luminescent Iridium(III) Organometallic Complexes for Turn-On Sensing of TcO_4^- . <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15288-15297.	4.0	46
11015	Prediction of superheat limit temperatures for fuel mixtures using quantitative structure-property relationship model. <i>Journal of Loss Prevention in the Process Industries</i> , 2020, 64, 104087.	1.7	3
11016	Discovery of a Superatom inside the Fullerene Cage. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2694-2699.	1.1	5
11017	New class of cocogem surfactants based on hexamethylenediamine, propylene oxide, and long chain carboxylic acids: Theory and application. <i>Journal of Industrial and Engineering Chemistry</i> , 2020, 86, 123-135.	2.9	11
11018	Modeling the effect of ligands and solvation on hydrolysis variants in the Pd(II)-Catalyzed hydroxycarbonylation of pentenoic acids. <i>Journal of Organometallic Chemistry</i> , 2020, 914, 121221.	0.8	0

#	ARTICLE	IF	CITATIONS
11019	Computational Investigation into the Oxidation of Guanine to Form Imidazolone (Iz) and Related Degradation Products. <i>Chemical Research in Toxicology</i> , 2020, 33, 1010-1027.	1.7	5
11020	Computational studies of the mechanism of Pd-Catalyzed Intramolecular Friedel-Crafts allylic alkylation of phenols. <i>Tetrahedron</i> , 2020, 76, 131146.	1.0	2
11021	Insights into N-heterocyclic carbene and Lewis acid cooperatively catalyzed oxidative [3 + 3] annulation reactions of α,β -unsaturated aldehyde with 1,3-dicarbonyl compounds. <i>Organic Chemistry Frontiers</i> , 2020, 7, 1113-1121.	2.3	25
11022	Double Bonds Are Key to Fast Unimolecular Reactivity in First-Generation Monoterpene Hydroxy Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2885-2896.	1.1	37
11023	Äffnung der Valenzschale: Ein TÄÄrmiges Eisen(I)ÄMetalloradikal und sein Potential als Atomabstraktor. <i>Angewandte Chemie</i> , 2020, 132, 9535-9539.	1.6	4
11024	Planochromism of cyanoxime anions: Computational and mechanistic studies in solid state and solutions. <i>Inorganica Chimica Acta</i> , 2020, 507, 119570.	1.2	2
11025	Diketopyrrolopyrrole Derivatives Functionalized with NaÄAnnulated PDI and SeÄAnnulated PDI by Direct (Hetero)Arylation Methods. <i>Asian Journal of Organic Chemistry</i> , 2020, 9, 1291-1300.	1.3	6
11026	Liquid-phase decomposition mechanism for bis(triaminoguanidinium) azotetrazolate (TAGzT). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7314-7328.	1.3	6
11027	Theoretical Analysis of the Mechanism of the 1,3-Dipolar Cycloaddition of Benzodiazepine with N-Aryl-C-ethoxycarbonylnitrilimine. <i>Journal of Chemistry</i> , 2020, 2020, 1-8.	0.9	2
11028	Oxyaapa: A Picolinate-Based Ligand with Five Oxygen Donors that Strongly Chelates Lanthanides. <i>Inorganic Chemistry</i> , 2020, 59, 5116-5132.	1.9	14
11029	Kinetic investigation of the cyclopropanation process of fullerene C ₆₀ by halogenmethyl ketones under the conditions of the Bingel reaction. <i>New Journal of Chemistry</i> , 2020, 44, 7277-7285.	1.4	3
11030	To Bind or Not to Bind: Mechanistic Insights into CÄCO ₂ Bond Formation with Late Transition Metals. <i>Organometallics</i> , 2020, 39, 1339-1347.	1.1	21
11031	Exploring the Nature of the Energy Barriers on the Mechanism of the Zirconocene-Catalyzed Ethylene Polymerization: A Quantitative Study from Reaction Force Analysis. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8198-8209.	1.5	3
11032	Synthesis, characterisation and theoretical studies of a series of Iridium (III) heteroleptic complexes with Schiff base ligands. <i>Journal of Molecular Structure</i> , 2020, 1211, 128058.	1.8	15
11033	Bioluminescent NanoluciferaseÄFurimamide Complex: A Theoretical Study on Different Protonation States. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2539-2548.	1.2	5
11034	Oxone-DMSO Triggered Methylene Insertion and C(sp ²)ÄC(sp ³)-HÄC(sp ²) Bond Formation to Access Functional Bis-Heterocycles. <i>Journal of Organic Chemistry</i> , 2020, 85, 4951-4962.	1.7	23
11035	Cp*RuClÄVinyl Carbenes: Two Faces and the Bifunctional Role in Catalytic Processes. <i>Chemistry - A European Journal</i> , 2020, 26, 7470-7478.	1.7	6
11036	Exploring the effects of solvents on an organic explosive: Insights from the electron structure, electrostatic potential, and conformational transformations of 2,4,6,8,10,12ÄhexanitroÄ2,4,6,8,10,12Ähexaazaisowurtzitane. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26202.	1.0	1

#	ARTICLE	IF	CITATIONS
11037	Heteroatom engineering of polymeric carbon nitride heterojunctions for boosting photocatalytic reduction of hexavalent uranium. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 882-889.	1.7	21
11038	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26332.	1.0	63
11039	Semiglobal diabatic potential energy matrix for the N-H photodissociation of methylamine. <i>Journal of Chemical Physics</i> , 2020, 152, 244309.	1.2	7
11040	Insights into Ruthenium(II/IV)-Catalyzed Distal C-H Oxygenation by Weak Coordination. <i>Chemistry - A European Journal</i> , 2020, 26, 16450-16454.	1.7	15
11041	8-Hydroxyjulolidine aldimine as a fluorescent sensor for the dual detection of Al ³⁺ and Mg ²⁺ . <i>Sensing and Bio-Sensing Research</i> , 2020, 29, 100358.	2.2	4
11042	Computational Protocol To Predict Anti-Kasha Emissions: The Case of Azulene Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7228-7237.	1.1	35
11043	NH ₃ formation from N ₂ and H ₂ mediated by molecular tri-iron complexes. <i>Nature Chemistry</i> , 2020, 12, 740-746.	6.6	42
11044	A Bis-Chelating / Ligand for the Synthesis of Heterobimetallic Platinum(II)/Rhenium(I) Complexes: Tools for the Optimization of a New Class of Platinum(II) Anticancer Agents. <i>Chemistry - A European Journal</i> , 2020, 26, 12846-12861.	1.7	14
11045	Synthesis, Structures, and Antibacterial Activities of Four Similar 1D Metal-Organic Polymers with Different Metal Ions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 532-539.	0.6	4
11046	Synthesis, electronic structure and NH-tautomerism of novel mono- and dibenzoannelated phthalocyanines. <i>Dyes and Pigments</i> , 2020, 181, 108564.	2.0	6
11047	Engineering Electrical Conductivity in Stable Zirconium-Based PCN-222 MOFs with Permanent Mesoporosity. <i>Chemistry of Materials</i> , 2020, 32, 6137-6149.	3.2	34
11048	Tuning Activity and Selectivity during Alkyne Activation by Gold(I)/Platinum(0) Frustrated Lewis Pairs. <i>Organometallics</i> , 2020, 39, 2534-2544.	1.1	20
11049	Development of nuclear basis sets for multicomponent quantum chemistry methods. <i>Journal of Chemical Physics</i> , 2020, 152, 244123.	1.2	47
11050	Synthesis, characterization, and computational modeling of 6,6'-(((2-hydroxyethyl)azanediyl)bis(methylene))bis(2,4-di-tert-butylphenol) modified group 4 metal alkoxides. <i>Journal of Coordination Chemistry</i> , 2020, 73, 1389-1406.	0.8	1
11051	Anionic Copolymerization of Styrene Sulfide with Elemental Sulfur (S ₈). <i>Materials</i> , 2020, 13, 2597.	1.3	21
11052	Photoresponsive Dithienylethene-Containing Tris(8-hydroxyquinolino)aluminum(III) Complexes with Photocontrollable Electron-Transporting Properties for Solution-Processable Optical and Organic Resistive Memory Devices. <i>Journal of the American Chemical Society</i> , 2020, 142, 12193-12206.	6.6	42
11053	Fluconazole and fragments as corrosion inhibitors of API 5L X52 steel immersed in 1M HCl. <i>Corrosion Science</i> , 2020, 174, 108853.	3.0	27
11054	A concise synthesis of carbasugars isolated from <i>Streptomyces lincolnensis</i> . <i>Tetrahedron</i> , 2020, 76, 131346.	1.0	0

#	ARTICLE	IF	CITATIONS
11055	Assistance of DFT calculations on the design and rationalization of active pharmaceutical ingredients synthesis – Michael addition-isomerization steps in Oseltamivir synthesis. <i>Tetrahedron</i> , 2020, 76, 131373.	1.0	3
11056	Electronic structures and magnetism of Zr-, Th-, and U-based metal-organic frameworks (MOFs) by density functional theory. <i>Computational Materials Science</i> , 2020, 184, 109903.	1.4	25
11057	Identifying suitable ionic liquid electrolytes for Al dual-ion batteries: role of electrochemical window, conductivity and voltage. <i>Materials Advances</i> , 2020, 1, 1354-1363.	2.6	23
11058	Palladium-catalyzed C–H activation of anisole with electron-deficient auxiliary ligands: a mechanistic investigation. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 5857-5866.	1.5	8
11059	Spectral Characteristics and Sensor Ability of a New 1,8-Naphthalimide and Its Copolymer with Styrene. <i>Sensors</i> , 2020, 20, 3501.	2.1	3
11060	Excitonic Hamiltonians for Calculating Optical Absorption Spectra and Optoelectronic Properties of Molecular Aggregates and Solids. <i>Journal of Visualized Experiments</i> , 2020, , .	0.2	1
11061	Renewable diesel from oils and animal fat waste: implications of feedstock, technology, co-products and ILUC on life cycle GWP. <i>Resources, Conservation and Recycling</i> , 2020, 161, 104944.	5.3	14
11062	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15496-15508.	1.3	14
11063	Hydrogen bonding and charge transport in a protic polymerized ionic liquid. <i>Soft Matter</i> , 2020, 16, 6091-6101.	1.2	13
11064	Theoretical Characterization of Catalytically Active Species in Reductive Hydroxymethylation of Styrene with CO ₂ over a Bisphosphine-Ligated Copper Complex. <i>Inorganic Chemistry</i> , 2020, 59, 9667-9682.	1.9	8
11065	Intermolecular Allene Functionalization by Silver-Nitrene Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 13062-13071.	6.6	25
11066	SSAIMS – Stochastic-Selection <i>Ab Initio</i> Multiple Spawning for Efficient Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6133-6143.	1.1	13
11067	Doubly vinylogous and doubly rearomative functionalization of 2-alkyl-3-furfurals. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 5816-5821.	1.5	11
11068	Interaction of Nucleic Acid Bases (NABs) with Graphene (GR) and Boron Nitride Graphene (BNG). <i>Journal of Molecular Structure</i> , 2020, 1222, 128889.	1.8	4
11069	Effect of dehydrogenated hydrocarbon doping on the electronic properties of graphene-type nanosheets. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126702.	0.9	12
11070	Lignin Biodegradation by a Cytochrome P450 Enzyme: A Computational Study into Syringol Activation by GcoA. <i>Chemistry - A European Journal</i> , 2020, 26, 13093-13102.	1.7	34
11071	Unveiling the Role of Hydrogen Bonding and g-Tensor in the Interaction of Ru-Bis-DMSO with Amino Acid Residue and Human Serum Albumin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6459-6474.	1.2	2
11072	Connected three-body terms in single-reference unitary many-body theories: Iterative and perturbative approximations. <i>Journal of Chemical Physics</i> , 2020, 152, 234116.	1.2	5

#	ARTICLE	IF	CITATIONS
11073	Computational Study of Photo-oxidative Degradation Mechanisms of Boron-Containing Oligothiophenes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1390-1398.	1.1	0
11074	Local Dielectric Constant Density Analysis of High-k Dielectric Nanomaterial. , 2020, , 53-87.		0
11075	Towards better understanding of photophysical properties of rhenium(I) tricarbonyl complexes with terpy-like ligands. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 231, 118124.	2.0	13
11076	Electronic Transport Inhibiting of Carbon Nanotubes by 5f Elements. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900226.	1.3	2
11077	Mechanistic Insight into Palladium-Catalyzed Enantioselective Remote meta ³ H Arylation and Alkylation by Using Density Functional Theory (DFT) Calculations. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 1686-1695.	2.1	5
11078	A computational study on boron dipyrromethene ancillary acceptor-based dyes for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2020, 44, 4877-4886.	1.4	17
11079	Flame-retarding battery cathode materials based on reversible multi-electron redox chemistry of phenothiazine-based polymer. <i>Journal of Energy Chemistry</i> , 2020, 47, 256-262.	7.1	17
11080	Actinide 2-metallabiphenylenes that satisfy Hückel's rule. <i>Nature</i> , 2020, 578, 563-567.	13.7	43
11081	Trigonal Bipyramidal vs. Octahedral Coordination in Indium(III) Complexes with Potentially <i>S₂N₂S</i> Tridentate Thiosemicarbazones. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 1222-1229.	1.0	3
11082	Mechanistic Studies of Bioorthogonal ATP Analogues for Assessment of Histidine Kinase Autophosphorylation. <i>ACS Chemical Biology</i> , 2020, 15, 1252-1260.	1.6	11
11083	Intermediate state representation approach to physical properties of molecular electron-detached states. II. Benchmarking. <i>Journal of Chemical Physics</i> , 2020, 152, 024125.	1.2	15
11084	QSAR studies on benzothiophene derivatives as Plasmodium falciparum N-myristoyltransferase inhibitors: Molecular insights into affinity and selectivity. <i>Drug Development Research</i> , 2020, , .	1.4	6
11085	Theoretical and experimental electronic spectra of neutral, monoprotonated and diprotonated dapsone. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	4
11086	Vibrational spectroscopic investigations and biological activity of toxic material amitraz. <i>Materials Today: Proceedings</i> , 2020, 25, 278-284.	0.9	1
11087	Engineering stable radicals using photochromic triggers. <i>Nature Communications</i> , 2020, 11, 945.	5.8	25
11088	Microhydration of verbenone: how the chain of water molecules adapts its structure to the host molecule. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5855-5864.	1.3	11
11089	Double hybrids and time-dependent density functional theory: An implementation and benchmark on charge transfer excited states. <i>Journal of Computational Chemistry</i> , 2020, 41, 1242-1251.	1.5	42
11090	Prediction of the tautomer stability and acidity of phenacylpyridines in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	1

#	ARTICLE	IF	CITATIONS
11091	Difluoroacetaldehyde <i>N</i> -triflylhydrazones (DFHZTs) as a Bench-Stable Crystalline Diazo Surrogate for Diazoacetaldehyde and Difluorodiaoethane. <i>Angewandte Chemie</i> , 2020, 132, 6535-6543.	1.6	3
11092	Steric structure of 3-(5-phenyl-1H-pyrazol-3-yl)coumarins. <i>Journal of Molecular Structure</i> , 2020, 1207, 127765.	1.8	1
11093	Bright Luminescent Platinum(II)-Biaryl Emitters Synthesized Without Air-Sensitive Reagents. <i>Chemistry - A European Journal</i> , 2020, 26, 5449-5458.	1.7	8
11094	Phosphate and Water Sensing with a Zinc-Dipicolylamine-Based Charge-Transfer Dye. <i>ChemistrySelect</i> , 2020, 5, 1945-1949.	0.7	2
11095	Eu@C86 isomers: Calculated relative populations. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2020, 28, 565-570.	1.0	7
11096	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of water-octanol partition coefficients in the SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 471-483.	1.3	7
11097	Binuclear O ₂ activation and hydrogen transfer mechanism for aerobic oxidation of alcohols. <i>Catalysis Science and Technology</i> , 2020, 10, 2183-2192.	2.1	0
11098	Increasing the Cytotoxicity of Ru(II) Polypyridyl Complexes by Tuning the Electronic Structure of Dioxo Ligands. <i>Journal of the American Chemical Society</i> , 2020, 142, 6066-6084.	6.6	44
11099	A simple acidic "turn-on" fluorescent pH probe based on BOPYIN and its visual detection and cellular imaging. <i>Dyes and Pigments</i> , 2020, 177, 108318.	2.0	23
11100	Stabilization of Open-Shell Single Bonds within Endohedral Metallofullerene. <i>Inorganic Chemistry</i> , 2020, 59, 3606-3618.	1.9	11
11101	How CuCl and CuCl ₂ Insert into C-N Bonds of Diazo Compounds: An Electronic Structure and Mechanistic Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2029-2035.	1.1	5
11102	Nature of the Surface Intermediates Formed from Methane on Cu-ZSM-5 Zeolite: A Combined Solid-State Nuclear Magnetic Resonance and Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6242-6252.	1.5	38
11103	SERS and DFT Study of Noble-Metal-Anchored Cys-Trp/Trp-Cys Dipeptides: Influence of Main-Chain Direction and Terminal Modifications. <i>Journal of Physical Chemistry C</i> , 2020, 124, 7097-7116.	1.5	16
11104	Quantum Chemical Investigation of Dimerization in the Schlenk Equilibrium of Thiophene Grignard Reagents. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1480-1488.	1.1	7
11105	Efficient implementation of the interacting quantum atoms energy partition of the second-order Møller-Plesset energy. <i>Journal of Computational Chemistry</i> , 2020, 41, 1234-1241.	1.5	16
11106	Carbocatalytic Acetylene Cyclotrimerization: A Key Role of Unpaired Electron Delocalization. <i>Journal of the American Chemical Society</i> , 2020, 142, 3784-3796.	6.6	21
11107	O ₂ Activation by Non-Heme Thiolate-Based Dinuclear Fe Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 3249-3259.	1.9	17
11108	Color-tunable single-fluorophore supramolecular system with assembly-encoded emission. <i>Nature Communications</i> , 2020, 11, 158.	5.8	198

#	ARTICLE	IF	CITATIONS
11109	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4770-4777.	7.2	39
11110	Clar Rules the Electronic Properties of 2D π -Conjugated Frameworks: Mind the Gap. <i>Chemistry - A European Journal</i> , 2020, 26, 6569-6575.	1.7	8
11111	Elucidation of the chromatographic enantiomer elution order for praziquantel: An experimental and theoretical assessment. <i>Chirality</i> , 2020, 32, 353-358.	1.3	5
11112	Selective Oxidation of Benzylic C-H Bonds Catalyzed by Cu(II)/ PMo_{12} . <i>Journal of Organic Chemistry</i> , 2020, 85, 3101-3109.	1.7	29
11113	Feasibility of pristine, Al-doped and Ga-doped Boron Nitride nanotubes for detecting SF ₄ gas: A DFT, NBO and QTAIM investigation. <i>Applied Surface Science</i> , 2020, 510, 145490.	3.1	63
11114	Theoretical and experimental study of the influence of cationic Eriochrome complexes on the BDD anodic oxidation of Eriochrome Black T solutions. <i>Electrochemistry Communications</i> , 2020, 112, 106668.	2.3	13
11115	Helical Peptides Design for Molecular Dipoles Functionalization of Wide Band Gap Oxides. <i>Journal of the American Chemical Society</i> , 2020, 142, 3489-3498.	6.6	7
11116	Aluminum Alkyls as Highly Active Catalytic Chain Transfer Agents. <i>Macromolecular Reaction Engineering</i> , 2020, 14, 1900047.	0.9	1
11117	Electron donor substituents on the dppz-based ligands to control luminescence from dark to bright emissive state in Ir(III) complexes. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26167.	1.0	6
11118	Enhancing charge mobilities in self-assembled N^{π} halogen bonded organic semiconductors: A design approach based on experimental and computational perspectives. <i>Organic Electronics</i> , 2020, 79, 105637.	1.4	3
11119	Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4737-4750.	5.5	45
11120	Evidence for Genuine Bimetallic Frustrated Lewis Pair Activation of Dihydrogen with Gold(I)/Platinum(0) Systems. <i>Chemistry - A European Journal</i> , 2020, 26, 5982-5993.	1.7	37
11121	DFT Study on the Gold(I)-Catalyzed Dehydrogenative Heterocyclization of Alkynyl Alkenones to form 2,3-Furan fused Carbocycles: Effects of Additives $\text{C}_5\text{H}_5\text{NO}$ vs. PhNO . <i>Applied Organometallic Chemistry</i> , 2020, 34, e5443.	1.7	3
11122	Structural and spectral characterisation of 2-amino-2H-[1,2,3]triazolo[4,5-g]quinoline-4,9-dione polymorphs. Cytotoxic activity and molecular docking study with NQO1 enzyme. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 230, 118038.	2.0	8
11123	Scaling exchange and correlation in the on-top density functional of multiconfiguration pair-density functional theory: effect on electronic excitation energies and bond energies. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	3
11124	The effect of group-substitution on the sensitization properties of alkynylrhenium(I) tricarbonyl diimine complexes adsorbed to TiO ₂ (101) film surface: a theoretical study. <i>Journal of Molecular Modeling</i> , 2020, 26, 34.	0.8	4
11125	Exploring the Mechanism of the Palladium-Catalyzed 3-Butene-2-ol Amination Reaction: A DFT Study. <i>Frontiers in Chemistry</i> , 2020, 8, 48.	1.8	2
11126	Simultaneous formation of non-oxidovanadium(V^{IV}) and oxidovanadium(V^{V}) complexes incorporating phenol-based hydrazone ligands in aerobic conditions. <i>New Journal of Chemistry</i> , 2020, 44, 3700-3716.	1.4	9

#	ARTICLE	IF	CITATIONS
11127	Structural basis of second-generation HIV integrase inhibitor action and viral resistance. <i>Science</i> , 2020, 367, 806-810.	6.0	73
11128	Difluoroacetaldehyde <i>N</i> -triflylhydrazone (DFHZ-Tfs) as a Bench-Stable Crystalline Diazo Surrogate for Diazoacetaldehyde and Difluorodiaoethane. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 6473-6481.	7.2	45
11129	Dilution of the Electron Density in the π -Conjugated Skeleton of Organic Cathode Materials Improves the Discharge Voltage. <i>ChemSusChem</i> , 2020, 13, 2264-2270.	3.6	34
11130	Solar cells sensitized by porphyrin dyes containing a substituted carbazole donor with synergistically extended absorption and suppressed the dye aggregation. <i>Chinese Chemical Letters</i> , 2020, 31, 1927-1930.	4.8	31
11131	Luminescence of mononuclear Pt(II) complexes with glycolate: external stimuli-induced excimer emission changes to oligomer emissions. <i>Dalton Transactions</i> , 2020, 49, 1873-1882.	1.6	14
11132	A Combined Systematic-Stochastic Algorithm for the Conformational Search in Flexible Acyclic Molecules. <i>Frontiers in Chemistry</i> , 2020, 8, 16.	1.8	21
11133	Isothiourea-Catalyzed Atropselective Acylation of Biaryl Phenols via Sequential Desymmetrization/Kinetic Resolution. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7897-7905.	7.2	47
11134	Rational Development of Remote C-H Functionalization of Biphenyl: Experimental and Computational Studies. <i>Angewandte Chemie</i> , 2020, 132, 4800-4807.	1.6	3
11135	Local Aromaticity: An Important Indicator of the Surface Active Sites of Heterocyclic Nanostructures. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2583-2590.	1.5	4
11136	1,8-Dimercuri-Phenyl- <i>H</i> -Carbazole as a Monofacial Dinuclear Organometallic Nucleobase. <i>Chemistry - A European Journal</i> , 2020, 26, 2164-2168.	1.7	16
11137	A blind SAMPL6 challenge: insight into the octanol-water partition coefficients of drug-like molecules via a DFT approach. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 463-470.	1.3	13
11138	Hydrostatic Pressure-Induced Spectral Variation of Reichardt's Dye: A Polarity/Pressure Dual Indicator. <i>ACS Omega</i> , 2020, 5, 897-903.	1.6	13
11139	A Generalized Variational Principle with Applications to Excited State Mean Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1526-1540.	2.3	36
11140	Kinetic modelling of acyl glucuronide and glucoside reactivity and development of structure-property relationships. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 1389-1401.	1.5	5
11141	Asymmetric Organocatalyzed Aza-Henry Reaction of Hydrazones: Experimental and Computational Studies. <i>Chemistry - A European Journal</i> , 2020, 26, 5469-5478.	1.7	7
11142	Comparative quantum chemistry study of the F-center in lanthanum trifluoride. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2020, 474, 57-62.	0.6	9
11143	U ₂ O@C ₇₆ : Non-Isolated-Pentagon-Rule Cages Preval with the U ₂ O Configuration Determined by Cage Shape and Dominated by Multicenter Bonds. <i>Inorganic Chemistry</i> , 2020, 59, 7039-7048.	1.9	10
11144	Stepwise Activation of Water by Open-Shell Interactions, Cl(H ₂ O) _n =4 ^{8,17} . <i>Journal of Physical Chemistry A</i> , 2020, 124, 3417-3437.	1.1	6

#	ARTICLE	IF	CITATIONS
11145	Spontaneous Si-Si bonding of alkanethiols to Si(111)-H: towards Si-Si circuits. <i>Chemical Science</i> , 2020, 11, 5246-5256.	3.7	30
11146	Chlorosubstituted Copper Phthalocyanines: Spectral Study and Structure of Thin Films. <i>Molecules</i> , 2020, 25, 1620.	1.7	8
11147	Salt metathesis as an alternative approach to access aluminium(III) and gallium(III)-diketiminates. <i>Dalton Transactions</i> , 2020, 49, 6377-6383.	1.6	16
11148	Mechanistic Insights into the Chemo-Selective Dehydrogenative Silylation of Alkenes Catalyzed by Bis(imino)pyridine Cobalt Complex from DFT Computations. <i>ChemCatChem</i> , 2020, 12, 3890-3899.	1.8	2
11149	The unexpected effect of aqueous ion pairs on the forbidden n-π* transition in nitrate. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11678-11685.	1.3	2
11150	Bioinspired Design and Computational Prediction of SCS Nickel Pincer Complexes for Hydrogenation of Carbon Dioxide. <i>Catalysts</i> , 2020, 10, 319.	1.6	6
11151	All-electron basis sets augmented with diffuse functions for He, Ca, Sr, Ba, and lanthanides: application in calculations of atomic and molecular properties. <i>Journal of Molecular Modeling</i> , 2020, 26, 95.	0.8	3
11152	Study of the structures and photophysical properties of 1,3-diaza-5-phosphacyclohexanes using density functional theory and optical spectroscopy. <i>Russian Chemical Bulletin</i> , 2020, 69, 449-457.	0.4	3
11153	Mechanistic investigation of N-heterocyclic carbene and Na ₂ CO ₃ cooperatively catalyzed C(sp ³)-F bond activation reaction of fluoroenal. <i>Molecular Catalysis</i> , 2020, 489, 110944.	1.0	11
11154	Photophysical and theoretical studies on the solvatochromic effects and dipole moments evaluation of substituted 1-phenyl-3-naphthyl-5-(4-ethyl benzoate)-2-pyrazoline. <i>Journal of Molecular Liquids</i> , 2020, 307, 112967.	2.3	18
11155	Photo-dynamic and fluorescent zinc complex based on spiropyran ligand. <i>Journal of Molecular Structure</i> , 2020, 1211, 128105.	1.8	12
11156	Characterization of Magnetic Series of Iron-Carbon Clusters Fe _n C _{0,±1} (n = 13). <i>Journal of Physical Chemistry C</i> , 2020, 124, 9484-9495.	1.5	11
11157	Second Near-Infrared Aggregation-Induced Emission Fluorophores with Phenothiazine Derivatives as the Donor and 6,7-Diphenyl-[1,2,5]Thiadiazolo[3,4-g]Quinoxaline as the Acceptor for In Vivo Imaging. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20281-20286.	4.0	36
11158	Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8182-8192.	1.3	16
11159	Theoretical study of the mechanism behind the site- and enantio-selectivity of C-H functionalization catalysed by chiral dirhodium catalyst. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9561-9572.	1.3	5
11160	Tricarabrols: C, three anti-inflammatory sesquiterpene lactone trimers featuring a methylene-tethered linkage from <i>Carpesium faberi</i> . <i>Organic Chemistry Frontiers</i> , 2020, 7, 1374-1382.	2.3	14
11161	Acylation and deacylation mechanism and kinetics of penicillin G reaction with <i>Streptomyces</i> R61 DD-peptidase. <i>Journal of Computational Chemistry</i> , 2020, 41, 1685-1697.	1.5	4
11162	Quantum yields of singlet and triplet chemiexcitation of dimethyl 1,2-dioxetane: <i>ab initio</i> nonadiabatic molecular dynamic simulations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11440-11451.	1.3	17

#	ARTICLE	IF	CITATIONS
11163	Mono-, Di- and Tetra-iron Complexes with Selenium or Sulphur Functionalized Vinyliminium Ligands: Synthesis, Structural Characterization and Antiproliferative Activity. <i>Molecules</i> , 2020, 25, 1656.	1.7	20
11164	[Mo ₂ O ₂ S ₈] ²⁺ small molecule dimer as a basis for hydrogen evolution reaction (HER) catalyst materials. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	8
11165	Hydrogen Evolution Catalyzed by a Metal-Free Corrole: An Experimental and Theoretical Mechanistic Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10265-10271.	1.5	9
11166	Infrared photodissociation spectroscopy of D ₂ -tagged CH ₃ CO ₂ ⁻ (H ₂ O) ₀ ⁻² anions. <i>Molecular Physics</i> , 2020, 118, e1749953.	0.8	9
11167	Methylone screening with electropolymerized molecularly imprinted polymer on screen-printed electrodes. <i>Sensors and Actuators B: Chemical</i> , 2020, 316, 128133.	4.0	23
11168	Principal Descriptors of Ionic Liquid Co-catalysts for the Electrochemical Reduction of CO ₂ . <i>ACS Applied Energy Materials</i> , 2020, 3, 4690-4698.	2.5	10
11169	Organocatalytic <i>vs.</i> Ru-based electrochemical hydrogenation of nitrobenzene in competition with the hydrogen evolution reaction. <i>Dalton Transactions</i> , 2020, 49, 6446-6456.	1.6	17
11170	Evidence for Genuine Bimetallic Frustrated Lewis Pair Activation of Dihydrogen with Gold(I)/Platinum(0) Systems. <i>Chemistry - A European Journal</i> , 2020, 26, 5915-5915.	1.7	11
11171	Inhibitor design for 3- α -hydroxy- β -methylglutaryl-CoA reductase enzyme; molecular docking and determination of molecular and electronic properties of ligands by density functional theory method. <i>Journal of Heterocyclic Chemistry</i> , 2020, 57, 2875-2888.	1.4	8
11172	High-temperature rate constants for CH ₃ COOH + OH reactions: the effects of multiple structures and paths. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	4
11173	In vitro and computational studies of natural products related to perezone as anti-neoplastic agents. <i>Biochimie</i> , 2020, 171-172, 158-169.	1.3	9
11174	Clar model modified for nanographenes. <i>Chemical Physics Letters</i> , 2020, 750, 137487.	1.2	3
11175	Spectroscopic, thermogravimetric studies and DFT calculations of pentoxyverine citrate ion-pairs with sulfonephthalein dyes. <i>Journal of Molecular Structure</i> , 2020, 1212, 128074.	1.8	6
11176	Synthesis, characterization and crystal structure of two polymorphs of trans N-benzyl-3,9,9-trimethyl-1,2,3,4,4a,9,9a,10-octahydroacridine. <i>Journal of Molecular Structure</i> , 2020, 1215, 128222.	1.8	1
11177	Stronger Hydration of Eu(III) Impedes Its Competition against Am(III) in Binding with N-donor Extractants. <i>Inorganic Chemistry</i> , 2020, 59, 6267-6278.	1.9	15
11178	Undiscovered Effect of C ⁺ N Interchange Inside the Metal Carbonitride Clusterfullerenes: A Density Functional Theory Investigation. <i>Inorganic Chemistry</i> , 2020, 59, 6518-6527.	1.9	6
11179	Utilizing Essential Symmetry Breaking in Auxiliary-Field Quantum Monte Carlo: Application to the Spin Gaps of the C ₃₆ Fullerene and an Iron Porphyrin Model Complex. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3019-3027.	2.3	30
11180	Magnetism-Vanishing Stabilizes the Pyrite-Type 3d Transition Metal Peroxides at High Pressures. <i>Journal of Physical Chemistry C</i> , 2020, 124, 10085-10093.	1.5	1

#	ARTICLE	IF	CITATIONS
11181	Copper-Mediated Cascade Synthesis of Open-Cage Fullerenes. <i>Organic Letters</i> , 2020, 22, 3633-3636.	2.4	15
11182	Co(salen)-Catalyzed Oxidation of Lignin Models to Form Benzoquinones and Benzaldehydes: A Computational and Experimental Study. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 7225-7234.	3.2	18
11183	Metal-Free Thiophene-Sulfur Covalent Organic Frameworks: Precise and Controllable Synthesis of Catalytic Active Sites for Oxygen Reduction. <i>Journal of the American Chemical Society</i> , 2020, 142, 8104-8108.	6.6	226
11184	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). <i>Communications Chemistry</i> , 2020, 3, .	2.0	98
11185	The elusive dynamics of aqueous permanganate photochemistry. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 10043-10055.	1.3	7
11186	Identification of key functionalization species in the Cp*Ir(III)-catalyzed-ortho halogenation of benzamides. <i>Dalton Transactions</i> , 2020, 49, 16166-16174.	1.6	6
11187	Oxidative ability of organic iodine reagents: a theoretical assessment. <i>New Journal of Chemistry</i> , 2020, 44, 7051-7057.	1.4	17
11188	Nanomolar Detection of Palladium (II) through a Novel Seleno-Rhodamine-based fluorescent and colorimetric chemosensor. <i>Dyes and Pigments</i> , 2020, 179, 108355.	2.0	16
11189	Quantum chemical modeling of molecules under pressure. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26208.	1.0	14
11190	The complete catalytic mechanism of xanthine oxidase: a computational study. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 405-416.	3.0	14
11191	A DFT study of structure and stability of pleated and rippled cross-linked sheets with hydrophobic sidechains. <i>Biopolymers</i> , 2021, 112, e23391.	1.2	11
11192	pysisyphus: Exploring potential energy surfaces in ground and excited states. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26390.	1.0	29
11193	Thienyl/phenyl bay-substituted perylenebisimides: Intersystem crossing and application as heavy atom-free triplet photosensitizers. <i>Dyes and Pigments</i> , 2021, 184, 108708.	2.0	16
11194	Forming electron traps deactivates self-assembled crystalline organic nanosheets toward photocatalytic overall water splitting. <i>Science Bulletin</i> , 2021, 66, 265-274.	4.3	18
11195	Metal-ion-assisted structural and anomeric analysis of Amadori compounds by electrospray ionization mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e8960.	0.7	4
11196	Structural and thermochemical studies of pyrrolidine borane and piperidine borane by gas electron diffraction and quantum chemical calculations. <i>Structural Chemistry</i> , 2021, 32, 205-213.	1.0	1
11197	Synthesis, X-ray and complete assignments of ¹ H and ¹³ C nuclear magnetic resonance data for novel dichloro-1,4-dihydro-1,4-epoxynaphthalene derivatives. <i>Journal of Molecular Structure</i> , 2021, 1224, 129287.	1.8	2
11198	The adsorption of bromochlorodifluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. <i>Structural Chemistry</i> , 2021, 32, 481-494.	1.0	27

#	ARTICLE	IF	CITATIONS
11199	Rethinking the reaction pathways of chemical reduction of graphene oxide. <i>Carbon</i> , 2021, 171, 963-967.	5.4	15
11200	The adsorption of bromochlorodifluoromethane on pristine, Al, Ga, P, and As-doped boron nitride nanotubes: A study involving PBC-DFT, NBO analysis, and QTAIM. <i>Computational and Theoretical Chemistry</i> , 2021, 1193, 113047.	1.1	22
11201	Reactive atomistic simulations of Diels-Alder-type reactions: conformational and dynamic effects in the polar cycloaddition of 2,3-dibromobutadiene radical ions with maleic anhydride. <i>Molecular Physics</i> , 2021, 119, e1825852.	0.8	3
11202	A novel fluorescent chemosensor for Cu ²⁺ ion based on a new hexadentate ligand receptor: X-ray single crystal of the perchlorate salt of the ligand, ion selectivity assays and TD-DFT study. <i>Inorganica Chimica Acta</i> , 2021, 515, 120061.	1.2	5
11203	Adsorption of nitrosamine conformers on the C ₂₄ , B ₁₂ N ₁₂ , Be ₁₂ O ₁₂ and Al ₁₂ P ₁₂ nanocages and their conversion to nitrogen and water molecules: A DFT study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 127, 114506.	1.3	6
11204	Ab initio investigation of the ground and lowest excited states of the YAl molecule. <i>Computational and Theoretical Chemistry</i> , 2021, 1194, 113057.	1.1	0
11205	(â€“) â€“ Epicatechin gallate as a corrosion inhibitor for bronze in a saline medium and theoretical study. <i>Journal of Molecular Structure</i> , 2021, 1227, 129416.	1.8	9
11206	Multi-spectroscopic (FT-IR, FT-Raman, ¹ H NMR and ¹³ C NMR) investigations on syringaldehyde. <i>Journal of Molecular Structure</i> , 2021, 1229, 129490.	1.8	19
11207	ICT-modulated NIR water-soluble fluorescent probe with large Stokes shift for selective detection of cysteine in living cells and zebrafish. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119030.	2.0	20
11208	Immobilization of His-tagged proteins on NiO foams for recyclable enzymatic reactors. <i>Applied Surface Science</i> , 2021, 537, 147848.	3.1	5
11209	Mechanistic investigations <i>via</i> DFT support the cooperative heterobimetallic Câ€“H and Oâ€“H bond activation across Taâ€“r multiple bonds. <i>Dalton Transactions</i> , 2021, 50, 504-510.	1.6	13
11210	Impact of the macrocyclic structure and dynamic solvent effect on the reactivity of a localised singlet diradicaloid with Î€-single bonding character. <i>Chemical Science</i> , 2021, 12, 613-625.	3.7	16
11211	Control of the single atom/nanoparticle ratio in Pd/C catalysts to optimize the cooperative hydrogenation of alkenes. <i>Catalysis Science and Technology</i> , 2021, 11, 984-999.	2.1	30
11212	Neutral Chiral Tetrakisâ€“iodoâ€“Triazole Halogenâ€“Bond Donor for Chiral Recognition and Enantioselective Catalysis. <i>Chemistry - A European Journal</i> , 2021, 27, 2315-2320.	1.7	28
11213	Redox Modulation of the Reactivity and Regioselectivity in Dielsâ€“Alder Reaction of Metallofullerene La@C ₈₂ with Cyclopentadiene. <i>Chemistry - an Asian Journal</i> , 2021, 16, 80-86.	1.7	3
11214	DFT study on the [4+4] domino cycloaddition of ynones with benzylidenepyrazolones to access eight-membered cyclic ethers: effects of DBU <i>vs.</i> <i>Et</i> ₃ N. <i>New Journal of Chemistry</i> , 2021, 45, 131-140.	1.4	4
11215	Corrosion inhibition of mild steel in acidic medium by simple azole-based aromatic compounds. <i>Journal of Electroanalytical Chemistry</i> , 2021, 880, 114858.	1.9	43
11216	How to inverse the chemoselectivity of nucleophilic addition by using a Lewis acid/Brønsted base pair catalyst: A theoretical view. <i>Molecular Catalysis</i> , 2021, 499, 111318.	1.0	3

#	ARTICLE	IF	CITATIONS
11217	Molecular structure, spectroscopic (FT-IR, FT-Raman, NMR), HOMO-LUMO, chemical reactivity, AIM, ELF, LOL and Molecular docking studies on 1-Benzyl-4-(N-Boc-amino)piperidine. <i>Journal of Molecular Structure</i> , 2021, 1230, 129657.	1.8	72
11218	Effect of homonuclear boron bonds in the adsorption of DNA nucleobases on boron nitride nanosheets. <i>Journal of Molecular Liquids</i> , 2021, 322, 114951.	2.3	68
11219	Refined standards for simulating UV-vis absorption spectra of acceptors in organic solar cells by TD-DFT. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113087.	2.0	9
11220	Possible Mechanisms and Origin of Selectivities for Phosphine-Catalyzed [2+n] (n=3, 4) Annulations of Saturated Amines and α -Acetoxy Allenolates. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 619-625.	1.3	10
11221	Structural Changes in Five-Coordinate Bromido-bis(o-aminobenzo-semiquinonato)iron(III) Complex: Spin-Crossover or Ligand-Metal Antiferromagnetic Interactions?. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 756-762.	1.0	1
11222	SAMPL7: Host-guest binding prediction by molecular dynamics and quantum mechanics. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 63-77.	1.3	9
11223	Colorimetric metal ion (II) Sensors Based on imine boronic esters functionalized with pyridine. <i>Dyes and Pigments</i> , 2021, 186, 108991.	2.0	7
11224	Iridium(III) Sensitisers and Energy Upconversion: The Influence of Ligand Structure upon TTA-UC Performance. <i>Chemistry - A European Journal</i> , 2021, 27, 3427-3439.	1.7	20
11225	Predicting the origin of selectivity in NHC-catalyzed ring opening of formylcyclopropane: a theoretical investigation. <i>Catalysis Science and Technology</i> , 2021, 11, 332-337.	2.1	28
11226	Purple passion fruit seeds (<i>Passiflora edulis</i> f. <i>edulis</i> Sims) as a promising source of skin anti-aging agents: Enzymatic, antioxidant and multi-level computational studies. <i>Arabian Journal of Chemistry</i> , 2021, 14, 102905.	2.3	21
11227	A simple diaminomaleonitrile based molecular probe for selective detection of Cu(II) and Zn(II) ions in semi-aqueous medium. <i>Inorganica Chimica Acta</i> , 2021, 515, 120073.	1.2	9
11228	A DFT study of fulvic acid binding with bivalent metals: Cd, Cu, Mg, Ni, Pb, Zn. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107800.	1.3	18
11229	Green-Blue Phosphorescent Iridium(III) Complexes with Near Unitary Quantum Yield. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 601-604.	1.0	4
11230	Novel 2,5-bis(6-(trimethylammonium)hexyl)-3,6-diaryl-1,4-diketopyrrolo[3,4-c]pyrrole pigments as levelers for efficient electroplating applications. <i>Dyes and Pigments</i> , 2021, 186, 109064.	2.0	14
11231	The interaction of half-sandwich (η^5 -Cp*)Rh(III) cation with histidine containing peptides and their ternary species with (N,N) bidentate ligands. <i>Journal of Inorganic Biochemistry</i> , 2021, 216, 111330.	1.5	3
11232	Penta- and dinuclear carboxylate nickel(II) complexes with pyrazole-based ligands: Syntheses, magnetic properties and DFT calculations. <i>Polyhedron</i> , 2021, 195, 114971.	1.0	3
11233	Imaging and Monitoring the Hydrogen Peroxide Level in Heart Failure by a Fluorescent Probe with a Large Stokes Shift. <i>ACS Sensors</i> , 2021, 6, 54-62.	4.0	11
11234	Structure-antioxidant activity relationships in boldine and glaucine: a DFT study. <i>New Journal of Chemistry</i> , 2021, 45, 590-596.	1.4	2

#	ARTICLE	IF	CITATIONS
11235	An Ultimate Investigation on the Adsorption of Amantadine on Pristine and Decorated Fullerenes C59X (X=Si, Ge, B, Al, Ga, N, P, and As): A DFT, NBO, and QTAIM Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 23-39.	1.0	28
11236	Solidâ€State Molecular Motions in Organic THz Generators. <i>Advanced Optical Materials</i> , 2021, 9, 2001521.	3.6	15
11237	Investigations of structural, spectral (IR, 1H-, 9F-, 11B-, 13C-, 15ÂN-, 17O-NMR) and anticancer properties of 5FU@B12N12 complexes. <i>Chemical Papers</i> , 2021, 75, 1727-1737.	1.0	2
11238	Variable temperature FTIR spectra of polycrystalline purine nucleobases and estimating strengths of individual hydrogen bonds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 251, 119323.	2.0	7
11239	Analytic Energy, Gradient, and Hessian of Electrostatic Embedding QM/MM Based on Electrostatic Potential-Fitted Atomic Charges Scaling Linearly with the MM Subsystem Size. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 538-548.	2.3	11
11240	Unraveling the catalytically preferential pathway between the direct and indirect hydrogenation of CO₂ to CH₃OH using N-heterocyclic carbene-based Mn⁽ⁱ⁾ catalysts: a theoretical approach. <i>Catalysis Science and Technology</i> , 2021, 11, 1375-1385.	2.1	13
11241	Mechanistic Investigation on Chemiluminescent Formaldehyde Probes. <i>Chemistry - A European Journal</i> , 2021, 27, 5712-5720.	1.7	7
11242	Boronâ€Ligand Cooperation: The Concept and Applications. <i>Chemistry - A European Journal</i> , 2021, 27, 5615-5626.	1.7	12
11243	Preferential intermolecular interactions in a racemic mixture of amino acid Schiff base, conformational structures in solid state, and DFT studies. <i>New Journal of Chemistry</i> , 2021, 45, 1727-1733.	1.4	1
11244	Identifying the Molecular Origins of High-Performance in Organic Photodetectors Based on Highly Intermixed Bulk Heterojunction Blends. <i>ACS Nano</i> , 2021, 15, 1217-1228.	7.3	19
11245	Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of infrared spectra of arabidopsis thaliana plant cryptochrome. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1666-1674.	1.3	6
11246	Drug reservoir mechanism of Pt(II)-sulfur chelates based on pharmacokinetics of Pt(II) complex with thiols & thio-ethers: An experimental and theoretical approach. <i>Inorganica Chimica Acta</i> , 2021, 517, 120202.	1.2	4
11247	Synthesis, characterization and crystal structure of bis-(methylsulfonylmethyl) sulfone, a symmetric acyclic trisulfone. <i>Journal of Molecular Structure</i> , 2021, 1230, 129655.	1.8	1
11248	Synthesis and characterization of copper (II) complexes with arylmethylenebis-4-hydroxy-6-methyl-2-N-pyran-2-ones: A case of interesting keto-enol tautomerism. <i>Inorganica Chimica Acta</i> , 2021, 517, 120207.	1.2	3
11249	Study on the effect of substituents on the structure, volatility, and fluorescence of N-(Alkyl or Tj ETQqO O O rgBT /Overlock 10 Tf 50 187 121646.	0.8	3
11250	Metalloradical complex Coâ€CË™Ph3 catalyzes the CO2 reduction in gas phase: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1392-1400.	1.3	0
11251	Strong electron affinity PDI supramolecules form anion radicals for the degradation of organic pollutants <i>via</i> direct electrophilic attack. <i>Catalysis Science and Technology</i> , 2021, 11, 1899-1913.	2.1	7
11252	Modeling Molecules under Pressure with Gaussian Potentials. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 583-597.	2.3	17

#	ARTICLE	IF	CITATIONS
11253	Antioxidant properties of novel curcumin analogues: A combined experimental and computational study. <i>Journal of Food Biochemistry</i> , 2021, 45, e13584.	1.2	7
11254	Theoretical insight into the opposite redox activity of iron complexes toward the ring opening polymerization of lactide and epoxide. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1005-1014.	3.0	5
11255	Five lead(II) coordinated polymers assembled from asymmetric azoles carboxylate ligands: Synthesis, structures and fluorescence properties. <i>Inorganica Chimica Acta</i> , 2021, 514, 120035.	1.2	6
11256	Reactivity of Undissociated Molecular Nitric Acid at the Air–Water Interface. <i>Journal of the American Chemical Society</i> , 2021, 143, 453-462.	6.6	14
11257	Scale factor database for the vibration frequencies calculated in M06-2X, one of the DFT methods. <i>Vibrational Spectroscopy</i> , 2021, 112, 103189.	1.2	34
11258	¹ H and ¹⁹⁵ Pt NMR prediction for inclusion compounds formed by cisplatin and oxidized carbon nanostructures. <i>RSC Advances</i> , 2021, 11, 599-611.	1.7	4
11259	Reaction Pathway Discrimination in Alkene Oxidation Reactions by Designed Ti-Siloxo-Polyoxometalates. <i>ChemCatChem</i> , 2021, 13, 1220-1229.	1.8	13
11260	Ab-initio search for efficient red thermally activated delayed fluorescence molecules for organic light emitting diodes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 118952.	2.0	5
11261	Deeper insight into the multifaceted photodynamics of a potential organic functional material emphasizing aggregation induced emission enhancement (AIEE) properties. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 406, 112998.	2.0	7
11262	The HOX ⁻ SO ₂ ⁻ (X=F, Cl, Br, I) Binary Complexes: Implications for Atmospheric Chemistry. <i>ChemPhysChem</i> , 2021, 22, 112-126.	1.0	0
11263	De novo generation of optically active small organic molecules using Monte Carlo tree search combined with recurrent neural network. <i>Journal of Computational Chemistry</i> , 2021, 42, 136-143.	1.5	8
11264	What Determines the Selectivity of Arginine Dihydroxylation by the Nonheme Iron Enzyme OrfP?. <i>Chemistry - A European Journal</i> , 2021, 27, 1795-1809.	1.7	26
11265	Microsolvation of Co ²⁺ in water: Density functional theory calculations coupled with stochastic kicking method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 245, 118935.	2.0	8
11266	A study on the interaction of Nile blue with Uracils: A spectroscopic and computational approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119011.	2.0	5
11267	Calculated relative populations for the Eu@C84 isomers. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2021, 29, 144-148.	1.0	5
11268	The KOALA program: Wavefunction frozen-density embedding. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26351.	1.0	8
11269	Exploring the Reaction Paths on the Potential Energy Surfaces of the S ₁ and T ₁ States in Methylenecyclopropane. <i>Photochemistry and Photobiology</i> , 2021, 97, 126-135.	1.3	2
11270	Zinc oxide-quercetin nanocomposite as a smart nano-drug delivery system: Molecular-level interaction studies. <i>Applied Surface Science</i> , 2021, 536, 147741.	3.1	76

#	ARTICLE	IF	CITATIONS
11271	Influence of end-capped group on structural and electronic properties of the At-İc-Ac-İc-At small molecule donor for high-performance organic solar cells. <i>Structural Chemistry</i> , 2021, 32, 367-377.	1.0	0
11272	Unravelling the molecular basis of AM-6494 high potency at BACE1 in Alzheimerâ€™s disease: an integrated dynamic interaction investigation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-13.	2.0	10
11273	Proton-controlled non-exponential photoluminescence in a pyridylamidine-substituted Re(<i>scp</i>) complex. <i>Dalton Transactions</i> , 2021, 50, 7265-7276.	1.6	1
11274	Pseudo-octahedral nickel(<i>scp</i>) complexes of strongly absorbing benzannulated pincer-type amido ligands: ligand-based redox and non-Aufbau electronic behaviour. <i>RSC Advances</i> , 2021, 11, 3547-3555.	1.7	3
11275	Pereskia aculeata vibrational model by Raman characterization and DFT method. <i>International Journal for Innovation Education and Research</i> , 2021, 9, 485-505.	0.0	1
11276	Dâ€™A dyads and Aâ€™Dâ€™A triads based on ferrocene: pushâ€™pull dyes with unusual behaviours in solution. <i>New Journal of Chemistry</i> , 2021, 45, 13475-13498.	1.4	6
11277	Synthesis, photophysical, electrochemical and computational study of indolocarbazole based donor acceptor type conjugated polymers. <i>Chemical Papers</i> , 2021, 75, 1969-1980.	1.0	1
11278	Multi PCET in symmetrically substituted benzimidazoles. <i>Chemical Science</i> , 2021, 12, 12667-12675.	3.7	5
11279	Aerobic oxidation of primary amines to amides catalyzed by an annulated mesoionic carbene (MIC) stabilized Ru complex. <i>Catalysis Science and Technology</i> , 2021, 11, 7018-7028.	2.1	6
11280	Vapochromic behaviour of a nickel(<i>scp</i>)-quinonoid complex with dimensional changes between 1D and higher. <i>Dalton Transactions</i> , 2021, 50, 8696-8703.	1.6	7
11281	A Theoretical Study of Product Selectivity in Rhodium Catalyzed Oxidative Coupling Reaction Caused by the Solvation Effect. <i>Heterocycles</i> , 2021, 103, 952.	0.4	0
11282	A simplified charge projection scheme for long-range electrostatics in <i>ab initio</i> QM/MM calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024115.	1.2	18
11283	Doubly Strapped Redox-Switchable 5,10,15,20-Tetraaryl-5,15-diazaporphyrinoids: Promising Platforms for the Evaluation of Paratropic and Diatropic Ring-Current Effects. <i>Journal of Organic Chemistry</i> , 2021, 86, 2283-2296.	1.7	12
11284	Selective catalytic reduction of NO with NH ₃ over Cu-exchanged CHA, GME, and AFX zeolites: a density functional theory study. <i>Catalysis Science and Technology</i> , 2021, 11, 1780-1790.	2.1	12
11285	Tailoring Lewis/Brønsted acid properties of MOF nodes <i>via</i> hydrothermal and solvothermal synthesis: simple approach with exceptional catalytic implications. <i>Chemical Science</i> , 2021, 12, 10106-10115.	3.7	40
11286	Polyeutectic-based stable and effective electrolytes for high-performance energy storage systems. <i>Energy and Environmental Science</i> , 2021, 14, 931-939.	15.6	21
11287	Long-lived localised singlet diradicaloids with carbonâ€™carbon İc-single bonding (Câ€™İc). <i>Chemical Communications</i> , 2021, 57, 11301-11309.	2.2	6
11288	Equivalent Loading of Directed Arenes in Pd(II)-Catalyzed Oxidative Cross-Coupling of Aryl Câ€™H Bonds at Room Temperature. <i>Journal of Organic Chemistry</i> , 2021, 86, 2714-2733.	1.7	7

#	ARTICLE	IF	CITATIONS
11289	Electron-ion coincidence measurements of molecular dynamics with intense X-ray pulses. <i>Scientific Reports</i> , 2021, 11, 505.	1.6	11
11290	C _{sp} -C _{sp} bond cleavage and fragment coupling: a transition metal-free extrusion and recombination approach towards synthesis of 1,2-diketones. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5389-5396.	2.3	4
11291	Significant Roles of a Particularly Stable Two-Center Two-Electron Lu ^{II} Lu ^{III} Bond in Lu ₂ @C ₈₆ : Electronic Structure of Lu and Radius of Lu ²⁺ . <i>Inorganic Chemistry</i> , 2021, 60, 2425-2436.	1.9	8
11292	Chelates of 3- and 5-hydroxyflavone: Quantum chemical study. <i>Chemical Physics Letters</i> , 2021, 762, 138142.	1.2	3
11293	Mechanistic study of C-H bond activation by O ₂ on negatively charged Au clusters: β , γ -dehydrogenation of 1-methyl-4-piperidone by supported Au catalysts. <i>Catalysis Science and Technology</i> , 2021, 11, 3333-3346.	2.1	5
11294	DFT Study on the Chemical Degradation Mechanism of Perfluorobis(sulfonyl)imide Sulfonic Acid Ionomer Membranes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1929-1939.	1.5	5
11295	Quantitative analysis of liquid-phase adsorption over chromium-containing metal-organic frameworks of MTN topology. <i>Adsorption</i> , 2021, 27, 953-962.	1.4	0
11296	Fitting quantum machine learning potentials to experimental free energy data: predicting tautomer ratios in solution. <i>Chemical Science</i> , 2021, 12, 11364-11381.	3.7	15
11297	An effective potential for Frenkel excitons. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1923-1935.	1.3	2
11298	Aerobic α -hydroxylation of 2-Me-1-tetralone in 1-alkyl-3-methylimidazolium ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 5864-5869.	1.3	6
11299	How stable can the pentanitrogen cation be in kinetics?. <i>Chemical Communications</i> , 2021, 57, 4432-4435.	2.2	2
11300	Manganese complexes with chelating and bridging di-triazolylidene ligands: synthesis and reactivity. <i>Dalton Transactions</i> , 2021, 50, 5911-5920.	1.6	10
11301	Gaussian Basis Sets for Solid State Calculations. <i>Lecture Notes in Quantum Chemistry II</i> , 2021, , 157-181.	0.3	5
11302	Climbing to the Top of Mount Fuji: Uniting Theory and Observations of Oxygen Triple Isotope Systematics. <i>Reviews in Mineralogy and Geochemistry</i> , 2021, 86, 97-135.	2.2	8
11303	Tuning the hyperconjugative aromaticity in Au(ⁱⁱⁱ)-substituted indoliums. <i>Dalton Transactions</i> , 2021, 50, 8096-8101.	1.6	6
11304	Evaluation of nine condensed-phase force fields of the GROMOS, CHARMM, OPLS, AMBER, and OpenFF families against experimental cross-solvation free energies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13055-13074.	1.3	9
11305	Understanding the reaction mechanism of gold-catalyzed reactions of 2,1-benzisoxazoles with propiolates and ynamides. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3342-3353.	2.3	3
11306	Heterometallic Molecular Clusters Featuring Triple Bonds Between Uranium and Transition Metals. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0

#	ARTICLE	IF	CITATIONS
11307	Carbon nanohorns as nanocontainers for cisplatin: insight into their interaction with the plasma membranes of normal and breast cancer cells. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16376-16389.	1.3	6
11308	Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double- ζ Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. <i>Australian Journal of Chemistry</i> , 2021, , .	0.5	2
11309	Hantzsch Ester-Mediated Photochemical Transformations in the Ketone Series: Remote C(sp ³) ³ Arylation and Cyclopentene Synthesis through Strain Release. <i>Journal of Organic Chemistry</i> , 2021, 86, 3232-3248.	1.7	9
11310	Computational study of 4,4-dimethoxy triphenylamine donor linked with low band gap π -spacers by single and double bonds for DSSC applications. <i>New Journal of Chemistry</i> , 2021, 45, 16989-17001.	1.4	5
11311	Characteristic activity of phosphorous acid in the dehydration condensation of a chitin-derived nitrogen-containing sugar alcohol. <i>Green Chemistry</i> , 2021, 23, 7228-7234.	4.6	7
11312	Theoretical study of the NHC-catalyzed C=S bond cleavage and reconstruction reaction: mechanism, stereoselectivity, and role of catalysts. <i>Organic Chemistry Frontiers</i> , 2021, 8, 5352-5360.	2.3	16
11313	Can a gas phase contact ion pair containing a hydrocarbon carbocation be formed in the ground state?. <i>RSC Advances</i> , 2021, 11, 4221-4230.	1.7	4
11314	Benchmark <i>ab initio</i> proton affinity of glycine. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9663-9671.	1.3	9
11315	Design of robust 2,2-bipyridine ligand linkers for the stable immobilization of molecular catalysts on silicon(111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9921-9929.	1.3	6
11316	Exploring the redox decomposition of ethylene carbonate \rightarrow propylene carbonate in Li-ion batteries. <i>Materials Advances</i> , 2021, 2, 1747-1751.	2.6	18
11317	Catalyzed reaction of isocyanates (RNCO) with water. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18535-18546.	1.3	6
11318	Catalytic and non-catalytic hydroboration of carbonyls: quantum-chemical studies. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 3004-3015.	1.5	7
11319	Theoretical insight on antioxidant potency of kanzakiflavone-2 and its derivatives. <i>Structural Chemistry</i> , 2021, 32, 1451-1458.	1.0	1
11320	Impact of tensile and compressive forces on the hydrolysis of cellulose and chitin. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15908-15916.	1.3	15
11321	An Introduction and Overview of Basis Sets for Molecular and Solid-State Calculations. <i>Lecture Notes in Quantum Chemistry II</i> , 2021, , 1-16.	0.3	3
11322	Acenes and phenacenes in their lowest-lying triplet states. Does kinked remain more stable than straight?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13574-13582.	1.3	18
11323	Physico-chemical properties of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) diazonium ion: a theoretical investigation. <i>RSC Advances</i> , 2021, 11, 26750-26762.	1.7	0
11324	Formation of atmospheric molecular clusters from organic waste products and sulfuric acid molecules: a DFT study. <i>Environmental Science Atmospheres</i> , 2021, 1, 267-275.	0.9	2

#	ARTICLE	IF	CITATIONS
11325	Mechanistic Insights into Selective Hydrogenation of C=C Bonds Catalyzed by CCC Cobalt Pincer Complexes: A DFT Study. <i>Catalysts</i> , 2021, 11, 168.	1.6	4
11326	Modular Counter-Fischer Indole Synthesis through Radical-Enolate Coupling. <i>Organic Letters</i> , 2021, 23, 1096-1102.	2.4	11
11327	Hetero-Diels Alder reactions of 2H-phospholes with allenes: synthesis and functionalization of 6-methylene-1-phosphanorbornenes. <i>Organic Chemistry Frontiers</i> , 2021, 8, 3740-3745.	2.3	10
11328	Differences between Gaussian and GAMESS Basis Sets (II) 6-31G and 6-31G*. <i>Journal of Computer Chemistry Japan -International Edition</i> , 2021, 7, n/a.	0.2	1
11329	Reactive force fields for modeling oxidative degradation of organic matter in geological formations. <i>RSC Advances</i> , 2021, 11, 29298-29307.	1.7	6
11330	Hydrogen bond donor functionalized poly(ionic liquid)s for efficient synergistic conversion of CO ₂ to cyclic carbonates. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2005-2014.	1.3	37
11331	Solvent effect on xylose-to-furfural reaction in biphasic systems: combined experiments with theoretical calculations. <i>Green Chemistry</i> , 2021, 23, 8510-8518.	4.6	41
11332	Paramagnetic solid-state NMR assignment and novel chemical conversion of the aldehyde group to dihydrogen <i>ortho</i> ester and hemiacetal moieties in copper(II)- and cobalt(II)-pyridinecarboxaldehyde complexes. <i>RSC Advances</i> , 2021, 11, 20216-20231.	1.7	9
11333	Hydrogenation of Cyclic 1,3-Diones to Their 1,3-Diols Using Heterogeneous Catalysts: Toward a Facile, Robust, Scalable, and Potentially Bio-Based Route. <i>ACS Omega</i> , 2021, 6, 4313-4328.	1.6	4
11334	A computational approach to understand the role of metals and axial ligands in artificial heme enzyme catalyzed C-H insertion. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9500-9511.	1.3	15
11335	Theoretical inspection of the spin-crossover [Fe(tzpy) ₂ (NCS) ₂] complex on Au(100) surface. <i>Journal of Chemical Physics</i> , 2021, 154, 034701.	1.2	6
11336	Role of substituents in the Hofmann Löffler Freytag reaction. A quantum-chemical case study on nicotine synthesis. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 854-865.	1.5	4
11337	Cyclic polylactide synthesis initiated by a lithium anthraquinoid: understanding the selectivity through DFT and diffusion NMR. <i>Polymer Chemistry</i> , 2021, 12, 4083-4092.	1.9	4
11338	The complex between molecular oxygen and an organic molecule: modeling optical transitions to the intermolecular charge-transfer state. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15038-15048.	1.3	6
11339	Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light. <i>BBA Advances</i> , 2021, 1, 100019.	0.7	6
11340	Benchmarking Antioxidant-Related Properties for Gallic Acid through the Use of DFT, MP2, CCSD, and CCSD(T) Approaches. <i>Journal of Physical Chemistry A</i> , 2021, 125, 198-208.	1.1	49
11341	Electroanalytical profiling of cocaine samples by means of an electropolymerized molecularly imprinted polymer using benzocaine as the template molecule. <i>Analyst</i> , 2021, 146, 1747-1759.	1.7	12
11342	C _N -Coupled naphthylisoquinoline alkaloids: a versatile new class of axially chiral natural products. <i>Natural Product Reports</i> , 2021, 38, 2154-2186.	5.2	24

#	ARTICLE	IF	CITATIONS
11343	Understanding polyoxometalates as water oxidation catalysts through iron vs. cobalt reactivity. <i>Chemical Science</i> , 2021, 12, 8755-8766.	3.7	23
11344	Reactivity of 1,3-dichloro-1,3-bis(dimethylamino)-propenium salts with primary amines. <i>New Journal of Chemistry</i> , 2021, 45, 13558-13570.	1.4	2
11345	Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. <i>Inorganic Chemistry</i> , 2021, 60, 807-815.	1.9	5
11346	trans-cis Photoisomerization of a biomimetic cyclocurcumin analogue rationalized by molecular modelling. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 12842-12849.	1.3	12
11347	Ruthenium(II)-catalyzed regioselective direct C4- and C5-diamidation of indoles and mechanistic studies. <i>Chemical Science</i> , 2021, 12, 11427-11437.	3.7	11
11348	Imaging intramolecular hydrogen migration with time- and momentum-resolved photoelectron diffraction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20174-20182.	1.3	11
11349	Host-Guest Complexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone). <i>Journal of Physical Chemistry A</i> , 2021, 125, 536-542.	1.1	6
11350	Tuning the reduction potentials of benzoquinone through the coordination to Lewis acids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9822-9831.	1.3	6
11351	Influence of the Solvent Environment on the Ultrafast Relaxation Pathways of a Sunscreen Molecule Diethylamino Hydroxybenzoyl Hexyl Benzoate. <i>Journal of Physical Chemistry A</i> , 2021, 125, 636-645.	1.1	20
11352	Pyromellitic-Based Low Molecular Weight Gelators and Computational Studies of Intermolecular Interactions: A Potential Additive for Lubricant. <i>Langmuir</i> , 2021, 37, 2954-2962.	1.6	15
11353	Optoelectronic properties of diketopyrrolopyrrole homopolymers compared to donor-acceptor copolymers. <i>Journal of Chemical Physics</i> , 2021, 154, 054309.	1.2	2
11354	Computational mechanistic studies of the carbon-carbon double bond difunctionalization via epoxidation and subsequent aminolysis in vegetable oils. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26609.	1.0	1
11355	Zeolite catalyzed hydroarylation of alkenes with aromatic amines under organic ligand-free conditions. <i>Journal of Catalysis</i> , 2021, 394, 18-29.	3.1	6
11356	Quadrupole Moment Induced Morphology Control Via a Highly Volatile Small Molecule in Efficient Organic Solar Cells. <i>Advanced Functional Materials</i> , 2021, 31, 2010535.	7.8	55
11357	HMNTA Complexes of Tetravalent Metal Ions: On the Roles of Carbonyl Oxygen and Amine Nitrogen in the Stabilization of Gas-Phase M(HMNTA) ₂ ⁴⁺ Complexes. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 700-706.	1.2	2
11358	Scale factors of Gaussian type orbitals optimized in molecule's local environments. <i>Chemical Physics Letters</i> , 2021, 765, 138285.	1.2	3
11359	Imidazole-containing photoinitiators for fabrication of sub-micron structures by 3D two-photon polymerization. <i>European Polymer Journal</i> , 2021, 145, 110209.	2.6	11
11360	Collision-induced dissociation of protonated fentanyl: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113117.	1.1	5

#	ARTICLE	IF	CITATIONS
11361	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	6.2	84
11362	Spinâ€projected QM/MM Free Energy Simulations for Oxidation Reaction of Guanine in BâˆDNA by Singlet Oxygen. ChemPhysChem, 2021, 22, 561-568.	1.0	5
11363	Computationalâ€driven synthesis of pentothal sodium. International Journal of Quantum Chemistry, 2021, 121, e26624.	1.0	0
11364	Effect of varying the TD-Ic-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. Journal of Chemical Physics, 2021, 154, 054102.	1.2	9
11365	Explicit environmental and vibronic effects in simulations of linear and nonlinear optical spectroscopy. Journal of Chemical Physics, 2021, 154, 084116.	1.2	10
11366	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101.	1.2	70
11367	The role of precursor decomposition in the formation of samarium doped ceria nanoparticles via solid-state microwave synthesis. SN Applied Sciences, 2021, 3, 1.	1.5	1
11368	Synthesis, crystal structure, Hirshfeld surface analysis and energy framework calculations of <i>trans</i>-3,7,9-tetramethyl-10-(prop-2-yn-1-yl)-1,2,3,4,4a,9,9a,10-octahydroacridine. Acta Crystallographica Section E: Crystallographic Communications, 2021, 77, 226-232.	0.2	0
11369	Effective suppression of conductance in multichannel molecular wires. Cell Reports Physical Science, 2021, 2, 100342.	2.8	8
11370	3,4-Methylenedioxypropylvalerone (MDPV) Sensing Based on Electropolymerized Molecularly Imprinted Polymers on Silver Nanoparticles and Carboxylated Multi-Walled Carbon Nanotubes. Nanomaterials, 2021, 11, 353.	1.9	10
11371	High throughput virtual screening of 230 billion molecular solar heat battery candidates. PeerJ Physical Chemistry, 0, 3, e16.	0.0	15
11372	Quantum Simulations of Hydrogen Bonding Effects in Glycerol Carbonate Electrolyte Solutions. Journal of Physical Chemistry B, 2021, 125, 2157-2166.	1.2	7
11373	Use of Imidazo[1,5-a]pyridinâ€acylidene as a Platform for Metalâ€imidazole Cooperative Catalysis: Silverâ€Catalyzed Cyclization of Alkyneâ€Tethered Carboxylic Acids. Advanced Synthesis and Catalysis, 2021, 363, 1631-1637.	2.1	5
11374	Beryllium (II) Chloride Complexes with Phosphoryl Ligands: A DFT Study. International Research Journal of Pure and Applied Chemistry, 0, , 38-46.	0.2	0
11375	Colloidal CdSe nanocrystals are inherently defective. Nature Communications, 2021, 12, 890.	5.8	22
11376	Computational exploration of Î±-lactone rearrangements and the cyclic halonium zwitterion from bromination of acrylate anion in water: Implicit vs. explicit solvation. Tetrahedron, 2021, 84, 131989.	1.0	0
11377	A Water/Toluene Biphasic Medium Improves Yields and Deuterium Incorporation into Alcohols in the Transfer Hydrogenation of Aldehydes. European Journal of Inorganic Chemistry, 2021, 2021, 1358-1372.	1.0	0
11378	Direct Formation of Metal Layer on Anion Exchange Membrane Using Electroless Deposition Process. Electrochemistry, 2021, 89, 192-196.	0.6	3

#	ARTICLE	IF	CITATIONS
11379	When Does Fusing Two Rings Not Yield a Larger Ring? The Curious Case of BOPHY. <i>Journal of Organic Chemistry</i> , 2021, 86, 4547-4556.	1.7	4
11380	Regioselective Synthesis of 1,2,3,4-Tetrasubstituted Arenes by Vicinal Functionalization of Arynes Derived from Aryl(Mes)iodonium Salts**. <i>Chemistry - A European Journal</i> , 2021, 27, 7168-7175.	1.7	21
11381	Balancing Cost and Accuracy in Quantum Mechanical Simulations on Collagen Protein Models. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2566-2574.	2.3	9
11382	Engineering couplings for exciton transport using synthetic DNA scaffolds. <i>CheM</i> , 2021, 7, 752-773.	5.8	50
11383	Systematic Detection and Characterization of Hydrogen Bonding in Proteins via Local Vibrational Modes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2551-2565.	1.2	15
11384	Theoretical Determination of Binding Energies of Small Molecules on Interstellar Ice Surfaces. <i>Frontiers in Astronomy and Space Sciences</i> , 2021, 8, .	1.1	20
11385	Geometric, optical, and phosphorescent properties of cationic Ir(III) and Rh(III) complexes with cyclometalated ligands: DFT/TDDFT investigations. <i>Monatshefte für Chemie</i> , 2021, 152, 315-322.	0.9	2
11386	C=C versus C-H Activation: Understanding How the Carbene π -Accepting Ability Controls the Intramolecular Reactivities of Mono(carbene)-Stabilized Borylenes. <i>Organometallics</i> , 2021, 40, 766-775.	1.1	8
11387	Confinement of the antitumoral drug cisplatin inside edge-functionalized carbon nanotubes and its release near lipid membrane. <i>European Physical Journal D</i> , 2021, 75, 1.	0.6	4
11388	Understanding the Effectiveness of Phospholane Electrolyte Additives in Lithium-Ion Batteries under High-Voltage Conditions. <i>ChemElectroChem</i> , 2021, 8, 972-982.	1.7	5
11389	Theoretical Study of closo-Borate Anions $[B_nH_n]^{2-}$ ($n = 5-12$): Bonding, Atomic Charges, and Reactivity Analysis. <i>Symmetry</i> , 2021, 13, 464.	1.1	21
11390	Dynamic Effects in Intramolecular Schmidt Reactions: Entropy, Electrostatic Drag, and Selectivity Prediction. <i>ChemPhysChem</i> , 2021, 22, 649-656.	1.0	2
11391	Ultrafast Charge Transfer Dynamics at the Origin of Photoconductivity in Doped Organic Solids. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7086-7096.	1.5	4
11392	QM-Cluster Model Study of the Guaiacol Hydrogen Atom Transfer and Oxygen Rebound with Cytochrome P450 Enzyme GcoA. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3296-3306.	1.2	13
11393	Conformational Dependence of Triplet Energies in Rotationally Hindered N- and S-Heterocyclic Dimers: New Design and Measurement Rules for High Triplet Energy OLED Host Materials. <i>Chemistry - A European Journal</i> , 2021, 27, 6545-6556.	1.7	29
11394	Intermediate state representation approach to physical properties of molecular electron-attached states: Theory, implementation, and benchmarking. <i>Journal of Chemical Physics</i> , 2021, 154, 104117.	1.2	15
11395	Thermochemical and Quantum Descriptor Calculations for Gaining Insight into Ricin Toxin A (RTA) Inhibitors. <i>ACS Omega</i> , 2021, 6, 8764-8777.	1.6	6
11396	Anion-Radical Polymerization of Sulfur- and Selenium-Substituted N-Type Conjugated Polymers. <i>Macromolecules</i> , 2021, 54, 3130-3138.	2.2	7

#	ARTICLE	IF	CITATIONS
11397	Indene Derived Phosphorusâ€”Thioether Ligands for the Irâ€”Catalyzed Asymmetric Hydrogenation of Olefins with Diverse Substitution Patterns and Different Functional Groups. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 4561-4574.	2.1	12
11398	Highly Sterically Encumbered Gold Acyclic Diaminocarbene Complexes: Overriding Electronic Control in Regiodivergent Gold Catalysis. <i>Organometallics</i> , 2021, 40, 1416-1433.	1.1	10
11399	Development of a Radical Silylzincation of (Het)Arylâ€”Substituted Alkynes and Computational Insights into the Origin of the <i>trans</i> -â€”Stereoselectivity. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 2634-2647.	2.1	9
11400	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. <i>ChemPhysChem</i> , 2021, 22, 788-795.	1.0	1
11401	Peripherally octamethyl zinc(II) phthalocyanines with various axial substituents. <i>Polyhedron</i> , 2021, 197, 115024.	1.0	5
11402	Implications for an Imidazole-2-yl Carbene Intermediate in the Rhodanase-Catalyzed Câ€”S Bond Formation Reaction of Anaerobic Ergothioneine Biosynthesis. <i>ACS Catalysis</i> , 2021, 11, 3319-3334.	5.5	12
11403	Synchronized Câ€”H Activations at Proximate Dinuclear Pd ²⁺ Sites on Silicotungstate for Oxidative Câ€”C Coupling. <i>ACS Catalysis</i> , 2021, 11, 3455-3465.	5.5	3
11404	Catalytic mechanism and endo-to-exo selectivity reversion of an octalin-forming natural Dielsâ€”Alderase. <i>Nature Catalysis</i> , 2021, 4, 223-232.	16.1	35
11405	A revised formulation of the generalized subsystem vibrational analysis (GSVA). <i>Theoretical Chemistry Accounts</i> , 2021, 140, 31.	0.5	6
11406	Mechanistic insight into the fluorescence activity of forensic fingerprinting reagents. <i>Journal of Chemical Physics</i> , 2021, 154, 124313.	1.2	3
11407	Smooth potential-energy surfaces in fragmentation-based local correlation methods for periodic systems. <i>Molecular Physics</i> , 2021, 119, e1896046.	0.8	0
11408	MgZnO Dual Gate Thin Film Transistor for the Sensitive Determination of Modified Folic Acid. <i>IEEE Sensors Journal</i> , 2021, 21, 7242-7249.	2.4	1
11409	Mechanistic Insights into the Nickel-Catalyzed Regioselective Carboxylation of Allylic Alcohols. <i>Organometallics</i> , 2021, 40, 869-879.	1.1	15
11410	Determination of Triplet State Energy and the Absorption Spectrum for a Lanthanide Complex. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7022-7033.	1.5	13
11411	A nitrogen-rich covalent organic framework for simultaneous dynamic capture of iodine and methyl iodide. <i>CheM</i> , 2021, 7, 699-714.	5.8	197
11412	Substituent effect on emission of flavonolate-boron difluoride complexes: The role of ï€-system for dual-state (solution and solid) emission. <i>Dyes and Pigments</i> , 2021, 187, 109081.	2.0	17
11413	DFT Study on the Electrocatalytic Reduction of CO ₂ to CO by a Molecular Chromium Complex. <i>Inorganic Chemistry</i> , 2021, 60, 3635-3650.	1.9	18
11414	Free Radical Isomerizations in Acetylene Bromoboration Reaction. <i>Molecules</i> , 2021, 26, 2501.	1.7	1

#	ARTICLE	IF	CITATIONS
11415	Hydrogen Bonding in Natural and Unnatural Base Pairs—A Local Vibrational Mode Study. <i>Molecules</i> , 2021, 26, 2268.	1.7	26
11416	One-Pot Synthesis of Tertiary Amides from Organic Trichlorides through Oxygen Atom Incorporation from Air by Convergent Paired Electrolysis. <i>Journal of Organic Chemistry</i> , 2021, 86, 5983-5990.	1.7	20
11417	Isolated boron in zeolite for oxidative dehydrogenation of propane. <i>Science</i> , 2021, 372, 76-80.	6.0	155
11418	Koopmans's Type Theorem in Kohn-Sham Theory with Optimally Tuned Long-Range-Corrected (LC) Functionals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3489-3502.	1.1	16
11419	Stereoselective protonation of 2-methyl-1-tetralone lithium enolate catalyzed by salan-type diamines. <i>Tetrahedron</i> , 2021, 86, 132085.	1.0	2
11420	Tribological behavior of stainless steel in sulfuric acid in the presence of <i>Thymus zygis</i> subsp. <i>gracilis</i> essential oil: experimental and quantum chemical studies. <i>Corrosion Reviews</i> , 2021, 39, 279-295.	1.0	3
11421	Structure Elucidation and Confirmation of Phloroglucinols from the Roots of <i>Garcinia dauphinensis</i> by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. <i>Journal of Natural Products</i> , 2021, 84, 1163-1174.	1.5	2
11422	Total Synthesis and Computational Investigations of Sesquiterpene-Tropolones Ameliorate Stereochemical Inconsistencies and Resolve an Ambiguous Biosynthetic Relationship. <i>Journal of the American Chemical Society</i> , 2021, 143, 6006-6017.	6.6	32
11423	A general RNA force field: comprehensive analysis of energy minima of molecular fragments of RNA. <i>Journal of Molecular Modeling</i> , 2021, 27, 137.	0.8	1
11424	Revisited the reaction mechanism of cobalt catalyzed [3+2] cycloaddition reactions between the derivatives of cyclopropanols and allenes: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2021, 937, 121744.	0.8	4
11425	Molecular engineering of near-infrared active boron dipyrromethene moiety with various donors and acceptors for tuning the absorption behavior and electron injection of the resultant dyes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 410, 113161.	2.0	12
11426	Non-adiabatic dynamic of atmospheric unimolecular photochemical reactions of 4,4-difluoroacrolein using TD-DFT and TSH approaches. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26663.	1.0	2
11427	Theoretical Studies on the Electronic Structure of Nano-graphenes for Applications in Nonlinear Optics. <i>Chemical Research in Chinese Universities</i> , 2022, 38, 579-587.	1.3	6
11428	C-N and C-H Activation of an N-Heterocyclic Carbene by Magnesium(II) Hydride and Magnesium(I) Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 6065-6072.	1.9	5
11429	Reactive Metabolites from Thiazole-Containing Drugs: Quantum Chemical Insights into Biotransformation and Toxicity. <i>Chemical Research in Toxicology</i> , 2021, 34, 1503-1517.	1.7	13
11430	Manganese-Catalyzed Hydrogenation of Ketones under Mild and Base-free Conditions. <i>Organometallics</i> , 2021, 40, 1388-1394.	1.1	31
11431	Snapshots of the Fragmentation for C70@Single-Walled Carbon Nanotube: Tight-Binding Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3929.	1.8	3
11432	Boronic Acids as Prospective Inhibitors of Metallo- β -Lactamases: Efficient Chemical Reaction in the Enzymatic Active Site Revealed by Molecular Modeling. <i>Molecules</i> , 2021, 26, 2026.	1.7	11

#	ARTICLE	IF	CITATIONS
11433	Effects of Structural Dynamics on Charge Carrier Transfer in B-DNA: A Combined MD and RT-TDDFT Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3986-4003.	1.2	8
11434	Selective, Base-Free Hydrogenation of Aldehydes Catalyzed by Ir Complexes Based on Proton-Responsive Lutidine-Derived CNP Ligands. <i>Organometallics</i> , 2021, 40, 1314-1327.	1.1	12
11435	Structure and phase transition in 1-(diaminomethylene)thiourea-1-ium m-nitrobenzoate monohydrate and the structure of its anhydrous deuterated analogue. <i>Journal of Molecular Structure</i> , 2021, 1230, 129626.	1.8	5
11436	Unitary coupled-cluster approach for the calculation of core-excited states and x-ray absorption spectra. <i>Journal of Chemical Physics</i> , 2021, 154, 154108.	1.2	4
11437	Structures and Conducting Properties of Molecular Conductors Based on Dimethyl-Substituted DTDA-TTP and DTDH-TTP. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 1273-1284.	2.0	3
11438	Effects of Magnesium, Calcium, and Aluminum Chelation on Fluoroquinolone Absorption Rate and Bioavailability: A Computational Study. <i>Pharmaceutics</i> , 2021, 13, 594.	2.0	15
11439	Structure-property study of pristine and dehydrofluorinated poly(vinylidene fluoride) using density functional theory. <i>Monatshefte für Chemie</i> , 2021, 152, 559-567.	0.9	4
11440	Zn(II) complexes of substituted oxyacridinate ligands. Synthesis, structure and properties. <i>Journal of Molecular Structure</i> , 2021, 1229, 129798.	1.8	2
11441	Palladium-Catalyzed Regioselective and Stereospecific Ring-Opening Suzuki-Miyaura Arylative Cross-Coupling of 2-Arylazetidines with Arylboronic Acids. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 2796-2805.	2.1	6
11442	Synthesis of uranium complexes incorporating extended azo-imine ligands: Molecular and electronic structure. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100049.	1.3	0
11443	Reaction of Singlet Oxygen with the Ethylene Group: Implications for Electrolyte Stability in Li-Ion and Li-O ₂ Batteries. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2876-2884.	1.1	13
11444	Chemical, spectroscopic characterization, molecular modeling and antibacterial activity assays of a silver (I) complex with succinic acid. <i>Ecletica Quimica</i> , 2021, 46, 26-35.	0.2	6
11445	Organic Conductors with Narrow Bandwidth Based on 2-(Pyran-4-ylidene)-1,3-dithiole. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 1331-1339.	2.0	2
11446	Application of the Molecular Invariom Model for the Study of Interactions Involving Fluorine Atoms in the $\{Yb\}_2\{Zr\}_2\{Al\}_2\{O\}_{42}OCH(CF_3)_2\{OCH(CF_3)_2\}_3\{OCH(CF_3)_2\}_2YbIII(OCH(CF_3)_2)_2(THF)(Et_2O)\}$ Complex. <i>Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya</i> , 2021, 47, 235-243.	0.3	3
11447	On the Mechanism of Dimerization of Stable Organic Radicals. <i>Russian Journal of Organic Chemistry</i> , 2021, 57, 506-514.	0.3	1
11448	The density polarization reveals directions of electron displacements due to the substituent effect: Analysis performed on a metal-organic Mo=Oxo catalyst. <i>Journal of Computational Chemistry</i> , 2021, 42, 1118-1125.	1.5	0
11449	Quantum chemical calculation studies toward microscopic understanding of retention mechanism of Cs radioisotopes and other alkali metals in lichens. <i>Scientific Reports</i> , 2021, 11, 8228.	1.6	7
11450	New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. <i>Structural Chemistry</i> , 2021, 32, 2019-2033.	1.0	1

#	ARTICLE	IF	CITATIONS
11451	Discovery of Non-Isolated-Pentagon-Rule Fullerenes from Computational Characterization of U2O@C72. <i>Inorganic Chemistry</i> , 2021, 60, 6492-6502.	1.9	6
11452	Two Excited State Collaboration of Heteroleptic Ir(III)-Coumarin Complexes for H2 Evolution Dye-Sensitized Photocatalysts. <i>Energies</i> , 2021, 14, 2425.	1.6	4
11453	Metal diffusion model in polymer matrices in vapor phase infiltration. <i>Japanese Journal of Applied Physics</i> , 2021, 60, SCCC04.	0.8	5
11454	The thermochemical, structural, and spectroscopic analyses of the tautomers of sulfur and selenium modified emissive nucleobases. <i>Canadian Journal of Chemistry</i> , 2021, 99, 390-396.	0.6	0
11455	Effect of H ₂ O Molecules on the CO ₂ Replacement in CH ₄ Hydrate Behavior by Molecular Simulation. <i>Energy & Fuels</i> , 2021, 35, 8126-8140.	2.5	8
11456	Paving the Way to the First Functional Fulgide@MOF Hybrid Materials. <i>Chemistry of Materials</i> , 2021, 33, 3757-3766.	3.2	17
11457	Accurate prediction of the properties of materials using the CAM-B3LYP density functional. <i>Journal of Computational Chemistry</i> , 2021, 42, 1486-1497.	1.5	35
11458	Automating the IRC Analysis within Eyringpy. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26684.	1.0	7
11459	Efficient Open-Source Implementations of Linear-Scaling Polarizable Embedding: Use Octrees to Save the Trees. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3445-3454.	2.3	7
11460	Structural and Electronic Properties of Iron(0) PNP Pincer Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021, 647, 1429-1435.	0.6	2
11461	Reaction of a Molybdenum Bis(dinitrogen) Complex with Carbon Dioxide: A Combined Experimental and Computational Investigation. <i>Inorganic Chemistry</i> , 2021, 60, 7708-7718.	1.9	2
11462	Direct Dynamics Trajectories Reveal Nonstatistical Coordination Intermediates and Demonstrate that η^5 and η^6 -Coordination Are Not Required for Rhenium(I)-Mediated Ethylene C-H Activation. <i>Journal of the American Chemical Society</i> , 2021, 143, 8367-8374.	6.6	15
11463	The use of minimal topological differences to inspire the design of novel tetrahydroisoquinoline analogues with antimalarial activity. <i>Heliyon</i> , 2021, 7, e07032.	1.4	0
11464	Protecting Benzylic C-H Bonds by Deuteration Doubles the Operational Lifetime of Deep-Blue Ir-Phenylimidazole Dopants in Phosphorescent OLEDs. <i>Advanced Optical Materials</i> , 2021, 9, 2100630.	3.6	44
11465	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3599-3617.	2.3	6
11466	A guide to benchmarking enzymatically catalysed reactions: the importance of accurate reference energies and the chemical environment. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	6
11467	Molecularly Imprinted Polymer (MIP) for thiamethoxam: A theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2021, 1231, 129980.	1.8	32
11468	The chemical reactivity and QSPR of organic compounds applied to dye-sensitized solar cells using DFT. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107852.	1.3	1

#	ARTICLE	IF	CITATIONS
11469	Constructing photochromic diarylethene with NIR-absorption beyond 800 nm. <i>Dyes and Pigments</i> , 2021, 189, 109273.	2.0	3
11470	Mechanism of Oxidative Ring Closure as Part of the Hygromycin Biosynthesis Step by a Nonheme Iron Dioxygenase. <i>ChemCatChem</i> , 2021, 13, 3054-3066.	1.8	13
11471	Seven- and eight-coordinate lanthanide(III) amidophosphate complexes: synthesis, characterization and photoluminescence. <i>Journal of Coordination Chemistry</i> , 2021, 74, 1466-1481.	0.8	4
11472	Effect of the aniline fragment in Pt(II) and Pt(IV) complexes as anti-proliferative agents. Standard reduction potential as a more reliable parameter for Pt(IV) compounds than peak reduction potential. <i>Journal of Inorganic Biochemistry</i> , 2021, 218, 111403.	1.5	7
11473	Thermal Degradation and Bimolecular Decomposition of 2-Ethoxyethanol in Binary Ethanol and Isobutanol Solvent Mixtures: A Computational Mechanistic Study. <i>ACS Omega</i> , 2021, 6, 13365-13374.	1.6	1
11474	In(III)-Catalyzed Direct Regioselective Syntheses of 1-Naphthaldehyde Derivatives via a Hidden Aldehyde 1,3-Translocation and Disjointed CO ₂ Extrusion. <i>ACS Catalysis</i> , 2021, 11, 6467-6473.	5.5	6
11475	Combined MD and QM/MM Investigations of Hydride Reduction of 5 α -Dihydrotestosterone Catalyzed by Human 3 α -Hydroxysteroid Dehydrogenase Type 3: Importance of Noncovalent Interactions. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4998-5008.	1.2	4
11476	Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4258-4265.	1.1	11
11477	DFT Approach for Predicting ¹³ C NMR Shifts of Atoms Directly Coordinated to Nickel. <i>Organometallics</i> , 2021, 40, 1614-1625.	1.1	8
11478	Predicting Dinitrogen Activation via Transition-Metal-Involved [4+2] Cycloaddition Reaction. <i>Chemistry - an Asian Journal</i> , 2021, 16, 1626-1633.	1.7	13
11479	Mechanistic Insights into Activation of Carbon Monoxide, Carbon Dioxide, and Nitrous Oxide by Acyclic Silylene. <i>Inorganic Chemistry</i> , 2021, 60, 8998-9007.	1.9	6
11480	Organic molecules with inverted gaps between first excited singlet and triplet states and appreciable fluorescence rates. <i>Matter</i> , 2021, 4, 1654-1682.	5.0	67
11481	Dyes with tunable absorption properties from the visible to the near infrared range: 2,4,5,7-Tetranitrofluorene (TNF) as a unique electron acceptor. <i>Dyes and Pigments</i> , 2021, 189, 109250.	2.0	2
11482	Robust, Enantioselective Construction of Challenging, Biologically Relevant Tertiary Ether Stereocenters. <i>ACS Catalysis</i> , 2021, 11, 6325-6333.	5.5	17
11483	Factors Governing Selectivity of Dopamine Receptor Binding Compounds for D2R and D3R Subtypes. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2829-2843.	2.5	2
11484	Role of hydrogen bond alternation and charge transfer states in photoactivation of the Orange Carotenoid Protein. <i>Communications Biology</i> , 2021, 4, 539.	2.0	30
11485	<i>In vitro</i> investigation of biophysical interactions between Ag(I) complexes of bis(methyl)(thia/selena)salen and ctDNA via multi-spectroscopic, physicochemical and molecular docking methods along with cytotoxicity study. <i>Luminescence</i> , 2021, 36, 1277-1284.	1.5	2
11486	NO Reduction to N ₂ O Triggered by a Dinuclear Dinitrosyl Iron Complex via the Associated Pathways of Hyponitrite Formation and NO Disproportionation. <i>Inorganic Chemistry</i> , 2021, 60, 15874-15889.	1.9	10

#	ARTICLE	IF	CITATIONS
11487	Nucleophilic Reactions of Osmanaphthalynes with PMe_3 and H_2O . Chemistry - A European Journal, 2021, 27, 9328-9335.	1.7	7
11488	DFT insights into the structure, reactivity and radical scavenging activity of cycloartocarpesin. Journal of Physical Organic Chemistry, 2021, 34, e4245.	0.9	5
11489	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. Chemical Physics Letters, 2021, 771, 138550.	1.2	2
11490	Redox-active binary eutectics: Preparation and their electrochemical properties. Electrochemistry Communications, 2021, 126, 107028.	2.3	3
11491	Synthetic and Computational Studies on Rh^{III} -Catalyzed Redox-Neutral Cascade of Carbenoid Functionalization and Dephosphonylative Annulation. Journal of Organic Chemistry, 2021, 86, 7069-7077.	1.7	13
11492	Ultrafast time-resolved x-ray absorption spectroscopy of ionized urea and its dimer through <i>ab initio</i> nonadiabatic dynamics. Structural Dynamics, 2021, 8, 034102.	0.9	3
11493	Metal-Free Deoxygenation of Amine $\text{N}=\text{O}$ Oxides: Synthetic and Mechanistic Studies. ChemPhysChem, 2021, 22, 1237-1242.	1.0	2
11494	A Key Piece in the Global N-Cycle: The $\text{N}=\text{N}$ Bond Formation Presented by Heme-Dependent Hydrazine Synthase. ACS Catalysis, 2021, 11, 6489-6498.	5.5	9
11495	Linear and Helical Carbonic Acid Clusters. Journal of Physical Chemistry A, 2021, 125, 4589-4597.	1.1	3
11496	Accurate Electronic Excitation Energies in Full-Valence Active Space via Bootstrap Embedding. Journal of Chemical Theory and Computation, 2021, 17, 3335-3347.	2.3	8
11497	NaBr -Assisted Photoelectrochemical and Photochemical Integrated Process for Isomerization of Maleate Esters to Fumarate Esters. ACS Sustainable Chemistry and Engineering, 2021, 9, 6886-6893.	3.2	5
11498	Soluble polymers with intrinsic porosity for efficient removal of phenolic compounds from water. Microporous and Mesoporous Materials, 2021, 319, 111068.	2.2	19
11499	Catalytic hydrolysis mechanism of aminocarboxylester substrate by human carboxylesterase 1: A theoretical study on methylphenidate hydrolysis. Computational and Theoretical Chemistry, 2021, 1199, 113198.	1.1	0
11500	The C5 -substituent effects on the formic acid-assisted tautomerization of protonated cytosine: A lower isomerization barrier and potential biological importance. Journal of Physical Organic Chemistry, 2021, 34, e4220.	0.9	0
11501	Substituent Effects on the Quantum Interference of Two-Center One-Electron Bonds: $[\text{B}_2\text{X}_6]^{+}$ ($\text{X} = \text{H}, \text{F}, \text{Cl}, \text{CN}, \text{OH}, \text{CH}_3$, and Tj) $\text{ETQ}000\text{rgBT}$ Overlock $10\text{Tf}5017$		
11502	The Emergence of Multiple Coordination Numbers in Gold-Cyanoarene Complexes: A Study of the On-Surface Coordination Mechanism. Journal of Physical Chemistry C, 2021, 125, 9937-9946.	1.5	6
11503	Intramolecular hydrogen-bonding effects on structural and electronic properties of pyrrole-furan derivatives: a density functional calculation. Optical and Quantum Electronics, 2021, 53, 1.	1.5	0
11504	Mechanisms of Co^{II} and Acid Jointly Catalyzed Domino Conversion of CO_2 , H_2 , and CH_3OH to Dialkoxymethane: A DFT Study. ACS Catalysis, 2021, 11, 6908-6919.	5.5	9

#	ARTICLE	IF	CITATIONS
11505	Cooperativity and Anticooperativity in Ion-Water Interactions: Implications for the Aqueous Solvation of Ions. <i>ChemPhysChem</i> , 2021, 22, 1269-1285.	1.0	10
11506	Highly Stereoselective Glycosylation Reactions of Furanoside Derivatives via Rhenium (V) Catalysis. <i>Journal of Organic Chemistry</i> , 2021, 86, 7672-7686.	1.7	3
11507	Synthesis and Photoswitching Properties of Bioinspired Dissymmetric β -Pyrone, an Analogue of Cyclocurcumin. <i>Journal of Organic Chemistry</i> , 2021, 86, 8112-8126.	1.7	12
11508	Broadening the Scope of the Zwitterionic 1,3-Diaza-Claisen Rearrangement through a Tethering Strategy. <i>Journal of Organic Chemistry</i> , 2021, 86, 8197-8215.	1.7	2
11509	The effects of protecting and acyl groups on the conformation of benzyl β -L-rhamnopyranosides: An in silico study. <i>Turkish Computational and Theoretical Chemistry</i> , 2021, 5, 39-50.	0.5	5
11510	Significant Enhancement of the Polarization Holographic Performance of Photopolymeric Materials by Introducing Graphene Oxide. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27500-27512.	4.0	25
11511	BOPYIN-anil and BOPYIN-boranil complex: Synthesis, spectroscopic properties and ESIPT process. <i>Journal of Porphyrins and Phthalocyanines</i> , 0, , A-H.	0.4	0
11512	Molecular Dynamics Simulations of a Cytochrome P450 from <i>Tepidiphilus thermophilus</i> (P450-TT) Reveal How Its Substrate-Binding Channel Opens. <i>Molecules</i> , 2021, 26, 3614.	1.7	4
11513	Development of Linear-Scaling Relativistic Quantum Chemistry Covering the Periodic Table. <i>Bulletin of the Chemical Society of Japan</i> , 2021, 94, 1664-1681.	2.0	5
11514	Structural insights of the conserved "priming loop" of hepatitis B virus pre-genomic RNA. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 9761-9773.	2.0	14
11515	Pathways to Metal-Ligand Cooperation in Quinoline-Based Titanium(IV) Pincers: Nonelectrophilic N-methylation, Deprotonation, and Dihydropyridine Formation. <i>Organometallics</i> , 2021, 40, 1838-1847.	1.1	2
11516	Electrocatalytic Water Oxidation by a Trinuclear Copper(II) Complex. <i>ACS Catalysis</i> , 2021, 11, 7223-7240.	5.5	35
11517	<i>In-Situ</i> -Generated Active Hf-hydride in Zeolites for the Tandem N-Alkylation of Amines with Benzyl Alcohol. <i>ACS Catalysis</i> , 2021, 11, 8049-8061.	5.5	29
11518	Development of a Tunable Chiral Pyridine Ligand Unit for Enantioselective Iridium-Catalyzed C-H Borylation. <i>ACS Catalysis</i> , 2021, 11, 7339-7349.	5.5	51
11519	Cations Derived from Fentanils Generated by Atmospheric Pressure Photoionization in the Presence of Ammonia: An IMS-MS Study. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 1700-1706.	1.2	0
11520	Boosted spintronic properties in triangular Si-based nanoflakes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 130, 114699.	1.3	11
11521	Catalytic asymmetric nucleophilic fluorination using $\text{BF}_3 \cdot \text{Et}_2\text{O}$ as fluorine source and activating reagent. <i>Nature Communications</i> , 2021, 12, 3957.	5.8	27
11522	Computational Chemistry: The Exciting Opportunities and the Boring Details. <i>Israel Journal of Chemistry</i> , 2022, 62, .	1.0	5

#	ARTICLE	IF	CITATIONS
11523	Generation, Characterization, and Dissociation of Radical Cations Derived from Prolyl-glycyl-glycine. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6121-6129.	1.2	1
11524	Multiwavelets applied to metal–ligand interactions: Energies free from basis set errors. <i>Journal of Chemical Physics</i> , 2021, 154, 214302.	1.2	5
11525	SAMPL7 blind challenge: quantum–mechanical prediction of partition coefficients and acid dissociation constants for small drug-like molecules. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 841-851.	1.3	10
11526	Evaluation of acrylamide-based molecularly imprinted polymer thin-sheets for specific protein capture—a myoglobin model. <i>Biomedical Physics and Engineering Express</i> , 2021, 7, 045025.	0.6	11
11527	Amphiphilic Pd@micro-organohydrogels with controlled wettability for enhancing gas-liquid-solid triphasic catalytic performance. <i>Nano Research</i> , 2022, 15, 557-563.	5.8	15
11528	Enzymatic N–N bond formation: Mechanism for the N-nitroso synthesis catalyzed by non-heme iron SznF enzyme. <i>Journal of Catalysis</i> , 2021, 398, 44-53.	3.1	7
11529	From Oligo(Phenyleneethynylene) Monomers to Supramolecular Helices: The Role of Intermolecular Interactions in Aggregation. <i>Molecules</i> , 2021, 26, 3530.	1.7	2
11530	Optical Response of Sila-Fullerenes in Interaction With Glycoproteins for Environmental Monitoring. <i>Frontiers in Physics</i> , 2021, 9, .	1.0	2
11531	Dissecting Transmetalation Reactions at the Molecular Level: Role of the Coordinated Anion in Gas-Phase Models for the Transmetalation Step of the Hiyama Cross-Coupling Reaction. <i>Organometallics</i> , 2021, 40, 1822-1829.	1.1	5
11532	Pseudo Jahn-Teller Origin of the Proton-transfer Energy Barrier in the Hydrogen-bonded [FHF]-System. <i>Chemistry Journal of Moldova</i> , 2021, 16, 115-120.	0.3	4
11533	Mechanistic Studies of the Pd- and Pt-Catalyzed Selective Cyclization of Propargyl/Allenyl Complexes. <i>Journal of Organic Chemistry</i> , 2021, 86, 9670-9681.	1.7	1
11534	Antioxidant properties of anthocyanin revealed through the hydrogen atom transfer: combined effects of temperature and pH *. <i>Molecular Physics</i> , 2021, 119, e1936246.	0.8	6
11535	A tautomeric ligand enables directed C–H hydroxylation with molecular oxygen. <i>Science</i> , 2021, 372, 1452-1457.	6.0	84
11536	Density Functional Theory Study into the Reaction Mechanism of Isonitrile Biosynthesis by the Nonheme Iron Enzyme ScoE. <i>Topics in Catalysis</i> , 2022, 65, 528-543.	1.3	8
11537	Inactivation Mechanism of Neuronal Nitric Oxide Synthase by (<i>S</i>)-2-Amino-5-(2-(methylthio)acetimidamido)pentanoic Acid: Chemical Conversion of the Inactivator in the Active Site. <i>Inorganic Chemistry</i> , 2021, 60, 9345-9358.	1.9	1
11538	Next Generation Cuprous Phenanthroline MLCT Photosensitizer Featuring Cyclohexyl Substituents. <i>Inorganic Chemistry</i> , 2021, 60, 8394-8403.	1.9	31
11539	Iron Redox Shuttles with Wide Optical Gap Dyes for High-Voltage Dye-Sensitized Solar Cells. <i>ChemSusChem</i> , 2021, 14, 3084-3096.	3.6	8
11540	Ionic Carbazole-Based Water-Soluble Two-Photon Photoinitiator and the Fabrication of Biocompatible 3D Hydrogel Scaffold. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27796-27805.	4.0	31

#	ARTICLE	IF	CITATIONS
11541	Theoretical insights about the possibility of removing Pb ²⁺ and Hg ²⁺ metal ions using adsorptive processes and matrices of carboxymethyl diethylaminoethyl cellulose and cellulose nitrate biopolymers. <i>Journal of Molecular Liquids</i> , 2021, 331, 115730.	2.3	17
11542	Electrostatic Perturbations from the Protein Affect C-H Bond Strengths of the Substrate and Enable Negative Catalysis in the TmpA Biosynthesis Enzyme. <i>Chemistry - A European Journal</i> , 2021, 27, 8851-8864.	1.7	20
11543	Perturbation approach to constrained electron transfer in density functional theory. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
11544	New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach. <i>Molecular Diversity</i> , 2022, 26, 1373-1381.	2.1	17
11545	A novel BODIPY-based fluorescent probe for sensitive and selective detection of nerve agent simulants through base-assisted photo-induced electron transfer process. <i>Sensors and Actuators B: Chemical</i> , 2021, 337, 129804.	4.0	17
11546	Direct Conversion of Alginate Oligo- and Polysaccharides into Biodegradable and Non-ecotoxic Anionic Furanic Surfactants: An Experimental and Mechanistic Study. <i>Advanced Sustainable Systems</i> , 2021, 5, 2100108.	2.7	5
11547	2-Phenylethyne-1-Sulfonamide Derivatives as New Drugs Candidates for Heat Shock Protein 70 and Doublecortin-like Kinase. <i>Turkish Computational and Theoretical Chemistry</i> , 2021, 5, 1-12.	0.5	2
11548	Efficient Molybdenum Hydrazonato Epoxidation Catalysts Operating under Green Chemistry Conditions: Water vs. Decane Competition. <i>Catalysts</i> , 2021, 11, 756.	1.6	3
11549	Temperature-dependent oxidation of BSCAPE molecule in methanol medium. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 105, 107850.	1.3	0
11550	Understanding Ball Milling Mechanochemical Processes with DFT Calculations and Microkinetic Modeling. <i>ChemSusChem</i> , 2021, 14, 2763-2768.	3.6	17
11551	Stabilization of Bicontinuous Cubic Phase and Its Two-sided Nature Produced by Use of Siloxane Tails and Introduction of Molecular Nonsymmetry. <i>Chemistry - A European Journal</i> , 2021, 27, 10293-10302.	1.7	2
11552	Telluracarboraphyrins and a Related Palladium(II) Complex: Evidence for Hypervalent Interactions. <i>Inorganic Chemistry</i> , 2021, 60, 9833-9847.	1.9	11
11553	Small Amount Makes a Big Difference: Critical (<i>n</i> - 1)d Valence Orbitals of Heavy Alkaline Earth Metals inside Cage Clusters. <i>Inorganic Chemistry</i> , 2021, 60, 8621-8630.	1.9	2
11554	Py-Macrodipa: A Janus Chelator Capable of Binding Medicinally Relevant Rare-Earth Radiometals of Disparate Sizes. <i>Journal of the American Chemical Society</i> , 2021, 143, 10429-10440.	6.6	30
11555	Degradation mechanism of tris(2-chloroethyl) phosphate (TCEP) as an emerging contaminant in advanced oxidation processes: A DFT modelling approach. <i>Chemosphere</i> , 2021, 273, 129674.	4.2	12
11556	A Proton-responsive Pyridyl(benzamide)-functionalized NHC Ligand on Ir Complex for Alkylation of Ketones and Secondary Alcohols. <i>Chemistry - A European Journal</i> , 2021, 27, 10737-10748.	1.7	27
11557	3,9-Disubstituted Bis[1]benzothieno[3,2- <i>b</i>][2,3- <i>e</i>][1,4]thiazines with Low Oxidation Potentials and Enhanced Emission. <i>Journal of Organic Chemistry</i> , 2021, 86, 8000-8014.	1.7	5
11558	Mechanistic Insights into Promoted Hydrolysis of Phosphoester Bonds by MoO ₂ Cl ₂ (DMF) ₂ . <i>Inorganic Chemistry</i> , 2021, 60, 11177-11191.	1.9	5

#	ARTICLE	IF	CITATIONS
11559	Probing the origin of ambiphilic reactivity in osmapentalyne complexes: Interplay of ring strain, aromaticity, and phosphonium substituent. <i>Journal of Organometallic Chemistry</i> , 2021, 945, 121866.	0.8	1
11560	Novel synthesis, structural characterization, DFT and TDDFT investigation of "Butterfly" like Ag(I)-Structure, 2021, 1235, 130188.	1.8	2
11561	Benzylnickel(II) Complexes of 2-Iminopyrrolyl Chelating Ligands: Synthesis, Structure, and Catalytic Oligo-/Polymerization of Ethylene to Hyperbranched Polyethylene. <i>Organometallics</i> , 2021, 40, 2594-2609.	1.1	15
11562	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5419-5427.	2.3	8
11563	Adiabatic Molecular Orbital Tracking in Ab Initio Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4675-4685.	2.3	3
11564	Optical and structural properties of the new triblock copolymer (A-B-C) based on p-terphenyl, PVK and MEH-PPV for organic electronics: Experimental and theoretical study. <i>Materials Research Express</i> , 2021, 8, 075304.	0.8	1
11565	Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic \hat{H}^{SCF} . <i>Journal of Chemical Physics</i> , 2021, 155, 014103.	1.2	5
11566	Bridging the 12-6-4 Model and the Fluctuating Charge Model. <i>Frontiers in Chemistry</i> , 2021, 9, 721960.	1.8	4
11567	Water in Protic Ionic Liquid Electrolytes: From Solvent Separated Ion Pairs to Water Clusters. <i>ChemSusChem</i> , 2021, 14, 3315-3324.	3.6	8
11568	One-Pot and Two-Chamber Methodologies for Using Acetylene Surrogates in the Synthesis of Pyridazines and Their D_4 -Labeled Derivatives. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2286-2297.	1.7	9
11569	A Mechanistic Probe into 1,2-cis Glycoside Formation Catalyzed by Phenanthroline and Further Expansion of Scope. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 4054-4066.	2.1	4
11570	Determining Factor of the Quantum Yield of the Cyclization Reaction via Triplet States for Dye-Attached Diarylethene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5895-5902.	1.1	7
11571	Verification of corrosion inhibition of Mild steel by some 4-Aminoantipyrine-based Schiff bases "Impact of adsorbate substituent and cross-conjugation. <i>Journal of Molecular Liquids</i> , 2021, 333, 115960.	2.3	35
11572	Understanding the Dynamics of Molecular Water Oxidation Catalysts with Liquid-Phase Transmission Electron Microscopy: The Case of Vitamin B ₁₂ . <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 9494-9505.	3.2	17
11573	Wide-Bite-Angle Diphosphine Ligands in Thermally Activated Delayed Fluorescent Copper(I) Complexes: Impact on the Performance of Electroluminescence Applications. <i>Inorganic Chemistry</i> , 2021, 60, 10323-10339.	1.9	28
11574	Optimizing two-electron repulsion integral calculations with McMurchie "Davidson method on graphic processing unit. <i>Journal of Chemical Physics</i> , 2021, 155, 034112.	1.2	6
11575	Synthesis of D- π -A high-emissive 6-arylalkynyl-1,8-naphthalimides for application in Organic Field-Effect Transistors and optical waveguides. <i>Dyes and Pigments</i> , 2021, 191, 109358.	2.0	12
11576	A community-powered search of machine learning strategy space to find NMR property prediction models. <i>PLoS ONE</i> , 2021, 16, e0253612.	1.1	9

#	ARTICLE	IF	CITATIONS
11577	Acridone-amine D-A-D thermally activated delayed fluorescence emitters with narrow resolved electroluminescence and their electrochromic properties. <i>Electrochimica Acta</i> , 2021, 384, 138347.	2.6	10
11578	<i>syn</i> -Selective Construction of Fused Heterocycles by Catalytic Reductive Tandem Functionalization of N-Heteroarenes. <i>ACS Catalysis</i> , 2021, 11, 9271-9278.	5.5	32
11579	Comparative study of structural order, thermal desorption behavior, and work function change of self-assembled monolayers of pentafluorobenzenethiols and tetrafluorobenzenethiols on Au(1 1 1). <i>Applied Surface Science</i> , 2021, 555, 149671.	3.1	15
11580	H ₂ Evolution from Electrocatalysts with Redox-Active Ligands: Mechanistic Insights from Theory and Experiment vis-à-vis Co-Mabiq. <i>Inorganic Chemistry</i> , 2021, 60, 13888-13902.	1.9	7
11581	Cationic Co(I) Catalysts for Regiodivergent Hydroalkenylation of 1,6-Enynes: An Uncommon <i>cis</i> - β -C-H Activation Leads to <i>Z</i> -Selective Coupling of Acrylates. <i>ACS Catalysis</i> , 2021, 11, 9605-9617.	5.5	32
11582	Revisited the mechanism of cobalt(III) catalyzed cyanation of arenes and heteroarenes: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113289.	1.1	2
11583	Theoretical Investigation on the Elusive Reaction Mechanism of Spirooxindole Formation Mediated by Cytochrome P450s: A Nascent Feasible Charge-Shift C=O Bond Makes a Difference. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8419-8430.	1.2	4
11584	Insights into the Dual Shuttle Catalytic Mechanism of Guanine Deaminase. <i>Journal of Physical Chemistry B</i> , 2021, 125, 8814-8826.	1.2	4
11585	An improved Slater's transition state approximation. <i>Journal of Chemical Physics</i> , 2021, 155, 034101.	1.2	12
11586	Machine learning based energy-free structure predictions of molecules, transition states, and solids. <i>Nature Communications</i> , 2021, 12, 4468.	5.8	53
11587	Photoluminescence of Homoleptic Lanthanide Complexes With Tris(benzotriazol-1-yl)borate. <i>Journal of Fluorescence</i> , 2021, 31, 1433-1443.	1.3	5
11588	Novel Hybrid Compounds Containing Benzofuroxan and Aminothiazole Scaffolds: Synthesis and Evaluation of Their Anticancer Activity. <i>International Journal of Molecular Sciences</i> , 2021, 22, 7497.	1.8	8
11589	Electrophilic Properties of 2-Deoxyadenosine-Thymine Dimer: Photoelectron Spectroscopy and DFT Studies. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6591-6599.	1.1	0
11590	Tight electrostatic regulation of the OH production rate from the photolysis of hydrogen peroxide adsorbed on surfaces. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	9
11591	Product Distributions of Cytochrome P450 OleTJE with Phenyl-Substituted Fatty Acids: A Computational Study. <i>International Journal of Molecular Sciences</i> , 2021, 22, 7172.	1.8	6
11592	How Can the σ -Type Fullerene-Metal Bond Survive? A Systematic Survey of Reactions between Mono-EMFs and (M ²⁺ Ln) ₂ Dimers. <i>Inorganic Chemistry</i> , 2021, 60, 11287-11296.	1.9	0
11593	Formation and Reactivity with ^t BuCN of a Thorium Phosphinidide through a Combined Experimental and Computational Analysis. <i>Organometallics</i> , 2021, 40, 2701-2708.	1.1	4
11594	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890.	2.3	22

#	ARTICLE	IF	CITATIONS
11595	Amide imidic prototropic tautomerization of efavirenz, NBO analysis, hyperpolarizability, polarizability and HOMO–LUMO calculations using density functional theory. Computational and Theoretical Chemistry, 2021, 1201, 113273.	1.1	8
11596	On the Low-Lying Electronically Excited States of Azobenzene Dimers: Transition Density Matrix Analysis. Molecules, 2021, 26, 4245.	1.7	9
11597	Deciphering the Mechanistic Details of Manganese-Catalyzed Formic Acid Dehydrogenation: Insights from DFT Calculations. Inorganic Chemistry, 2021, 60, 11038-11047.	1.9	7
11598	Energy Decomposition Analysis of Lewis Acid/Base Adducts and Frustrated Lewis Pairs: The Use of Orbital Steric Ratios as a Reaction Parameter. Inorganic Chemistry, 2021, 60, 13797-13805.	1.9	9
11599	Structural studies of ligand stabilized Ni/Ga clusters by means of vibrational spectroscopy and theoretical calculations. Journal of Raman Spectroscopy, 2021, 52, 2317-2337.	1.2	4
11600	Carbon-Based Hybrid Interlayer to Anchor the Shuttling of Polysulfides for High-Performance Lithium–Sulfur Batteries. ACS Applied Energy Materials, 2021, 4, 8294-8302.	2.5	7
11601	Controlled Regulation of the Nitrile Activation of a Peroxocobalt(III) Complex with Redox-Inactive Lewis Acidic Metals. Journal of the American Chemical Society, 2021, 143, 11382-11392.	6.6	12
11602	Pathways of the Extremely Reactive Iron(IV)–oxido complexes with Tetradentate Bispidine Ligands. Chemistry - A European Journal, 2021, 27, 11377-11390.	1.7	13
11603	A novel water-soluble platinum(II) complex with the amino acid deoxyalliin: synthesis, crystal structure, theoretical studies and investigations about its antibacterial activity. Journal of Molecular Structure, 2021, 1236, 130316.	1.8	2
11604	Methane Adsorption on Heteroatom-Modified Maquettes of Porous Carbon Surfaces. Journal of Physical Chemistry A, 2021, 125, 6042-6058.	1.1	5
11605	Carbohydrate-Based NK1R Antagonists with Broad-Spectrum Anticancer Activity. Journal of Medicinal Chemistry, 2021, 64, 10350-10370.	2.9	10
11606	Catalytic Performance of Cycloalkyl-Fused Aryliminopyridyl Nickel Complexes toward Ethylene Polymerization by QSPR Modeling. Catalysts, 2021, 11, 920.	1.6	3
11607	Single Solvent Molecules Induce Dual Nucleophiles in Gas-Phase Ion–Molecule Nucleophilic Substitution Reactions. Journal of Physical Chemistry Letters, 2021, 12, 7134-7139.	2.1	8
11608	Exploring the Concept of Dimerization-Induced Intersystem Crossing: At the Origins of Spin–Orbit Coupling Selection Rules. Journal of Physical Chemistry B, 2021, 125, 8572-8580.	1.2	8
11609	Calculated Relative Thermodynamic Stabilities of the Gd@C ₈₂ Isomers. ECS Journal of Solid State Science and Technology, 2021, 10, 071013.	0.9	8
11610	Spatial Generation of Molecules with Transformers. , 2021, , .		0
11611	Theoretical investigation on conversion of CO ₂ with epoxides to cyclic carbonates by bifunctional metal-salen complexes bearing ionic liquid substituents. Molecular Catalysis, 2021, 511, 111733.	1.0	5
11612	Light-Driven Carbene Catalysis for the Synthesis of Aliphatic and α -Amino Ketones. Angewandte Chemie, 2021, 133, 18069-18075.	1.6	6

#	ARTICLE	IF	CITATIONS
11613	Light-Driven Carbene Catalysis for the Synthesis of Aliphatic and α -Amino Ketones. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17925-17931.	7.2	68
11614	Electrocoagulation/oxidation/flotation by direct pulsed current applied to the removal of antibiotics from Brazilian WWTP effluents. <i>Electrochimica Acta</i> , 2021, 388, 138499.	2.6	25
11615	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
11616	Polyfluorinated triphenyl-4,5-dihydro-1H-pyrazoles with dendroid arylsulfanyl moieties as donor blocks in donor-acceptor chromophores. <i>Journal of Fluorine Chemistry</i> , 2021, 248, 109841.	0.9	2
11617	Computational approach to (ZnS) _i nanoclusters in ionic liquids. <i>Physical Review E</i> , 2021, 104, 024604.	0.8	1
11618	Unraveling the Ultrafast Self-assembly and Photoluminescence in Zero-Dimensional Mn ²⁺ -Based Halides with Narrow-Band Green Emissions. <i>ACS Applied Electronic Materials</i> , 2021, 3, 4144-4150.	2.0	16
11619	A Statistically Supported Antioxidant Activity DFT Benchmark—The Effects of Hartree–Fock Exchange and Basis Set Selection on Accuracy and Resources Uptake. <i>Molecules</i> , 2021, 26, 5058.	1.7	21
11620	Computational and NMR Conformational Analysis of Galactofuranoside Cycles Presented in Bacterial and Fungal Polysaccharide Antigens. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 719396.	1.6	2
11621	SOMO→HOMO Conversion in Triplet Cyclopentane-1,3-diyl Diradicals. <i>ACS Omega</i> , 2021, 6, 22773-22779.	1.6	8
11622	Infrared, Electronic Absorption and Emission Spectra of Tris (4-methyl-1-methyl-1H-benzo [d]) Tj ETQq1 1 0.784314 rg Axial Substitution. <i>Photochemistry and Photobiology</i> , 2021, , .	1.3	0
11623	Elucidating active sites and decomposition mechanisms for oxythiomolybdate clusters (Mo ₂ O ₂ S _x , x=6;8) as catalyzers for hydrogen evolution reactions. <i>Electrochemical Science Advances</i> , 2022, 2, e2100088.	1.2	2
11624	Dipole-bound states and substituent effects of Breslow intermediates in the enolate form. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 2060-2070.	0.8	2
11625	[(C ₆₀)Au(N ₆₀ N)] ⁺ Complexes as a New Family of Anticancer Candidates: Synthesis, Characterization and Exploration of the Antiproliferative Properties. <i>Chemistry - A European Journal</i> , 2021, 27, 15773-15785.	1.7	11
11626	Solvatomorphism of Moxidectin. <i>Molecules</i> , 2021, 26, 4869.	1.7	1
11627	Interaction of Fe ²⁺ , Co ²⁺ , Ni ²⁺ , Cu ²⁺ , Zn ²⁺ , Pb ²⁺ , and Cr ³⁺ metal ions on B12N12 fullerene-like cages: a theoretical study. <i>Monatshefte für Chemie</i> , 2021, 152, 915-922.	0.9	2
11628	Anti-inflammatory dihydroxanthones from a <i>Diaporthe</i> species. <i>Biological Chemistry</i> , 2022, 403, 89-101.	1.2	0
11629	Direct Detection of Singlet Cyclopentane-1,3-diyl Diradicals By Infrared and Ultraviolet-Visible Spectroscopy at Cryogenic Temperature and Their Photoreactivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 12046-12053.	1.7	2
11630	On deformability of atoms—comparative study between atoms and atomic nuclei. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2021, 54, 165201.	0.6	3

#	ARTICLE	IF	CITATIONS
11631	Structure and Absolute Configuration of Phenanthro-perylene Quinone Pigments from the Deep-Sea Crinoid <i>Hyalocrinus naresianus</i> . <i>Marine Drugs</i> , 2021, 19, 445.	2.2	6
11632	A Covalent-Like Feature of Intermolecular Hydrogen Bonding in Energetic Molecules 3,6-Dihydrazino- ϵ -s-tetrazine (DHT). <i>Advanced Theory and Simulations</i> , 2021, 4, 2100179.	1.3	2
11633	Constraints on the Structure of Fibrils Formed by a Racemic Mixture of Amyloid- β Peptides from Solid-State NMR, Electron Microscopy, and Theory. <i>Journal of the American Chemical Society</i> , 2021, 143, 13299-13313.	6.6	17
11634	Evidence for ligand- and solvent-induced disproportionation of uranium(IV). <i>Nature Communications</i> , 2021, 12, 4832.	5.8	13
11635	Extending π -Conjugation and Integrating Multi-Redox Centers into One Molecule for High-Capacity Organic Cathodes. <i>ChemSusChem</i> , 2021, 14, 3858-3866.	3.6	17
11636	Structure and Functional Differences of Cysteine and β -Mercaptopropionate Dioxygenases: A Computational Study. <i>Chemistry - A European Journal</i> , 2021, 27, 13793-13806.	1.7	12
11637	Photodissociation of aliphatic PAH derivatives under relevant astrophysical conditions. <i>Astronomy and Astrophysics</i> , 2021, 652, A42.	2.1	8
11638	Active Thermochemical Tables: the thermophysical and thermochemical properties of methyl, CH ₃ , and methylene, CH ₂ , corrected for nonrigid rotor and anharmonic oscillator effects. <i>Molecular Physics</i> , 0, , e1969046.	0.8	12
11639	Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Light-Emitting Diodes. <i>Advanced Materials</i> , 2021, 33, e2100677.	11.1	99
11640	Naphthodithiophene Diimide Based Chiral π -Conjugated Nanopillar Molecules. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24543-24548.	7.2	19
11641	Modulation of the Second Order Nonlinear Optical Properties of Helical Graphene Nanoribbons Through Introducing Azulene Defects or/and BN Units. <i>Chemical Research in Chinese Universities</i> , 2022, 38, 974-984.	1.3	3
11642	Gas-phase structure, bonding, and fragmentation chemistry of the An (IV)-TMPDCAM complexes studied using mass spectrometry and theoretical calculation (An = Th and U). <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e9168.	0.7	1
11643	Symmetrized systematic molecular fragmentation model and its application for molecular properties. <i>Computational and Theoretical Chemistry</i> , 2021, 1202, 113303.	1.1	5
11644	Pyridine-containing octadentate ligand NE3TA-PY for formation of neutral complex with ¹⁷⁷ Lu(III) and ^{90Y} (III) for radiopharmaceutical applications: Synthesis, DFT calculation, radiolabeling, and in vitro complex stability. <i>Journal of Inorganic Biochemistry</i> , 2021, 221, 111436.	1.5	1
11645	Ab initio and steady-state models for uranium isotope fractionation in multi-step biotic and abiotic reduction. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 307, 212-227.	1.6	5
11646	New Insights on the Interaction of Phenanthroline Based Ligands and Metal Complexes and Polyoxometalates with Duplex DNA and G-Quadruplexes. <i>Molecules</i> , 2021, 26, 4737.	1.7	21
11647	$x\tilde{r}^{\sim}[\text{Pd}(\text{dmit})_2]_2$ as a quasi-one-dimensional scalene Heisenberg model. <i>Physical Review Materials</i> , 2021, 5, .	0.9	2
11648	Effect of dimethyl sulfoxide intercalation into kaolinite on etheramine adsorption: experimental and theoretical investigation. <i>Journal of Environmental Chemical Engineering</i> , 2021, 9, 105503.	3.3	14

#	ARTICLE	IF	CITATIONS
11649	Adaptive-Partitioning Multilayer Dynamics Simulations: 1. On-the-Fly Switch between Two Quantum Levels of Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5456-5465.	2.3	7
11650	Implication of oxidant activation on olefin epoxidation catalysed by Molybdenum catalysts with aroylhydrazonato ligands: Experimental and theoretical studies. <i>Molecular Catalysis</i> , 2021, 512, 111764.	1.0	9
11651	Selectively Fluorinated Furan-Phenylene Co-Oligomers Pave the Way to Bright Ambipolar Light-Emitting Electronic Devices. <i>Advanced Functional Materials</i> , 2021, 31, 2104638.	7.8	12
11652	Naphthodithiophene Diimide Based Chiral π -Conjugated Nanopillar Molecules. <i>Angewandte Chemie</i> , 2021, 133, 24748.	1.6	3
11653	Expansion of Photostable Luminescent Radicals by <i>Meta</i> -Substitution. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2538-2544.	1.7	13
11654	Accurate fragment-based 51-V chemical shift predictions in molecular crystals. <i>Solid State Nuclear Magnetic Resonance</i> , 2021, 114, 101733.	1.5	3
11655	Light-responsive and Protic Ruthenium Compounds Bearing Bathophenanthroline and Dihydroxybipyridine Ligands Achieve Nanomolar Toxicity towards Breast Cancer Cells. <i>Photochemistry and Photobiology</i> , 2021, , .	1.3	6
11656	Simple Synthesis of Complex Amines from the Diels-Alder Adducts of (α)-Cytisine. <i>Synthesis</i> , 0, , .	1.2	2
11657	Insights into the BPO 4 α -Driven Catalytic Mechanism for the Formation of Cyclic Carbonates from CO ₂ and Epoxides. <i>ChemistrySelect</i> , 2021, 6, 7489-7498.	0.7	2
11658	Electronic Spectra of C ₆₀ Films Using Screened Range Separated Hybrid Functionals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7625-7632.	1.1	5
11659	Theoretical analysis of structures and electronic spectra of molecular colloidal cadmium sulfide clusters and nanoplatelets. <i>Journal of Chemical Physics</i> , 2021, 155, 094302.	1.2	4
11660	A partial least squares and artificial neural network study for a series of arylpiperazines as antidepressant agents. <i>Journal of Molecular Modeling</i> , 2021, 27, 297.	0.8	5
11661	Microextraction by packed molecularly imprinted polymer followed by ultra-high performance liquid chromatography for determination of fipronil and fluzaron residues in drinking water and veterinary clinic wastewater. <i>Microchemical Journal</i> , 2021, 168, 106405.	2.3	12
11662	Theoretical study on pentiptycene molecular brake: photoinduced isomerization and photoinduced electron transfer. <i>Journal of Molecular Modeling</i> , 2021, 27, 289.	0.8	0
11663	Numerical integration of overlap electron densities: Parallelization strategies for a good load balancing using OpenMP. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113457.	1.1	6
11664	Synchronous construction of a porous intramolecular D-A conjugated polymer via electron donors for superior photocatalytic decontamination. <i>Journal of Hazardous Materials</i> , 2022, 424, 127379.	6.5	12
11665	Coordination of reduced Schiff base anion to Pd(II): Synthesis, characterization, DFT calculation and catecholase activity. <i>Journal of the Indian Chemical Society</i> , 2021, 98, 100186.	1.3	1
11666	Electronic structure investigation of the stability, reactivity, NBO analysis, thermodynamics, and the nature of the interactions in methyl-substituted imidazolium-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2021, 337, 116458.	2.3	68

#	ARTICLE	IF	CITATIONS
11667	Origin of Regioselectivity in the Dehydrogenation of Alkanes by Pincer Iridium Complexes: A Combined Experimental and Computational Study. <i>ACS Catalysis</i> , 2021, 11, 12038-12051.	5.5	7
11669	New Compound of Pyridine-4-Boronic Acid Cation and Pt(CN) ₄ Anion Salt: Synthesis, Structural Properties, Hirshfeld Surface Analysis and Density Functional Theory Calculations. <i>Journal of the Institute of Science and Technology</i> , 0, , 1990-2000.	0.3	0
11671	The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain. <i>International Journal of Biological Macromolecules</i> , 2021, 186, 54-70.	3.6	7
11672	Water hydrogen-bonding effects on the ground and low-lying excited states of dipyrindyl isomers. <i>Journal of Molecular Liquids</i> , 2021, 338, 116767.	2.3	5
11673	Computational Mechanistic Study of Fused Phenol Formations from 1,6-Heptadiyne Involving Carbyne Complexes. <i>ChemCatChem</i> , 0, , .	1.8	2
11674	Distorted Copper(II) Complex with Unusually Short CF ₃ -Cu Distances. <i>Inorganic Chemistry</i> , 2021, 60, 14759-14764.	1.9	1
11675	Absolute configuration of a [1]rotaxane determined from vibrational and electronic circular dichroism spectra. <i>Chirality</i> , 2021, 33, 773-782.	1.3	2
11676	Controlled Asymmetric Charge Distribution of Active Centers in Conjugated Polymers for Oxygen Reduction. <i>Angewandte Chemie</i> , 0, , .	1.6	7
11677	A computational study of a reduced dye and its O ₂ reduction: Implication on H ₂ O ₂ production with dye-sensitized photocathodes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 418, 113437.	2.0	1
11678	Robust fluorogenic non-porphyrin interaction of Zn(II) and Hg(II) naphthadiazacrown macrocyclic complexes with C ₆₀ : Spectroscopic and dispersion-corrected DFT study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 418, 113414.	2.0	4
11679	Using structure-function relationships to understand the mechanism of phenazine-mediated extracellular electron transfer in <i>Escherichia coli</i> . <i>IScience</i> , 2021, 24, 103033.	1.9	27
11680	Estimation of ground and excited-state dipole moments of three symmetric carbocyanine dyes via the analysis of luminescence properties. <i>Journal of Molecular Liquids</i> , 2021, 337, 116476.	2.3	5
11681	Small Transition-Metal Mixed Clusters as Activators of the C=O Bond. Fe _n Cu _m -CO (n + m = 6): A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7940-7955.	1.1	3
11682	Computational Study of Benzosultam Formation through Gold(I)-Catalyzed Ammoniumation/Nucleophilic Substitution Reaction. <i>Helvetica Chimica Acta</i> , 2021, 104, e2100133.	1.0	3
11683	Electronic properties and reactivity patterns of high-valent metal-oxo species of Mn, Fe, Co, and Ni. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 1506-1512.	1.0	9
11684	How acid can become a dihydrogen complex in water? A DFT study. <i>Journal of Organometallic Chemistry</i> , 2021, 949, 121957.	0.8	3
11685	Analysis of Local and Global Aromaticity in Si ₃ C ₅ and Si ₄ C ₈ Clusters. <i>Aromatic Species Containing Planar Tetracoordinate Carbon</i> . <i>Chemistry</i> , 2021, 3, 1101-1112.	0.9	7
11686	Nonsymmetrical Benzene-Pyridine-Based Nickel Pincer Complexes Featuring Borohydride, Formate, Ethyl, and Nitrosyl Ligands. <i>Organometallics</i> , 2021, 40, 3331-3340.	1.1	3

#	ARTICLE	IF	CITATIONS
11687	Dysphania ambrosioides Essential Oil: An Eco-friendly Inhibitor for Mild Steel Corrosion in Hydrochloric and Sulfuric Acid Medium. <i>Journal of Bio- and Tribo-Corrosion</i> , 2021, 7, 1.	1.2	3
11688	Nature of Oxygen Adsorption on Defective Carbonaceous Materials. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20686-20696.	1.5	11
11689	Quantitative Estimation of the Hydrogen-Atom-Donating Ability of 4-Substituted Hantzsch Ester Radical Cations. <i>ACS Omega</i> , 2021, 6, 23621-23629.	1.6	11
11690	Monomers of Glycine and Serine Have a Limited Ability to Hydrate in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8454-8467.	1.1	12
11691	Controlled Asymmetric Charge Distribution of Active Centers in Conjugated Polymers for Oxygen Reduction. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 26483-26488.	7.2	59
11692	Interaction of glyphosate in matrices of cellulose and diethylaminoethyl cellulose biopolymers: theoretical viewpoint of the adsorption process. <i>Journal of Molecular Modeling</i> , 2021, 27, 272.	0.8	3
11693	Ionic Inter-Particle Complexation Effect on the Performance of Waterborne Coatings. <i>Polymers</i> , 2021, 13, 3098.	2.0	17
11694	A black-box, general purpose quadratic self-consistent field code with and without Cholesky decomposition of the two-electron integrals. <i>Molecular Physics</i> , 2021, 119, .	0.8	8
11695	Mass Spectrometry-Based Techniques to Elucidate the Sugar Code. <i>Chemical Reviews</i> , 2022, 122, 7840-7908.	23.0	67
11696	Mechanistic exploration of Rh(III)-catalyzed C-H allylation of benzamides with allyl bromide. <i>Journal of Organometallic Chemistry</i> , 2021, 949, 121888.	0.8	1
11697	A Metallic Ion-Induced Self-Assembly Enabling Nanowire-Based Aerogels. <i>Small</i> , 2021, 17, e2103406.	5.2	3
11698	A Two-Step Baromechanical Cycle for Repeated Activation and Deactivation of Mechanophores. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9470-9474.	2.1	5
11699	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4582-4593.	2.5	4
11700	Atypical and Asymmetric 1,3- λ^5 -N Ligands: Synthesis, Coordination and Catalytic Performance of Cycloiminophosphanes. <i>Chemistry - A European Journal</i> , 2021, 27, 14007-14016.	1.7	2
11701	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. <i>Biophysical Journal</i> , 2021, 120, 3577-3587.	0.2	7
11702	Half-Pancake Bonding in Asphaltenes. <i>Energy & Fuels</i> , 0, , .	2.5	5
11703	Ceratonia Siliqua L seeds extract as eco-friendly corrosion inhibitor for carbon steel in 1M HCl: Characterization, electrochemical, surface analysis, and theoretical studies. <i>Journal of Molecular Structure</i> , 2021, 1240, 130611.	1.8	34
11704	N-Confused Pyritriphyrin: A New Class of Triphyrin and Its Calixphyrin Analogue. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 5222-5226.	1.2	3

#	ARTICLE	IF	CITATIONS
11705	Electrocatalytic Behavior of Tetrathiafulvalene (TTF) and Extended Tetrathiafulvalene (exTTF) [FeFe] Hydrogenase Mimics. ACS Organic & Inorganic Au, 2022, 2, 23-33.	1.9	5
11706	Protein Response Effects on Cofactor Excitation Energies from First Principles: Augmenting Subsystem Time-Dependent Density-Functional Theory with Many-Body Expansion Techniques. Journal of Chemical Theory and Computation, 2021, 17, 6105-6121.	2.3	9
11707	Machine Learning to Predict Diels-Alder Reaction Barriers from the Reactant State Electron Density. Journal of Chemical Theory and Computation, 2021, 17, 6203-6213.	2.3	16
11708	Singlet O ₂ Produced by Ultraviolet Dissociation of the Î ² -ionone-O ₂ Complex. Journal of Physical Chemistry A, 2021, 125, 8649-8657.	1.1	3
11709	Mechanistic Investigation of Palladium-Catalyzed <i>meta</i> -C-H Bond Activation of Arenes with a Carboxyl Directing Group. Journal of Organic Chemistry, 2021, 86, 13475-13480.	1.7	4
11710	Isomerization of a cationic (Î ⁵ -C ₅ Me ₅)Ir(III) complex involving remote C-C and C-H bond formation. Polyhedron, 2021, 207, 115363.	1.0	2
11711	Supramolecular architecture formed between amidinothiourea and 2-pyridinecarboxylic acid. Journal of Molecular Structure, 2021, 1242, 130736.	1.8	3
11712	A computational approach on engineering short spacer for carbazole-based dyes for dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 419, 113447.	2.0	6
11713	Fast and automated identification of reactions with low barriers: the decomposition of 3-hydroperoxypropanal. SciPost Chemistry, 2021, 1, .	2.0	7
11714	Synthesis, optical and electrochemical properties of a series of push-pull dyes based on the 4,4-bis(4-methoxy phenyl)butadienyl donor. Dyes and Pigments, 2021, 194, 109552.	2.0	4
11715	Preparation of anatase-free hierarchical titanosilicalite-1 in favor of allyl chloride epoxidation. Microporous and Mesoporous Materials, 2021, 326, 111388.	2.2	15
11716	Adsorption and activation of CO ₂ molecule on subnanometer-sized anionic vanadium carbide clusters V _n C _{4n} ⁻ (n = 1-6): A theoretical study. Molecular Catalysis, 2021, 515, 111871.	1.0	2
11717	Oxidation mechanism of ammonia in water clusters. Molecular Physics, 0, , .	0.8	0
11718	Double-layer novel zinc porphyrin based on axial coordination self-assembly for dye-sensitized solar cells. Journal of Molecular Structure, 2021, 1242, 130819.	1.8	6
11719	Structural defects on (5,5) single-walled carbon nanotubes: Impact on their electronic properties and chemical reactivity from a DFT perspective. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 134, 114874.	1.3	6
11720	Resonance Raman characterization of poly(benzidine) in different oxidation states. Journal of Molecular Structure, 2021, 1242, 130751.	1.8	3
11721	Red light-emitting Carborane-BODIPY dyes: Synthesis and properties of visible-light tuned fluorophores with enhanced boron content. Dyes and Pigments, 2021, 194, 109644.	2.0	9
11722	Dissociative adsorption of NO introduces flexibility in gas phase Rh ₆ ⁺ clusters leading to a rich isomeric distribution. Chemical Physics Letters, 2021, 780, 138937.	1.2	5

#	ARTICLE	IF	CITATIONS
11723	Electrochemically driven efficient enzymatic conversion of CO ₂ to formic acid with artificial cofactors. <i>Journal of CO₂ Utilization</i> , 2021, 52, 101679.	3.3	18
11724	Lowering Electrocatalytic CO ₂ Reduction Overpotential Using N-Annulated Perylene Diimide Rhenium Bipyridine Dyads with Variable Tether Length. <i>Journal of the American Chemical Society</i> , 2021, 143, 16849-16864.	6.6	15
11725	Synthesis, characterization and catalytic activity of a mononuclear nonheme copper(II)-iodosylbenzene adduct. <i>Journal of Inorganic Biochemistry</i> , 2021, 223, 111524.	1.5	3
11726	The alcohol catalytic mechanism for Schiff base 1,3-proton transfer. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113419.	1.1	1
11727	Structural and spectroscopic analysis of the Cis-Trans isomers of the captopril in the gaseous and aqueous phases. <i>Journal of Molecular Structure</i> , 2021, 1243, 130872.	1.8	2
11728	New models involving quantum chemical parameters for assessing the chromatographic retention process. <i>Microchemical Journal</i> , 2021, 170, 106693.	2.3	1
11729	Photochromism of dye containing Schiff base-metal complex: A revisit through spectro-kinetic, thermodynamic and theoretical analyses for the design of a molecular logic gate. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 420, 113505.	2.0	18
11730	Carbonate anion photolyzed by solar radiation or combined with peracetic acid to form reactive species for dye degradation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 420, 113511.	2.0	8
11731	Nanomolar inhibition of human OGA by 2-acetamido-2-deoxy-d-glucono-1,5-lactone semicarbazone derivatives. <i>European Journal of Medicinal Chemistry</i> , 2021, 223, 113649.	2.6	6
11732	Highly selective and sensitive optical discrimination of pyrophosphate ion by a Zn(II)-terpyridine complex in aqueous medium at physiological pH. <i>Journal of Molecular Structure</i> , 2021, 1243, 130868.	1.8	4
11733	Spectroscopy and a theoretical study of colorimetric sensing of fluoride ions by salicylidene based Schiff base derivatives. <i>Journal of Molecular Structure</i> , 2021, 1245, 131132.	1.8	7
11734	Phyllanthus emblica seed extract as corrosion inhibitor for stainless steel used in petroleum industry (SS-410) in acidic medium. <i>Chemical Physics Impact</i> , 2021, 3, 100038.	1.7	11
11735	Synthesis, spectroscopic characterization and in vitro antibacterial and antiviral activities of novel silver(I) complexes with mafenide and ethyl-mafenide. <i>Journal of Molecular Structure</i> , 2021, 1246, 131261.	1.8	9
11736	Two-dimensional quantum dots for highly efficient heterojunction solar cells. <i>Journal of Colloid and Interface Science</i> , 2021, 603, 48-57.	5.0	31
11737	Solubility measurement and thermodynamic correlation of (2,4-dichlorophenoxy)acetic acid in fifteen pure solvents. <i>Journal of Chemical Thermodynamics</i> , 2021, 163, 106589.	1.0	12
11738	Characterization, Hirshfeld surface analysis, DFT study and an in vitro α -glucosidase/ α -amylase/radical scavenging profiling of novel 5-styryl-2-(4-tolylsulfonamido) chalcones. <i>Journal of Molecular Structure</i> , 2021, 1245, 131090.	1.8	5
11739	In vitro and in silico studies of radical scavenging activity of salicylaldehyde benzoylhydrazones. <i>Journal of Molecular Structure</i> , 2021, 1245, 131021.	1.8	9
11740	Ultrahigh rate and high-performance lithium-sulfur batteries with resorcinol-formaldehyde xerogel derived highly porous carbon matrix as sulfur cathode host. <i>Chemical Engineering Journal</i> , 2021, 425, 131521.	6.6	21

#	ARTICLE	IF	CITATIONS
11741	UV/Fe ^{III} /NTA as a novel photoreductive system for the degradation of perfluorooctane sulfonate (PFOS) via a photoinduced intramolecular electron transfer mechanism. <i>Chemical Engineering Journal</i> , 2022, 427, 130923.	6.6	18
11742	Computational insight into biotransformation of halophenols by cytochrome P450: Mechanism and reactivity for epoxidation. <i>Chemosphere</i> , 2022, 286, 131708.	4.2	8
11743	819 molecular knot: a theoretical analysis of the electronic structure using an ONIOM approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 39.	0.8	1
11744	Adsorption of SO ₂ on pristine and defective single-walled MgO nanotubes: a dispersion-corrected density-functional theory (DFT-D) study. <i>Materials Research Express</i> , 2021, 8, 015023.	0.8	4
11745	Adsorption of 1-chloro-1,2,2,2-tetrafluoroethane on pristine, Al, Ga-doped boron nitride nanotubes: a study involving PBC-DFT, NBO analysis, and QTAIM. <i>Canadian Journal of Chemistry</i> , 2021, 99, 51-62.	0.6	27
11746	Titanium complexes of pyrrolylaldiminato ligands and their exploitation for the ring-opening polymerization of cyclic esters. <i>Dalton Transactions</i> , 2021, 50, 10964-10981.	1.6	7
11747	Lanthanide-Bisphosphonate Coordination Chemistry: Biocompatible Fluorescent Labeling Strategy for Hydrogel. <i>ACS Applied Bio Materials</i> , 2021, 4, 1057-1064.	2.3	8
11748	The mechanism behind the photochromism and photomagnetism of type II biindenylidenediones: multiconfigurational, perturbative and density functional theory studies. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 17453-17465.	1.3	0
11749	Submonomer synthesis of peptoids containing <i>trans</i> -inducing <i>N</i> -imino- and <i>N</i> -alkylamino-glycines. <i>Chemical Science</i> , 2021, 12, 8401-8410.	3.7	16
11750	Mechanistic Understanding of Rh(III)-Catalyzed Redox-Neutral C-H Activation/Annulation Reactions of <i>N</i> -Phenoxyacetamides and Methyleneoxetanones. <i>Chinese Journal of Organic Chemistry</i> , 2021, 41, 3272.	0.6	0
11751	Computational Investigation of Adsorptive Removal of Pb ²⁺ from Water by the UiO-66 Metal-Organic Framework: Comparison of Adsorption Sites on Defects and Functionalised Linkers. <i>Australian Journal of Chemistry</i> , 2021, , .	0.5	1
11752	Resolving the ultrafast dynamics of the anionic green fluorescent protein chromophore in water. <i>Chemical Science</i> , 2021, 12, 11347-11363.	3.7	28
11753	Identifying the preferential pathways of CO ₂ capture and hydrogenation to methanol over an Mn-PNP catalyst: a computational study. <i>Dalton Transactions</i> , 2021, 50, 9598-9609.	1.6	5
11754	Mechanism of iron complexes catalyzed in the <i>N</i> -formylation of amines with CO ₂ and H ₂ : the superior performance of ¹ H ligand methylated complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16675-16689.	1.3	3
11755	Predicting phosphorescence energies and inferring wavefunction localization with machine learning. <i>Chemical Science</i> , 2021, 12, 10207-10217.	3.7	14
11756	Synthesis and Catalytic Reactivity of Cobalt Pincer Nitrosyl Hydride Complexes. <i>Organometallics</i> , 2021, 40, 278-285.	1.1	12
11757	Cis-Bis(2,2'-Azopyridinido)dicarbonylruthenium(II). <i>MolBank</i> , 2021, 2021, M1182.	0.2	1
11758	[8+2] vs [4+2] Cycloadditions of Cyclohexadienamines to Tropone and Heptafulvenes: Mechanisms and Selectivities. <i>Journal of the American Chemical Society</i> , 2021, 143, 934-944.	6.6	23

#	ARTICLE	IF	CITATIONS
11759	Disentangling the complex network of non-covalent interactions in fenchone hydrates <i>via</i> rotational spectroscopy and quantum chemistry. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20686-20694.	1.3	12
11760	Excited-state behavior and photoinduced electron transfer of pH-sensitive Ir(III) complexes with cyclometallation (C/Nâ€“) ratios between 0/6 and 3/3. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 405, 112957.	2.0	8
11761	Hartree-Fock and Density Functional Calculations on Graphics Processing Unit. <i>Acta Chimica Sinica</i> , 2021, 79, 653.	0.5	2
11762	Computational modelling of Pd-catalysed alkoxy carbonylation of alkenes and alkynes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15869-15880.	1.3	7
11763	Mechanistic insight into B(C ₆ F ₅) ₃ catalyzed imine reduction with PhSiH ₃ under stoichiometric water conditions. <i>RSC Advances</i> , 2021, 11, 20961-20969.	1.7	4
11764	Photoreduction Mechanism of CO ₂ to CO Catalyzed by a Three-Component Hybrid Construct with a Bimetallic Rhenium Catalyst. <i>ACS Catalysis</i> , 2021, 11, 1495-1504.	5.5	19
11765	Computational exploration of copper catalyzed vinylogous aerobic oxidation of unsaturated compounds. <i>Scientific Reports</i> , 2021, 11, 1304.	1.6	2
11766	The mechanism studies of catalytic chemoselective conjugate addition of amino alcohols to α,β -unsaturated ester. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	0
11767	A mechanistic study of the manganese porphyrin-catalyzed Câ€“H isocyanation reaction. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1858-1866.	2.3	7
11768	Role of the base Cs ₂ CO ₃ on the palladium-catalyzed intramolecular cyclization of two bromoindole derivatives to yield paullone-type products. <i>Journal of Molecular Modeling</i> , 2021, 27, 9.	0.8	0
11769	Nonlinear Optical and Spectroscopical Properties of Functionalized Oligoanilines. <i>ChemistrySelect</i> , 2021, 6, 542-550.	0.7	1
11770	Relative Rates of Krypton and Rubidium Release from Zeolite Getters. <i>Journal of Physical Chemistry C</i> , 2021, 125, 1323-1333.	1.5	0
11771	Theoretical insight into dihydrogen activation with β^2 -diketiminato ligand supported Group 13 and 14 elements: mechanism and activity difference. <i>New Journal of Chemistry</i> , 2021, 45, 14789-14796.	1.4	0
11772	Protective interlayer for trapping polysulfides and a conducting host for sulfur: dual role of candle soot carbon for the development of high performance lithiumâ€“sulfur batteries. <i>Materials Advances</i> , 2021, 2, 3031-3041.	2.6	12
11773	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. <i>Journal of Materials Chemistry C</i> , 2021, 9, 13557-13583.	2.7	20
11774	Prediction of the standard potentials for one-electron oxidation of <i>N,N,N',N'</i> -tetrasubstituted <i>p</i> -phenylenediamines by calculation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20340-20351.	1.3	3
11775	Distiboranes based on <i>ortho</i> -phenylene backbones as bidentate Lewis acids for fluoride anion chelation. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 4949-4957.	1.5	14
11776	DFT Mechanism of Cu Catalyzed Coupling Reaction to Alkyl Aryl Ethers. <i>Acta Chimica Sinica</i> , 2021, 79, 948.	0.5	1

#	ARTICLE	IF	CITATIONS
11777	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 801-815.	1.1	8
11778	Tuning the edge states in X-type carbon based molecules for applications in nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7713-7722.	1.3	7
11779	Generation, contraction, and polarisation of Gaussian basis sets for atomic and molecular calculations using the generator coordinate method with polynomial discretisation: atoms from Na through Cl. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16989-16997.	1.3	0
11780	A quantum chemical model for a series of self-assembled nanocages: the origin of stability behind the coordination-driven formation of transition metal complexes up to $[M_{12}L_{24}]^{24+}$. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 866-877.	1.3	4
11781	Symmetric and Non-symmetric Anthracen-diyl Bis(alkylidynes). <i>Dalton Transactions</i> , 2021, 50, 15502-15523.	1.6	4
11782	Molecular dynamics simulation of the Pb(II) coordination in biological media via cationic dummy atom models. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	19
11783	Manganese and iron PCP pincer complexes – the influence of sterics on structure and reactivity. <i>Dalton Transactions</i> , 2021, 50, 13915-13924.	1.6	6
11784	Nickel(II) di-aqua complex containing a water cluster: synthesis, X-ray structure and catecholase activity. <i>New Journal of Chemistry</i> , 2021, 45, 2221-2227.	1.4	6
11785	On the role of symmetry in XDW-CASPT2. <i>Journal of Chemical Physics</i> , 2021, 154, 034102.	1.2	20
11786	On the question of steric repulsion versus noncovalent attractive interactions in chiral phosphoric acid catalyzed asymmetric reactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18936-18950.	1.3	10
11788	Olefin Polymerization Using Homogeneous Group IV Metallocenes. , 0, , 149-179.		4
11789	Isothiourea-Catalyzed Atropselective Acylation of Biaryl Phenols via Sequential Desymmetrization/Kinetic Resolution. <i>Angewandte Chemie</i> , 2020, 132, 7971-7979.	1.6	13
11790	Boron-Nitrogen-Doped Nanographenes: A Synthetic Tale from Borazine Precursors. <i>Chemistry - A European Journal</i> , 2020, 26, 6608-6621.	1.7	20
11791	Following the evolution of excited states along photochemical reaction pathways. <i>Journal of Computational Chemistry</i> , 2020, 41, 1156-1164.	1.5	5
11792	Ab initio effective one-electron potential operators: Applications for charge-transfer energy in effective fragment potentials. <i>Journal of Computational Chemistry</i> , 2021, 42, 398-411.	1.5	2
11793	Origins of relative acidity: First and second period hydrides. <i>Journal of Computational Chemistry</i> , 1996, 17, 1771-1781.	1.5	5
11794	The Nature of Silicon-oxygen Bonds in Silica Polymorphs. <i>Topics in Molecular Organization and Engineering</i> , 1997, , 179-199.	0.1	21
11795	Theoretical Prediction of Bond Dissociation Energies for Transition Metal Compounds and Main Group Complexes with Standard Quantum-Chemical Methods. , 2001, , 199-233.		4

#	ARTICLE	IF	CITATIONS
11796	Substrate-Enzyme Interactions from Modeling and Isotope Effects. Challenges and Advances in Computational Chemistry and Physics, 2007, , 341-363.	0.6	2
11797	Performance Analysis and Derived Parallelization Strategy for a SCF Program at the Hartree Fock Level. Lecture Notes in Computer Science, 1999, , 163-172.	1.0	7
11798	Foundations and recent developments on molecular quantum similarity. Topics in Current Chemistry, 1995, , 31-62.	4.0	72
11799	User-Friendly Quantum Mechanics: Applications for Drug Discovery. Methods in Molecular Biology, 2020, 2114, 231-255.	0.4	11
11800	QM Calculations in ADMET Prediction. Methods in Molecular Biology, 2020, 2114, 285-305.	0.4	7
11801	Quantum Chemistry. Theory of Geometries and Energies of Small Molecules. , 1973, , 11-22.		1
11802	Carbonium Ions: Structural and Energetic Investigations. , 1977, , 277-331.		4
11803	Informing Saccharide Structural NMR Studies with Density Functional Theory Calculations. Methods in Molecular Biology, 2015, 1273, 289-331.	0.4	24
11804	Electron momentum spectroscopy of metal carbonyls: a reinvestigation of the role of nuclear dynamics. Highlights in Theoretical Chemistry, 2014, , 95-109.	0.0	1
11805	Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods. Progress in Theoretical Chemistry and Physics, 2009, , 131-195.	0.2	5
11806	Divide-and-Conquer Approaches to Quantum Chemistry: Theory and Implementation. Challenges and Advances in Computational Chemistry and Physics, 2011, , 97-127.	0.6	27
11807	Design of Catalysts for Asymmetric Organic Reactions Through Density Functional Calculations. Challenges and Advances in Computational Chemistry and Physics, 2010, , 107-136.	0.6	2
11808	Identifying the Reaction Mechanisms of Inteins with QM/MM Multiscale Methods. , 2010, , 469-489.		1
11809	Neutral Hydrolysis of Methyl Formate from Ab initio Potentials and Molecular Dynamics Simulation. Progress in Theoretical Chemistry and Physics, 2012, , 395-403.	0.2	1
11810	First Steps Towards Quantum Refinement of Protein X-Ray Structures. , 2012, , 87-120.		7
11811	Theoretical Investigation of the NO ₃ Initiated Reaction of VOCs. NATO Science for Peace and Security Series C: Environmental Security, 2013, , 163-171.	0.1	1
11812	Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2015, , 1-67.		5
11813	Practical Ab Initio Methods for Molecular Electronic Structure Studies. II. Finite Basis Sets and the Algebraic Approximation. , 1997, , 109-158.		13

#	ARTICLE	IF	CITATIONS
11814	Quantum Mechanical AB Initio Investigation of Metal-Ligand Interactions in Transition-Metal Carbonyl Complexes. , 1996, , 185-232.		3
11815	A Reappraisal of the Hydrogen Bonding Interaction Obtained by Combining Energy Decomposition Analyses and Counterpoise Corrections. Topics in Molecular Organization and Engineering, 1988, , 507-559.	0.1	15
11816	Hydrocarbon Radical Cations in Condensed Phases. Topics in Molecular Organization and Engineering, 1989, , 259-300.	0.1	11
11817	The Ethane Problem. , 1974, , 177-190.		2
11818	Carbon-13 Chemical Shielding Tensors in Sugars: Sucrose and Methyl- β -D-Glucopyranoside. , 1993, , 367-384.		26
11819	Structure and Bonding of $M(CO)_3(H_2O)$, $M(CO)_5(NH_3)$, and $M(CO)_5(PH_3)$ ($M = Cr, Mo, W$)1. , 2000, , 73-89.		2
11820	General Suggestions and Applications of Quantum Molecular Similarity Measures from ab initio Fitted Electron Densities. , 1995, , 89-111.		5
11821	Using the Reaction Path Concept to Obtain Rate Constants From ab initio Calculations. , 1995, , 191-228.		2
11823	Size and Conformation-Selective Infrared Spectroscopy of Neutral Hydrogen-Bonded Clusters. , 2000, , 83-99.		1
11824	A Quantum Chemistry Approach for the Design and Analysis of Nanosensors for Fissile Materials. Challenges and Advances in Computational Chemistry and Physics, 2014, , 1-29.	0.6	1
11825	Functionalized Graphene and Cobalt Phthalocyanine Based Materials with Potential Use for Electrical Conduction. Challenges and Advances in Computational Chemistry and Physics, 2014, , 185-215.	0.6	1
11826	Multipole electrostatic model for MNDO-like techniques with minimal valence spd-basis sets. , 2005, 114, 159.		2
11827	A DFT and wave function theory study of hydrogen adsorption on small beryllium oxide clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	7
11828	Extending the Marcus $\hat{1}/4$ -Scale of Solvent Softness Using Conceptual Density Functional Theory and the Orbital Overlap Distance: Method and Application to Ionic Liquids. Journal of Solution Chemistry, 2020, 49, 614-628.	0.6	2
11829	Kinetic analysis of formation of boron trioxide from thermal decomposition of boric acid under non-isothermal conditions. Journal of Thermal Analysis and Calorimetry, 2018, 131, 2443-2455.	2.0	37
11830	Properties of Crystalline Organic Molecules. , 2001, , 3-50.		3
11831	Ultrafast excited state dynamics in the green fluorescent protein chromophore. , 2004, , 425-432.		2
11833	Crystal and molecular structures, temperature dependence of the IR and Raman spectra and vibrational dynamics of aquo 4,6-dimethyl-5H-[1,2,3]triazolo[4,5-c]pyridine in a new zwitterionic form. Journal of Molecular Structure, 2017, 1144, 482-495.	1.8	4

#	ARTICLE	IF	CITATIONS
11834	The linear and non-linear optical absorption and asymmetrical electromagnetic interaction in chiral twisted bilayer graphene with hybrid edges. <i>Materials Today Physics</i> , 2020, 14, 100222.	2.9	52
11835	The interplay between X-ray crystallography and Ab initio calculations. <i>Advances in Molecular Structure Research</i> , 1995, , 201-226.	0.3	14
11836	TURTLE – A gradient VBSCF Program Theory and Studies of Aromaticity. <i>Theoretical and Computational Chemistry</i> , 2002, , 79-116.	0.2	25
11837	How similar are HF, MP2, and DFT charge distributions in the Cr(CO) ₆ complex?. <i>Advances in Molecular Similarity</i> , 1996, , 167-186.	0.5	2
11838	Homoleptic Tris-Cyclometalated Iridium Complexes with Substituted <i>o</i> -Carboranes: Green Phosphorescent Emitters for Highly Efficient Solution-Processed Organic Light-Emitting Diodes. <i>Inorganic Chemistry</i> , 2016, 55, 909-917.	1.9	63
11839	Charge Anisotropy of Nitrogen: Where Chemical Intuition Fails. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4443-4453.	2.3	8
11841	Low-Temperature Hypergolic Ignition of 1-Octene with Low Ignition Delay Time. <i>Journal of Physical Chemistry A</i> , 2021, 125, 423-434.	1.1	6
11842	The Relative Stability of Indole Isomers Is a Consequence of the Glidewell-Lloyd Rule. <i>Journal of Physical Chemistry A</i> , 2021, 125, 230-234.	1.1	16
11843	Density Functional Theory Study of the Solvent Effects on Systematically Substituted Dihydroazulene/Vinylheptafulvene Systems: Improving the Capability of Molecular Energy Storage. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8856-8865.	1.1	18
11844	Computing Proton-Coupled Redox Potentials of Fluorotyrosines in a Protein Environment. <i>Journal of Physical Chemistry B</i> , 2021, 125, 128-136.	1.2	7
11845	Unusual Electronic Structure of the Donor-Acceptor Cocrystal Formed by Dithieno[3,2- <i>a</i> :2',3'- <i>c</i>]phenazine and 7,7,8,8-Tetracyanoquinodimethane. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4510-4515.	2.1	15
11846	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 1314-1322.	4.0	13
11847	Water-Resistant Pt Sites in Hydrophobic Mesopores Effective for Low-Temperature Ethylene Oxidation. <i>ACS Catalysis</i> , 2020, 10, 13257-13268.	5.5	23
11848	A Facile N≡N Bond Cleavage by the Trinuclear Metal Center in Vanadium Carbide Cluster Anions V ₃ C ₄ ⁺ . <i>Journal of the American Chemical Society</i> , 2020, 142, 10747-10754.	6.6	57
11849	Cooperative Bond Activation by a Bimetallic Main-Group Complex. <i>Journal of the American Chemical Society</i> , 2021, 143, 142-148.	6.6	27
11850	Bottom-up synthesis of finite models of helical (n,m)-single-wall carbon nanotubes. , 0, .		1
11851	Isomerization versus dissociation of phenylalanylglycyltryptophan radical cations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 16923-16933.	1.3	1
11852	Metathesis of a U ^V imido complex: a route to a terminal U ^V sulfide. <i>Chemical Science</i> , 2017, 8, 5319-5328.	3.7	25

#	ARTICLE	IF	CITATIONS
11853	Cation influence on heterocyclic ammonium ionic liquids: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4472-4486.	1.3	17
11854	Mechanistic insight into Ni-mediated decarbonylation of unstrained ketones: the origin of decarbonylation catalytic activity. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2332-2339.	2.3	7
11855	Photochemical mechanism of DEACM uncaging: a combined time-resolved spectroscopic and computational study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13418-13430.	1.3	13
11856	C–F bond activation by pentamethylcyclopentadienyl-aluminium(σ): a combined experimental/computational exercise. <i>Chemical Communications</i> , 2020, 56, 7865-7868.	2.2	18
11857	Synthesis, crystal structures, DFT studies, antibacterial assays and interaction assessments with biomolecules of new platinum(σ) complexes with adamantane derivatives. <i>New Journal of Chemistry</i> , 2020, 44, 11546-11556.	1.4	11
11858	Understanding the structures and aromaticity of heteroporphyrins with computations. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 4415-4422.	1.5	7
11859	A novel dihydro phenylquinazolinone-based two-in-one colourimetric chemosensor for nickel(σ), copper(σ) and its copper complex for the fluorescent colourimetric nanomolar detection of the cyanide anion. <i>RSC Advances</i> , 2020, 10, 44860-44875.	1.7	30
11860	<i>Meso</i> -Zn(σ)porphyrins of tailored functional groups for intensifying the photoacoustic signal. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8546-8559.	2.7	4
11861	On the convergence of Z-averaged perturbation theory. <i>Journal of Chemical Physics</i> , 2008, 128, 074107.	1.2	15
11862	Isoenergetic two-photon excitation enhances solvent-to-solute excited-state proton transfer. <i>Journal of Chemical Physics</i> , 2020, 153, 224301.	1.2	4
11863	Coulomb explosion imaging for gas-phase molecular structure determination: An <i>ab initio</i> trajectory simulation study. <i>Journal of Chemical Physics</i> , 2020, 153, 184201.	1.2	15
11864	Excited state diabatisation on the cheap using DFT: Photoinduced electron and hole transfer. <i>Journal of Chemical Physics</i> , 2020, 153, 244111.	1.2	13
11865	Effect of Substitution for Insertion of CO ₂ into Epoxides and Aziridines: An <i>Ab Initio</i> Study. <i>Australian Journal of Chemistry</i> , 2020, 73, 30.	0.5	1
11866	Utilizing the Combined Power of Theory and Experiment to Understand Molecular Structure – Solid-State and Gas-Phase Investigation of Morpholine Borane. <i>Australian Journal of Chemistry</i> , 2020, 73, 794.	0.5	4
11867	Structural insights into a versatile macrocyclic family based on 2,5-diphenyl[1,3,4]oxadiazole: a combined X-ray diffraction and computational study. <i>Supramolecular Chemistry</i> , 2017, 29, 896-911.	1.5	3
11868	From simple molecules to nanotubes. Reliable predictions of ionization potentials from the $\hat{\Gamma}$ MP2-SCS methods. <i>New Journal of Physics</i> , 2020, 22, 083084.	1.2	4
11869	Numerical variational solution of hydrogen molecule and ions using one-dimensional hydrogen as basis functions. <i>New Journal of Physics</i> , 2020, 22, 093059.	1.2	8
11870	Thousands of reactants and transition states for competing E2 and S _N 2 reactions. <i>Machine Learning: Science and Technology</i> , 2020, 1, 045026.	2.4	33

#	ARTICLE	IF	CITATIONS
11891	Reactivity of Disulfidodicopper(II) Complexes and Its Theoretical Study by DFT Calculation. Transactions of the Materials Research Society of Japan, 2009, 34, 509-512.	0.2	2
11892	A Non-Hermitian Coupled Perturbed Hartree-Fock Method for Complex Potentials and Calculations of Electronic Structures with Electric Currents. Transactions of the Materials Research Society of Japan, 2013, 38, 397-404.	0.2	3
11893	Comparison of P- and As-core-modified porphyrins with the parental porphyrin: a computational study. Pure and Applied Chemistry, 2021, 93, 561-570.	0.9	2
11894	Synthesis of Hydroxy and Methoxy Perylene Quinones, Their Spectroscopic and Computational Characterization, and Their Antiviral Activity. Photochemistry and Photobiology, 2005, 81, 924.	1.3	14
11895	Topological Analysis and Frequency Dependent Hyperpolarizability Calculations of FDDNP: a DFT Study. Chemistry Journal of Moldova, 2016, 11, 84-92.	0.3	1
11896	Structural Distortions of Coordinated Ketene Molecule Induced by the Pseudo Jahn-Teller Effect. Chemistry Journal of Moldova, 2016, 11, 99-104.	0.3	1
11897	Joint Computational and Experimental Investigations on the Synthesis and Properties of Hantzsch-type Compounds: An Overview. Current Organic Chemistry, 2019, 23, 1421-1438.	0.9	4
11898	Kinetics of Decomposition Reactions of Acetic Acid Using DFT Approach. Open Chemical Engineering Journal, 2018, 12, 14-23.	0.4	8
11899	A New Configurational Analysis of 1,6,7-triacetoxy-8,13-epoxy-14-labden-11-one Isolated from Plectranthus ornatus Based on NMR and Theoretical Calculations. Open Natural Products Journal, 2009, 2, 1-5.	0.8	2
11900	Evaluation of Copper Oxide-Based Interconnecting Materials. The Open Surface Science Journal, 2010, 3, 123-130.	2.0	17
11902	Quantum-chemical calculations of the products and energies of electron induced ionization of 2-Furanmethanol, Tetrahydro-and 3-Furanol. Facta Universitatis - Series Physics Chemistry and Technology, 2008, 6, 127-139.	0.2	7
11903	A Quantum Chemical Study on Hydration of Ra (II): Comparison with the Other Hydrated Divalent Alkaline Earth Metal Ions. Journal of Computer Chemistry Japan, 2014, 13, 105-113.	0.0	9
11904	Periodic-Boundary-Condition Calculation using Heyd-Scuseria-Ernzerhof Screened Coulomb Hybrid Functional: Electronic Structure of Anatase and Rutile TiO ₂ . Journal of Computer Chemistry Japan, 2006, 5, 7-18.	0.0	22
11905	Estimation of Solvent Effects for the Complexing Reaction of Propylene and Nickel Dithiolene. Data Science Journal, 2007, 6, S837-S846.	0.6	8
11906	Peculiarities of sulfur dioxide sorption from air by weak base anion exchangers. Proceedings of the National Academy of Sciences of Belarus, Chemical Series, 2020, 56, 263-270.	0.1	2
11907	Thermochemical study of uranium by ab initio quantum chemical calculations. Journal of Nuclear Fuel Cycle and Environment, 2001, 7, 75-80.	0.1	2
11908	New Organic Materials Based on Thiophene for Photovoltaic Device: Theoretical investigation. Turkish Computational and Theoretical Chemistry, 2018, 2, 36-48.	0.5	5
11910	On the Efficient Evaluation of the Exchange Correlation Potential on Graphics Processing Unit Clusters. Frontiers in Chemistry, 2020, 8, 581058.	1.8	11

#	ARTICLE	IF	CITATIONS
11911	How Does Replacement of the Axial Histidine Ligand in Cytochrome c Peroxidase by N ¹ -Methyl Histidine Affect Its Properties and Functions? A Computational Study. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7133.	1.8	5
11912	Polymer designs for dense metal infiltration for higher dry-etch resistance. <i>Japanese Journal of Applied Physics</i> , 2020, 59, SIIC02.	0.8	4
11913	Electron Transport Materials: Synthesis, Properties and Device Performance. <i>International Journal of Organic Chemistry</i> , 2012, 02, 101-110.	0.3	7
11914	Pseudo Jahn-Teller Effect in Puckering and Planarization of Heterocyclic Compounds. <i>International Journal of Organic Chemistry</i> , 2018, 08, 142-159.	0.3	7
11915	Spin-Orbit Electronic Structure of the ScBr Molecule. <i>Journal of Modern Physics</i> , 2011, 02, 1172-1177.	0.3	5
11916	Theoretical Study on the Pyrolysis of Sulphonyl Oximes in the Gas Phase. <i>Bulletin of the Korean Chemical Society</i> , 2003, 24, 853-858.	1.0	4
11917	Protonation and Energetical Investigations of Calix[4]-cyclen-benzo-crown-6 and Its Complexes with Zinc and Copper. <i>Bulletin of the Korean Chemical Society</i> , 2004, 25, 819-822.	1.0	3
11918	Aromatic Formation from Vinyl Radical and Acetylene. A Mechanistic Study. <i>Bulletin of the Korean Chemical Society</i> , 2008, 29, 319-322.	1.0	4
11919	Uptake Effects of Two Electrons for Relative Stability and Atomic Structures of Carbon Cluster Isomers of C ₂₀ : ab initio Methods. <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 445-448.	1.0	4
11920	Adsorption Reactions of Trimethylgallium and Arsine on H/Si(100)-2x1 Surface. <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 1805-1810.	1.0	5
11921	Magnetic Exchange Interactions in a 2D Grid-like Copper(II) Polymer with Bridging End-on Cyanato and Pyrazine Ligands: A DFT Study. <i>Bulletin of the Korean Chemical Society</i> , 2010, 31, 1704-1710.	1.0	2
11922	Full Geometry Optimizations of Bond-Stretch Isomers of C ₂₀ +Fullerene Dication by the Hybrid Density Functional B3LYP Methods. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 277-280.	1.0	3
11923	Determination of Atomic Structures and Relative Stabilities of Diadduct Regioisomers of C ₂₀ X ₂ (X = H, F, Cl, Br, and OH) by the Hybrid Density-Functional B3LYP Method. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 3372-3376.	1.0	5
11924	DFT Study for Substitution Patterns of C ₂₀ H ₁₈ X ₂ Regioisomers (X) Tj ETQq _{1,0} 0.784314 rgBT	1.0	7
11925	Adsorption Mechanisms of NH ₃ on Chlorinated Si(100)-2x1 Surface. <i>Bulletin of the Korean Chemical Society</i> , 2012, 33, 775-778.	1.0	4
11926	DFT Study of the Effect of the Li ₂₀ Coating Pattern on the Volume and Band Gap of C ₂₀ Fullerene Cages. <i>Bulletin of the Korean Chemical Society</i> , 2013, 34, 365-366.	1.0	3
11927	Frontier Orbitals of Fifteen C ₂₀ H ₁₇ (OH) ₃ Regioisomers: Hybrid DFT B3LYP Study. <i>Bulletin of the Korean Chemical Society</i> , 2013, 34, 2403-2407.	1.0	2
11928	Analysis of Nonclassical Fullerene C ₂₄ Regioisomers Encapsulating H ₂ O using Hybrid Density Functional Methods B3LYP and M06-2X. <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 899-904.	1.0	1

#	ARTICLE	IF	CITATIONS
11929	Theoretical Study of the Hydroalumination Reaction of Cyclopropane with Alane. <i>Journal of the Korean Chemical Society</i> , 2013, 57, 216-220.	0.2	2
11930	Local Dielectric Property of Cubic, Tetragonal, and Monoclinic Hafnium Oxides. <i>Japanese Journal of Applied Physics</i> , 2012, 51, 031101.	0.8	4
11931	Fast and automatic estimation of transition state structures using tight binding quantum chemical calculations. <i>PeerJ Physical Chemistry</i> , 0, 2, e15.	0.0	15
11932	Will 1,2-dihydro-1,2-azaborine-based drugs resist metabolism by cytochrome P450 compound I?. <i>PeerJ</i> , 2016, 4, e2299.	0.9	1
11933	Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. <i>Journal of Organic Chemistry</i> , 2012, 77, 10824-10834.	1.7	14
11934	Unsupervised machine learning for unbiased chemical classification in X-ray absorption spectroscopy and X-ray emission spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23586-23601.	1.3	23
11935	Self-assembly of ultra-small-sized carbon nanoparticles in lipid membrane disrupts its integrity. <i>Nanoscale Advances</i> , 2021, 4, 163-172.	2.2	6
11936	On the rearrangements of biologically-relevant vinyl allene oxides to cis-cyclopentenones, ketols, and Favorskii-type carboxylic acids. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9460-9469.	1.5	2
11937	MD simulations and QM/MM calculations reveal the key mechanistic elements which are responsible for the efficient C-H amination reaction performed by a bioengineered P450 enzyme. <i>Chemical Science</i> , 2021, 12, 14507-14518.	3.7	21
11938	QM/MM modeling of class A β -lactamases reveals distinct acylation pathways for ampicillin and cefalexin. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9182-9189.	1.5	7
11939	Computational UV spectra for amorphous solids of small molecules. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24413-24420.	1.3	4
11940	Precise Recognition of Palladium Through Interlaminal Chelation in a Covalent Organic Framework. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
11941	Facile synthesis of hemiacetal ester-based dynamic covalent polymer networks combining fast reprocessability and high performance. <i>Green Chemistry</i> , 2021, 23, 9061-9070.	4.6	14
11942	Differences in the torsional anharmonicity between reactant and transition state: the case of 3-butenal + H abstraction reactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25414-25423.	1.3	3
11943	Catalytic approach to in vivo metabolism of atractylenolide III using biomimetic iron-porphyrin complexes. <i>RSC Advances</i> , 2021, 11, 33048-33054.	1.7	1
11944	Chiral Hypervalent Bromine(III) (Bromonium Salt): Hydrogen- and Halogen-Bonding Bifunctional Asymmetric Catalysis by Diaryl-bromanes. <i>ACS Catalysis</i> , 2021, 11, 13028-13033.	5.5	33
11945	Structures of Nitrogen Oxides Attached to Anionic Gold Clusters Au ₄ ⁺ Revealed by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9040-9047.	1.1	4
11946	Role of Methylene Diphenyl Diisocyanate (MDI) Additives on SBS-Modified Asphalt with Improved Thermal Stability and Mechanical Performance. <i>Energy & Fuels</i> , 2021, 35, 17629-17641.	2.5	9

#	ARTICLE	IF	CITATIONS
11947	Physicochemical and computational analysis of the melamine resin derivative for the glyphosate absorption from water using Langmuir-type model. <i>International Journal of Environmental Science and Technology</i> , 2022, 19, 7791-7802.	1.8	2
11948	Grassmann Extrapolation of Density Matrices for Born-Oppenheimer Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6965-6973.	2.3	10
11949	Switching Chemoselectivity Based on the Ring Size: How to Make Ring-Fused Indoles Using Transition-Metal-Mediated Cross-Coupling. <i>ACS Catalysis</i> , 2021, 11, 12821-12832.	5.5	7
11950	Shortwave Infrared Absorptive and Emissive Pentamethine-Bridged Indolizine Cyanine Dyes. <i>Journal of Organic Chemistry</i> , 2021, 86, 15376-15386.	1.7	16
11951	Large-Area Endohedral Metallofullerene Single-Crystal Arrays for High-Performance Field-Effect Transistors and Photodetectors. <i>Advanced Electronic Materials</i> , 2022, 8, 2100753.	2.6	4
11952	Double Tethered Metallacyclobutane Catalyst for Cyclic Polymer Synthesis. <i>Journal of the American Chemical Society</i> , 2021, 143, 17276-17283.	6.6	10
11953	Theoretical investigation on the mechanisms and kinetics of OH/NO ₃ -initiated atmospheric oxidation of vanillin and vanillic acid. <i>Chemosphere</i> , 2022, 288, 132544.	4.2	3
11954	PDG: A Composite Method Based on the Resolution of the Identity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9421-9429.	1.1	3
11955	Pancake Bonding Seen through the Eyes of Spectroscopy. , 0, , .		1
11956	Imidacloprid Crystal Polymorphs for Disease Vector Control and Pollinator Protection. <i>Journal of the American Chemical Society</i> , 2021, 143, 17144-17152.	6.6	27
11957	Corrosion Resistance of Sulfur-Selenium Alloy Coatings. <i>Advanced Materials</i> , 2021, 33, e2104467.	11.1	21
11958	Scope, Limitations and Mechanistic Analysis of the HyperBTM-Catalyzed Acylative Kinetic Resolution of Tertiary Heterocyclic Alcohols**. <i>European Journal of Organic Chemistry</i> , 2022, 2022, e202101111.	1.2	4
11959	Detection of Ylide Formation between an Alkylidenecarbene and Acetonitrile by Femtosecond Transient Absorption Spectroscopy. <i>Journal of the American Chemical Society</i> , 2021, 143, 17090-17096.	6.6	10
11960	DFT Probe into the Mechanism of Formic Acid Dehydrogenation Catalyzed by Cp*Co, Cp*Rh, and Cp*Ir Catalysts with 4,4'-Amino-/Alkylamino-Functionalized 2,2'-Bipyridine Ligands. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9478-9488.	1.1	7
11961	Bonding and Reactivity of a Pair of Neutral and Cationic Heterobimetallic RuZn ₂ Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 16256-16265.	1.9	7
11962	Achieving a Favorable Activation of the C-F Bond over the C-H Bond in Five- and Six-Membered Ring Complexes by a Coordination and Aromaticity Dually Driven Strategy. <i>Organometallics</i> , 2021, 40, 3397-3407.	1.1	11
11963	Density Functional Theory-Inspired Design of Ir/P,S-Catalysts for Asymmetric Hydrogenation of Olefins. <i>Organometallics</i> , 2021, 40, 3424-3435.	1.1	5
11964	Stepwise redox changes alter the speciation and mobilization of phosphorus in hydromorphic soils. <i>Chemosphere</i> , 2022, 288, 132652.	4.2	16

#	ARTICLE	IF	CITATIONS
11965	Univariate classification of phosphine ligation state and reactivity in cross-coupling catalysis. <i>Science</i> , 2021, 374, 301-308.	6.0	97
11966	Determination of the SmO ⁺ bond energy by threshold photodissociation of the cryogenically cooled ion. <i>Journal of Chemical Physics</i> , 2021, 155, 174303.	1.2	15
11967	Fe-carbon hybrid composite interlayer for improved electrochemical performance of Li-S battery. <i>Electrochimica Acta</i> , 2022, 401, 139466.	2.6	5
11968	Electronic Structure Theory Calculations Using Modern Architectures: KNL vs Haswell. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6910-6917.	2.3	1
11969	Quantum Chemical Calculations of Transition Metal Complexes. , 2003, , 361-380.		0
11971	Combined DFT and electrostatic calculations of pK _a s in proteins: study of cytochrome c oxidase. , 2006, , 53-78.		0
11972	Recent Trends in Quantum Chemical Calculations for Surface-Molecule Interacting Systems. <i>Hyomen Kagaku</i> , 2007, 28, 150-159.	0.0	0
11975	Density Functional Calculation of the Structure and Electronic Properties of Cu _n O _n (n=1-4) Clusters. <i>Lecture Notes in Computer Science</i> , 2009, , 122-130.	1.0	0
11976	Electronic Properties and Reactivities of Perfect, Defected, and Doped Single-Walled Carbon Nanotubes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 421-471.	0.6	1
11977	Theoretical Study of Cycloaddition Reactions of C ₆₀ on the Si(100)-2 \times 1 Surface. <i>Bulletin of the Korean Chemical Society</i> , 2010, 31, 1681-1688.	1.0	2
11979	Density functional study on chirospectra of bruguierols. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2011, 60, 043101.	0.2	0
11980	Exploring the Borderland between Physics and Chemistry. , 2011, , .		1
11982	Density Functional Study of the Origin of the Strongly Delocalized Electronic Structure of the CuA Site in Cytochrome c Oxidase. <i>Progress in Theoretical Chemistry and Physics</i> , 2012, , 513-524.	0.2	0
11983	Parallel Quantum Chemistry at the Crossroads. <i>Advances in Computer and Electrical Engineering Book Series</i> , 2012, , 239-266.	0.2	0
11984	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations. , 2012, , 21-36.		0
11985	Discovery of Chemical Principles: Symmetry Rules for Degenerate Excitations. <i>Journal of Computer Chemistry Japan</i> , 2012, 11, 1-16.	0.0	4
11986	Is the dynamical polarization a significant part of the contribution of the triples to the correlation energy?. <i>Highlights in Theoretical Chemistry</i> , 2013, , 135-141.	0.0	0
11987	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. <i>Highlights in Theoretical Chemistry</i> , 2014, , 39-47.	0.0	0

#	ARTICLE	IF	CITATIONS
11988	Mechanism of ketone hydrosilylation using NHC-Cu(I) catalysts: a computational study. Highlights in Theoretical Chemistry, 2014, , 135-147.	0.0	0
11989	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Highlights in Theoretical Chemistry, 2014, , 225-239.	0.0	0
11990	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O2. Highlights in Theoretical Chemistry, 2014, , 143-155.	0.0	0
11991	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. Highlights in Theoretical Chemistry, 2014, , 105-110.	0.0	0
11993	Ab Initio Molecular Orbital Calculations on the Boson Peak Frequencies of Molecular Glasses. Progress of Theoretical Physics Supplement, 2013, 126, 147-150.	0.2	0
11994	Strictly Localised Molecular Orbitals in QM/MM Methods. , 2014, , 71-89.		2
11995	Unidirectional Photo-induced Charge Separation and Thermal Charge Recombination of Cofacially Aligned Donor-Acceptor System Probed by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy. Bulletin of the Korean Chemical Society, 2014, 35, 587-596.	1.0	1
11996	Structure of Molecules in the Vapour Phase. Nihon Kessho Gakkaishi, 1975, 17, 21-35.	0.0	0
11997	Hydrogen Bonding between Molecules or Ions and in Molecular Crystals. , 1978, , 229-255.		0
11998	Gaussian Basis Sets. , 1981, , 15-20.		0
11999	INTRODUCTION AND COMPUTATIONAL METHODS. , 1981, , 1-52.		0
12000	Thermochemistry and Kinetics of Ionic and Radical Reactions in the Gas Phase. Topics in Molecular Organization and Engineering, 1989, , 233-257.	0.1	0
12001	Laboratory Projects in Computational Organic Chemistry. , 1991, , 411-428.		0
12002	A Computational Quantum Mechanical Study on Weakly Bonded Clusters of NH3 with SO2 and HNC. , 1992, , 211-216.		0
12003	Toward Quantitative Protein Structure Prediction. , 1994, , 507-548.		0
12005	An ab Initio Study on Adsorptive Interactions of Alcohols and Aromatic Compounds onto the Surface of Silica Gel. Kluwer International Series in Engineering and Computer Science, 1996, , 905-912.	0.2	3
12006	Vibrational Modulation Effects on EPR Spectra. Topics in Molecular Organization and Engineering, 1996, , 251-260.	0.1	0
12007	A Theoretical Study on Interactions between Silica Gel and Adsorbed Molecules by using ab initio MO Method. Kluwer International Series in Engineering and Computer Science, 1996, , 897-904.	0.2	4

#	ARTICLE	IF	CITATIONS
12008	Key features of quantum chemistry methods used in CAMD. , 1996, , 266-300.		0
12009	Comparison of reaction pathways calculated by different algorithms for disilane and water trimer. , 1997, , 229-235.		0
12010	Competitive Hydrogen Bonds and Conformational Equilibria in 2,6-Disubstituted Phenols Containing two Different Carbonyl Substituents. , 1999, , 59-72.		0
12011	The Dimer of Cyanodiacetylene: Stacking vs. Hydrogen Bonding. , 1999, , 73-86.		0
12013	Electronic Control of Molecular Configuration Instability via Vibronic Coupling. Pseudo Jahn-Teller Stabilization of Vertically Excited States of F2CO, N2H2 and H2C2O Molecules. Chemistry Journal of Moldova, 2014, 9, 80-89.	0.3	2
12014	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	0.2	0
12015	DFT STUDY ON HYDROGENATION REACTION OF ACETALDEHYDE TO ETHANOL IN GAS AND WATER PHASE. International Journal of Research in Engineering and Technology, 2016, 05, 53-57.	0.1	0
12016	4-Aminosubstituted 1,6-dihidropyrazolo[3,4-e][1,4] diazepines: the synthesis, NMR-spectral and quantum-chemical study. Journal of Organic and Pharmaceutical Chemistry, 2016, 14, 43-51.	0.0	0
12017	Origin of the chemical stability of phosphine-phosphoramidites: structural study of an UPPhos-type crystal and application of UPPhos in the asymmetric hydrogenation of imines. Acta Crystallographica Section C, Structural Chemistry, 2017, 73, 632-637.	0.2	1
12019	Selection of an Appropriate Basis Set for Accurate Description of Binding Energy: A First Principles Study. Journal of Natural and Applied Sciences, 2017, 21, 847.	0.1	0
12020	Development of the Divide-and-Conquer Based Single Reference Theory for Static Correlation Systems with Finite Temperature Scheme. Journal of Computer Chemistry Japan, 2018, 17, 212-214.	0.0	0
12021	Nitrogen Gas on Graphene: Pairwise Interaction Potentials. Lecture Notes in Computer Science, 2018, , 563-578.	1.0	3
12029	Electrical and vibrational properties of hydrogen bonds in glycine-water clusters. , 2019, , .		0
12030	The Template-Directed Synthesis of a Fully Conjugated 14-Porphyrin Nanoball. Springer Theses, 2020, , 151-221.	0.0	0
12032	Design, Synthesis and Characterization of Nâ€“Substituted Heteroaromatics: DFTâ€“Studies and Organic Light Emitting Device Application. ChemistrySelect, 2020, 5, 5903-5915.	0.7	4
12033	Crystal and geometry-optimized structure of an anthracene-based Dielsâ€“Alder adduct. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 639-646.	0.2	0
12034	Rotameric Isomers of La₂@C₈₀ & Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization. ECS Journal of Solid State Science and Technology, 2020, 9, 061014.	0.9	6
12035	Wirt-Gast-Komplexe von [bfu.bfu.bfu]: Vorhersage von IonenselektivitÃten mittels quantenchemischer Rechnungen XIII. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 769-775.	0.3	1

#	ARTICLE	IF	CITATIONS
12036	New spiro-borane and spiro-borate derived from dipyrromethane and their H/D exchange properties. <i>Polyhedron</i> , 2020, 186, 114612.	1.0	3
12038	Computational Exploration of the Efficacy of Fe(II)PNN Versus Fe(II)NNN Pincer Complexes in the Hydrogenation of Carbon Dioxide to Methanol. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24350-24362.	1.5	5
12039	Ascendancy of Nitrogen Heterocycles in the Computationally Designed Mn(I)PNN Pincer Catalysts on the Hydrogenation of Carbon Dioxide to Methanol. <i>Inorganic Chemistry</i> , 2022, 61, 1851-1868.	1.9	8
12040	Tuning azulene defects and doping of N atoms in graphene nanosheets: Improving nonlinear optical properties of carbon-based nano materials. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 136, 115040.	1.3	7
12041	SSIPTools: Software and Methodology for Surface Site Interaction Point (SSIP) Approach and Applications. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5331-5335.	2.5	6

12042

#	ARTICLE	IF	CITATIONS
12055	Group 11 metal complexes of the dinucleating triazole appended bisphosphine 1,4-bis(5-(diisopropylphosphaneyl)-1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)benzene. Dalton Transactions, 2021, 50, 16782-16794.	1.6	3
12056	Novel anthracene-based organic dyes as co-sensitizers of porphyrins for developing efficient dye-sensitized solar cells. New Journal of Chemistry, 0, , .	1.4	2
12057	Natural reaction orbitals for characterizing electron transfer responsive to nuclear coordinate displacement. Physical Chemistry Chemical Physics, 2022, 24, 3532-3545.	1.3	2
12058	Silicon $\hat{\nu}$ single molecule $\hat{\nu}$ silicon circuits. Chemical Science, 2021, 12, 15870-15881.	3.7	7
12059	Density functional theory studies on the excited-state properties of Bilirubin molecule. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 163101.	0.2	0
12060	Atomic-scale Modelling of Redox-active Organic Molecules and Polymers for Energy Applications. RSC Polymer Chemistry Series, 2020, , 93-136.	0.1	0
12061	^t Bu ₄ octapa-alkyl-NHS for metalloradiopeptide preparation. Dalton Transactions, 2020, 49, 7605-7619.	1.6	6
12062	When biomolecules meet 2-hydrazinopyrazine: from theory through experiment to molecular levels using a wide spectrum of techniques. RSC Advances, 2020, 10, 40673-40688.	1.7	1
12064	Radical chain monoalkylation of pyridines. Chemical Science, 2021, 12, 15362-15373.	3.7	7
12065	Excited-State Dynamics of a Substituted Fluorene Derivative. The Central Role of Hydrogen Bonding Interactions with the Solvent. Journal of Physical Chemistry B, 2021, 125, 12242-12253.	1.2	2
12066	Electromechanical Characteristics by a Vertical Flip of C70 Fullerene Prolate Spheroid in a Single-Electron Transistor: Hybrid Density Functional Methods. Nanomaterials, 2021, 11, 2995.	1.9	0
12067	Solvent-Dependent Photophysical Properties of a Semiconducting One-Dimensional Silver Cluster-Assembled Material. Inorganic Chemistry, 2021, 60, 18234-18241.	1.9	11
12068	Mechanistic insight into selective adsorption and easy regeneration of carboxyl-functionalized MOFs towards heavy metals. Journal of Hazardous Materials, 2022, 424, 127684.	6.5	35
12069	Exploring Guest-Host Interactions in Gas Hydrates: Insights from Quantum Mechanics. Energy & Fuels, 2021, 35, 18604-18614.	2.5	5
12070	Mechanistic insights into Rh(III)-catalyzed C-H activation/annulation of N-Aryloxyacetamides with alkynyloxiranes. Molecular Catalysis, 2021, 516, 111971.	1.0	1
12071	Toward a Generalized Hückel Rule: The Electronic Structure of Carbon Nanocones. Journal of Physical Chemistry A, 2021, 125, 9819-9825.	1.1	8
12072	Parallel Quantum Chemistry at the Crossroads. , 0, , 163-190.		0
12074	Theoretical Methods for Modeling Chemical Processes on Semiconductor Surfaces. , 2004, , 246-265.		0

#	ARTICLE	IF	CITATIONS
12076	Redox Catalysis and Reactivity of Metalloporphyrines. , 2009, , 201-212.		0
12077	Directed Assembly of Large-Sized, Mechanically Robust, Nature-Inspired Graphene Oxide/Sodium Alginate Nanocomposite Paper. <i>Macromolecular Materials and Engineering</i> , 2020, 305, 2000493.	1.7	3
12078	Single photon simultaneous K-shell ionization/excitation in $C_{60}H_{60}$: experiment and theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 244010.	0.6	5
12079	Thermal desorption and pyrolysis direct analysis in real time mass spectrometry of Nafion membrane. <i>Journal of Applied Polymer Science</i> , 2021, 138, 50172.	1.3	6
12080	Oxidative Addition of Biphenylene and Chlorobenzene to a Rh(CNC) Complex. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3899-3906.	1.0	12
12081	Synthesis and Biological Activity of N-(Indolyl)trifluoroacetamides Based on Substituted 6-Aminoindoles. <i>Moscow University Chemistry Bulletin</i> , 2020, 75, 382-387.	0.2	3
12082	Computational NMR Study of Ion Pairing of 1-Decyl-3-methyl-imidazolium Chloride in Molecular Solvents. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10776-10786.	1.2	6
12083	Spiro-based diamond-type nanogrids (DGs) <i>via</i> two ways: A_1B_1 -type + A_2B_2 -type gridization of vertical spiro-based fluorene synthons. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 10408-10416.		5
12084	The Effects of Oxidation States and Spin States of Chromium Interaction with Sargassum Sp. A Spectroscopic and Density Functional Theoretical Study. <i>Green and Sustainable Chemistry</i> , 2021, 11, 125-141.	0.8	2
12085	Aggregation-induced emission spectra of triphenylamine salicylaldehyde derivatives <i>via</i> excited-state intramolecular proton transfer revealed by molecular spectral and dynamics simulations. <i>RSC Advances</i> , 2021, 11, 37171-37180.	1.7	5
12086	<i>O</i> -Acetylated sugars in the gas phase: stability, migration, positional isomers and conformation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1016-1022.	1.3	4
12087	A mechanistic study on the regioselective Ni-catalyzed methylation-alkenylation of alkyne with $AlMe_3$ and allylic alcohol. <i>Organic Chemistry Frontiers</i> , 2021, 9, 163-172.	2.3	9
12088	Regioselectivity in metalloradical catalyzed C-H bond activation: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2022, 957, 122179.	0.8	1
12089	Influence of pseudo-polymorphism on the structure and thermal behavior of the new barium β -diketonate complexes $[Ba(adtf_a)_2(18\text{-crown-}6)]$ and $[Ba(adtf_a)_2(18\text{-crown-}6)](CDCl_3)_2$. <i>Inorganica Chimica Acta</i> , 2022, 531, 120734.	1.2	5
12090	Study on performance and charging dynamics of N/O codoped layered porous carbons derived from L-tyrosine for supercapacitors. <i>Applied Surface Science</i> , 2022, 578, 151888.	3.1	17
12091	Computational study of the interaction of heavy metal ions, Cd(II), Hg(II), and Pb(II) on lignin matrices. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 111, 108080.	1.3	7
12092	Effect of Lewis Acids on the Catalyst Activity for Alkene Metathesis, Z/E- Selectivity and Stability of Tungsten Oxo Alkylidenes. <i>Topics in Catalysis</i> , 2022, 65, 433-447.	1.3	3
12093	Molecular Dynamics Assessment of Doxorubicin Adsorption on Surface-Modified Boron Nitride Nanotubes (BNNTs). <i>Journal of Physical Chemistry B</i> , 2021, 125, 13168-13180.	1.2	7

#	ARTICLE	IF	CITATIONS
12094	Quantitative Theoretical Study of Molecular and Chain-Level Conformational Properties of Poly(ferrocenyldimethylsilanes). <i>Macromolecules</i> , 0, , .	2.2	0
12095	Learning to Measure: Adaptive Informationally Complete Generalized Measurements for Quantum Algorithms. <i>PRX Quantum</i> , 2021, 2, .	3.5	37
12096	Analysis of different sets of spin-adapted substitution operators in open-shell coupled cluster theory. <i>Molecular Physics</i> , 2022, 120, .	0.8	1
12097	An inexpensive density functional theory based protocol to predict accurate ¹⁹ F NMR chemical shifts. <i>Journal of Computational Chemistry</i> , 2022, 43, 170-183.	1.5	5
12098	Arbitrarily accurate quantum alchemy. <i>Journal of Chemical Physics</i> , 2021, 155, 224103.	1.2	9
12099	The kinetics and mechanism of B ₂ O ₃ formation from the chemically-synthesized HBO ₂ under non-isothermal conditions. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2022, 135, 349.	0.8	2
12100	The Role of (ⁱ t-Bu) ² POCOPIr(I) and Iridium(III) Pincer Complexes in the Catalytic Hydrogenolysis of Silyl Triflates into Hydrosilanes. <i>Organometallics</i> , 2022, 41, 1786-1796.	1.1	6
12101	Glycolonitrile (HOCH ₂ CH ₂ CN) Chemistry in Star-forming Regions. <i>Astrophysical Journal, Supplement Series</i> , 2021, 257, 26.	3.0	4
12102	Ammonia-Borane Dehydrogenation Catalyzed by Dual-Mode Proton-Responsive Ir-CNNH Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 18490-18502.	1.9	9
12103	Improved Methods for the Synthesis of KB ₃ H ₈ , NH ₃ B ₃ H ₇ , and N-Alkyl Analogues of NH ₃ B ₃ H ₇ . <i>Inorganic Chemistry</i> , 2021, 60, 18466-18472.	1.9	6
12104	Unraveling the Effect of Aromatic Groups in Mn(I)NNN Pincer Complexes on Carbon Dioxide Activation Using Density Functional Study. <i>Frontiers in Chemistry</i> , 2021, 9, 778718.	1.8	7
12105	The catalytic mechanism of Pd ₂ glutamine driven by a Cys-His-Glu triad: a computational study. <i>ChemBioChem</i> , 2021, , .	1.3	3
12106	Theoretical Investigation of Glycine Micro-Solvated. Energy and NMR Spin Spin Coupling Constants Calculations. <i>Sci</i> , 2021, 3, 41.	1.8	2
12107	The Crystal Structure of Cysteamine Dioxygenase Reveals the Origin of the Large Substrate Scope of This Vital Mammalian Enzyme. <i>Biochemistry</i> , 2021, 60, 3728-3737.	1.2	10
12108	Computational Study of CO ₂ Reduction Catalyzed by Iron(I) Complex at Different Spin States: Cooperativity of Hydrogen Bonding and Auxiliary Group Effect. <i>ACS Omega</i> , 2021, 6, 31971-31981.	1.6	0
12109	Assessing and rationalizing the performance of Hessian update schemes for reaction path Hamiltonian rate calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 204112.	1.2	1
12110	A global analysis of excited states: the global transition contribution grids. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
12111	Radical and Ionic Mechanisms in Rearrangements of <i>o</i> -Tolyl Aryl Ethers and Amines Initiated by the Grubbs-Stoltz Reagent, Et ₃ SiH/KOtBu. <i>Molecules</i> , 2021, 26, 6879.	1.7	4

#	ARTICLE	IF	CITATIONS
12112	Supramolecular structure and spectroscopic characterization of new 1,3,5-triaza-2-boracyclohex-3-en derivative formed under mild conditions between 2-imino-4-thiobiuret and boric acid. <i>Journal of Molecular Structure</i> , 2021, , 131968.	1.8	1
12113	Pincer iridium(III)-catalyzed enantioselective C(sp ³)-H functionalization via carbenoid C-H insertion of 3-diazooxindoles with 1,4-cyclohexadiene. <i>Chinese Chemical Letters</i> , 2022, 33, 2437-2441.	4.8	7
12114	Model studies on the formation of 2-vinylpyrazine and 2-vinyl-6-methylpyrazine in Maillard-type reactions. <i>Food Chemistry</i> , 2022, 374, 131652.	4.2	4
12115	Intramolecular Relaxation Dynamics Mediated by Solvent-Solute Interactions of Substituted Fluorene Derivatives. Solute Structural Dependence. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12486-12499.	1.2	0
12116	Nucleophilicity and CO ₂ fixation ability of phosphorus, nitrogen and sulfur ylides: insights on stereoelectronic factors from DFT study. <i>Journal of Chemical Sciences</i> , 2021, 133, 1.	0.7	0
12117	Synthesis and Physico-Chemical Properties of Homoleptic Copper(I) Complexes with Asymmetric Ligands as a DSSC Dye. <i>Molecules</i> , 2021, 26, 6835.	1.7	6
12118	Reaction-Controlled Phase-Transfer Process of Polyoxometalate-Based Catalyst for Cellulose Esterification: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 25478-25487.	1.5	3
12119	Evidence for Quantum Chemical Effects in Receptor-Ligand Binding Between Integrin and Collagen Fragments – A Computational Investigation With an Impact on Tissue Repair, Neurooncology and Glycobiology. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 756701.	1.6	2
12120	Low-temperature Hg ⁰ abatement by ionic liquid based on weak interaction. <i>Journal of Hazardous Materials</i> , 2022, 426, 127836.	6.5	3
12121	Oxygen Reduction Activity of N-Containing Organic Molecule Affected by Asymmetric Regulation. <i>Small</i> , 2022, 18, e2105524.	5.2	8
12122	Molecular dynamic simulation, quantum chemical calculation and electrochemical behaviour of Punica granatum peel extract as eco-friendly corrosion inhibitor for stainless steel (SS-410) in acidic medium. <i>Journal of Molecular Liquids</i> , 2022, 346, 118237.	2.3	31
12123	A New Member of the Growing Family of Interconvertible {RuNO} 6,7,8 Species. Redox and Acid-Base Characterization of [Ru((CH ₂) ₂ Me)[9]aneN ₃](NO)] ⁿ⁺ . <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 4842.	1.0	2
12124	Calculating Entropies of Large Molecules in Aqueous Phase. <i>Journal of Chemical Theory and Computation</i> , 2021, , .	2.3	6
12125	Ligand-controlled divergent dehydrogenative reactions of carboxylic acids via C-H activation. <i>Science</i> , 2021, 374, 1281-1285.	6.0	64
12126	Decomposition of nitric oxide by rhodium cluster cations at high temperatures. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26721-26728.	1.3	3
12127	Computational Methods in Organometallic Chemistry. , 2021, , .		1
12128	Ultrafast and efficient energy transfer in a one- and two-photon sensitized rhodamine-BODIPY dyad: a perspective for broadly absorbing photocages. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1795-1802.	1.3	4
12129	An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3043-3058.	1.3	6

#	ARTICLE	IF	CITATIONS
12130	Building toward the future in chemical and materials simulation with accessible and intelligently designed web applications. <i>Annual Reports in Computational Chemistry</i> , 2021, , 163-208.	0.9	5
12131	Mechanistic Study of Cu-Catalyzed Addition Reaction of Isocyanates. <i>Chinese Journal of Organic Chemistry</i> , 2021, 41, 4347.	0.6	4
12132	Fragmentation and rearrangement of Breslow intermediates: branches to both radical and ionic pathways. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 27377-27384.	1.3	2
12133	Photochemical conversion of CO ₂ to CO by a Re complex: theoretical insights into the formation of CO and HCO ₃ ⁺ from an experimentally detected monoalkyl carbonate complex. <i>RSC Advances</i> , 2021, 11, 37713-37725.	1.7	6
12134	Direct synthesis of ring-fused quinolines and pyridines catalyzed by <i>η</i> ⁵ -NNH ₂ -Y-ligated manganese complexes (Y = NR ₂ or SR). <i>Catalysis Science and Technology</i> , 2021, 11, 8026-8036.	2.1	9
12135	Structural parameters versus third-order optical susceptibility of zinc porphyrin molecules. <i>Journal of Materials Chemistry C</i> , 2021, 9, 17461-17470.	2.7	8
12136	Arsinocarbyne Reactivity. <i>Dalton Transactions</i> , 2022, , .	1.6	2
12137	Tris(Imidazolyl) Dicopper(I) Complex and its Reactivity to Exert Catalytic Oxidation of Sterically Hindered Phenol Substrates via a [Cu ₂ O] ²⁺ Core. <i>Dalton Transactions</i> , 2022, , .	1.6	0
12138	Platinum Assisted Tandem C Bond Cleavage and N Bond Formation in Amide Functionalized Bisphosphine <i>η</i> ⁵ -Ph ₂ PC ₆ H ₄ C(O)N(H)C ₆ H ₄ PPh ₂ : Synthesis, Mechanistic, and Catalytic Studies. <i>Inorganic Chemistry</i> , 2022, 61, 857-868.	1.9	5
12139	Understanding diversified chemoselectivities in Rh ₂ (II)-catalyzed intramolecular annulation reactions of diazo and N-Sulfonyl-1,2,3-triazole compounds: A DFT study. <i>Molecular Catalysis</i> , 2022, 517, 112047.	1.0	1
12140	Ti ₃ C ₂ T _x MXene nanosheets hybridized with bacteriochlorin ⁺ carotenoid conjugates for photocatalytic hydrogen evolution. <i>New Journal of Chemistry</i> , 2022, 46, 2166-2177.	1.4	8
12141	Theoretical Investigations on the Detecting Mechanism of a Typical 2,4,6-Trinitrophenol Fluorescence Sensor and Its Design Strategy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 230-238.	1.1	1
12142	A mechanistic study on the gold(⁺)-catalyzed cyclization of propargylic amide: revealing the impact of expanded-ring <i>η</i> ⁵ -N-heterocyclic carbenes. <i>Catalysis Science and Technology</i> , 2022, 12, 674-685.	2.1	7
12143	Raman spectroscopy and DFT calculations of PEDOT:PSS in a dipolar field. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 541-550.	1.3	24
12144	Biodegradation of Herbicides by a Plant Nonheme Iron Dioxygenase: Mechanism and Selectivity of Substrate Analogues. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	6
12145	Adiabatic projection: Bridging ab initio, density functional, semiempirical, and embedding approximations. <i>Journal of Chemical Physics</i> , 2022, 156, 014111.	1.2	5
12146	Design of twisted NIR BOPYIN with highly fluorescent intensity for monitoring viscosity. <i>Journal of Molecular Liquids</i> , 2022, 349, 118493.	2.3	4
12147	Protonation-induced fluorescence modulation of carbazole-based emitters. <i>Materials Advances</i> , 2022, 3, 1703-1712.	2.6	6

#	ARTICLE	IF	CITATIONS
12148	Some contribution to W(VI)-peroxo-chemistry: Synthesis, spectroscopic characterization, reactivity and DFT studies. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100327.	1.3	0
12149	Can aluminum, a non-redox metal, alter the thermodynamics of key biological redox processes? The DPPH-QH2 radical scavenging reaction as a test case. <i>Free Radical Biology and Medicine</i> , 2022, 179, 200-207.	1.3	2
12150	First-principles investigations on the feasibility of the GQD-PEB/PUB nanocomposites as the sensitizer of DSSC. <i>Chemical Physics Letters</i> , 2022, 789, 139306.	1.2	3
12151	Enantiomer stability of atropisomeric 1,5-disubstituted 1,2,3-triazoles. , 2022, 1, 100004.		5
12152	Conversion of CO ₂ to cyclic carbonates by metal-ethylenediamine complexes in ionic liquid: A DFT mechanistic study. <i>Journal of CO₂ Utilization</i> , 2022, 57, 101872.	3.3	5
12153	Aqueous zinc batteries using N-containing organic cathodes with Zn ²⁺ and H ⁺ Co-uptake. <i>Chemical Engineering Journal</i> , 2022, 431, 134253.	6.6	37
12154	Starburst configured imidazole-arylamine organic sensitizers for DSSC applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113735.	2.0	5
12155	Selective and swift-responsive "off-on" rhodamine B based chemosensors: Recognition of multi-metal ions, on-site sensing of Fe(III) in water samples and bioimaging in aqueous media. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 426, 113748.	2.0	9
12156	Quasi-Static Two-Dimensional Infrared Spectra of the Carboxyhemoglobin Subsystem under Electric Fields: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9570-9578.	1.2	3
12157	Organic Thermometers Based on Aggregation of Difluoroboron β^2 -Diketonate Chromophores. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10082-10089.	1.1	17
12158	KID Procedure Applied on the [(PY ₅ Me ₂)MoO] ⁺ Complex. <i>ACS Omega</i> , 2020, 5, 30549-30555.	1.6	2
12159	Extensive modelling and quantum chemical study of sterol C-22 desaturase mechanism: A commercially important cytochrome P450 family. <i>Catalysis Today</i> , 2021, , .	2.2	0
12160	New Isoquinoline Alkaloids from <i>Paraphaeosphaeria sporulosa</i> F03, a Fungal Endophyte Isolated from <i>Paepalanthus planifolius</i> . <i>Planta Medica</i> , 2022, 88, 994-1003.	0.7	3
12161	Ambient hydrogenation of carbon dioxide into liquid fuel by a heterogeneous synergetic dual single-atom catalyst. <i>Cell Reports Physical Science</i> , 2022, 3, 100705.	2.8	18
12162	Nitric oxide generation study of unsymmetrical β^2 -diketiminato copper(II) nitrite complexes. <i>Dalton Transactions</i> , 2022, 51, 3485-3496.	1.6	7
12163	Atomistic Molecular Dynamics Simulation Study on the Interaction between Atomically Precise Thiolate-Protected Gold Nanoclusters and Phospholipid Membranes. <i>Langmuir</i> , 2022, 38, 1653-1661.	1.6	4
12164	The Structural and Optical Properties of 1,2,4-Triazolo[4,3-a]pyridine-3-amine. <i>Molecules</i> , 2022, 27, 721.	1.7	4
12165	Computational Investigations of the Reactivity of Metalloporphyrins for Ammonia Oxidation. <i>Topics in Catalysis</i> , 2022, 65, 341-353.	1.3	4

#	ARTICLE	IF	CITATIONS
12166	A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics. <i>Nature Communications</i> , 2022, 13, 89.	5.8	77
12167	Taming salophen in rare earth metallocene chemistry. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 1325-1336.	3.0	7
12168	Role of Anion in Determining the Stereoselectivity of Mg-Ph-BOX-Catalyzed Diels-Alder Reactions: A Computational Study. <i>Organometallics</i> , 2022, 41, 105-114.	1.1	2
12169	Preparation, characterization and cell labelling of strong pH-controlled bicolor fluorescence carbonized polymer dots. <i>RSC Advances</i> , 2022, 12, 1258-1264.	1.7	3
12170	Computational Study of the Rh/phanephos-Catalyzed Enantioselective [2+2+2] Cyclization of Enediyne, Affording Lactone-Fused Cyclohexadiene Bearing a Quaternary Bridgehead Carbon. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 221-229.	2.0	0
12171	Reliability of computed molecular structures. <i>Journal of Computational Chemistry</i> , 2022, 43, 465-476.	1.5	3
12172	Mechanistic insights into the rhodium-catalyzed aryl C-H carboxylation. <i>Organic Chemistry Frontiers</i> , 2022, 9, 370-379.	2.3	4
12173	Heteroleptic Rare-Earth Tris(metallocenes) Containing a Dibenzocyclooctatetraene Dianion. <i>Inorganic Chemistry</i> , 2022, 61, 2444-2454.	1.9	9
12174	Chiral Binaphthyl-Based Iodonium Salt (Hypervalent Iodine(III)) as Hydrogen- and Halogen-Bonding Bifunctional Catalyst: Insight into Abnormal Counteranion Effect and Asymmetric Synthesis of α -N-S- α -Acetals. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 1091-1098.	2.1	22
12175	Insights into the gold(σ)-catalyzed intermolecular annulations of alkynes with α -allenamides: a mechanistic DFT study. <i>Dalton Transactions</i> , 2022, 51, 3734-3739.	1.6	3
12176	The mechanism and origin of selectivities for NHC-catalyzed synthesis of axially chiral benzothiophene/benzofuran-fused biaryls. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 1662-1670.	1.5	11
12177	Computational NMR of natural products. <i>Russian Chemical Reviews</i> , 2022, 91, .	2.5	13
12178	Computational insights into different regioselectivities in the Ir-porphyrin-catalyzed C-H insertion reaction of quinoid carbene. <i>Organic Chemistry Frontiers</i> , 2022, 9, 1143-1151.	2.3	2
12179	In Situ XAFS, XRD, and DFT Characterization of the Sulfur Adsorption Sites on Cu and Ce Exchanged Y Zeolites. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1496-1512.	1.5	8
12180	Enantioselective α -clip-cycle-synthesis of di-, tri- and spiro-substituted tetrahydropyrans. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 1181-1185.	1.5	4
12181	Study on the three-stage growth of silica nanoparticles prepared by the drop-by-drop precipitation method. <i>Powder Technology</i> , 2022, 397, 117115.	2.1	2
12182	C-H Bond Activation Mechanism by a Pd(II)(η^4 -O)-Au(0) Structure Unique to Heterogeneous Catalysts. <i>Jacs Au</i> , 2022, 2, 394-406.	3.6	6
12183	Adsorption Forms of NO on Iridium-Doped Rhodium Clusters in the Gas Phase Revealed by Infrared Multiple Photon Dissociation Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2022, 126, 36-43.	1.1	6

#	ARTICLE	IF	CITATIONS
12184	Mechanistic Investigation of Cu-Catalyzed Asymmetric Alkynylation of Cyclic N-Sulfonyl Ketimines with Terminal Alkynes. <i>Organometallics</i> , 0, , .	1.1	2
12185	Proton Affinity Values of Fentanyl and Fentanyl Analogues Pertinent to Ambient Ionization and Detection. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 482-490.	1.2	6
12186	Theoretical Design of Stable Pentacoordinate Boron Compounds. <i>ACS Omega</i> , 2022, 7, 2391-2397.	1.6	2
12187	Bis(2,6-diisopropylphenyl) tellurone: a well-defined monomeric diorganotellurone without cocrystallized solvents and without stabilizing intramolecular contacts. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 88-93.	0.2	1
12188	Nickel Phthalocyanines as Potential Aggregation-Induced Antibacterial Agents: Fenton-Like Pathways Driven by Near-Infrared Light. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	3
12189	Experimental and computational evidence for stabilising parallel, offset π -[C(=O)N(H)N=C] π -(phenyl) interactions in acetohydrazide derivatives. <i>CrystEngComm</i> , 2022, 24, 962-974.	1.3	0
12190	Hexabenzocoronene functionalized with antiaromatic S- and Se-core-modified porphyrins (isophlorins): comparison with the dyad with regular porphyrin. <i>Pure and Applied Chemistry</i> , 2022, 94, 747-765.	0.9	0
12191	Total Electron Detachment and Induced Cationic Fragmentation Cross Sections for Superoxide Anion ($O_2^{\cdot-}$) Collisions with Benzene (C_6H_6) Molecules. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1266.	1.8	1
12192	Role of imine isomerization in the stereocontrol of the Staudinger reaction between ketenes and imines. <i>RSC Advances</i> , 2021, 12, 104-117.	1.7	1
12193	Predominance of the second cycle in homogeneous Os-catalyzed dihydroxylation: the nature of Os(vi) \rightarrow Os(viii) reoxidation and unprecedented roles of amine-N-oxides. <i>Catalysis Science and Technology</i> , 2022, 12, 880-893.	2.1	2
12194	Purely Organic Emitters for Multiresonant Thermally Activated Delay Fluorescence: Design of Highly Efficient Sulfur and Selenium Derivatives. , 2022, 4, 440-447.		33
12195	A benchmark study of aromaticity indexes for benzene, pyridine and the diazines α -I. Ground state aromaticity. <i>RSC Advances</i> , 2022, 12, 2830-2842.	1.7	19
12196	Unveiling a key catalytic pocket for the ruthenium NHC-catalysed asymmetric heteroarene hydrogenation. <i>Chemical Science</i> , 2022, 13, 985-995.	3.7	12
12197	Insight into fragmentation of a phosphirane to form phosphinidene complexes: an illustration with the 1-phenylselenylphosphirane $W(CO)_5$ complex. <i>Dalton Transactions</i> , 2022, 51, 3046-3050.	1.6	0
12198	Data-driven approach towards identifying dyesensitizer molecules for higher power conversion efficiency in solar cells. <i>New Journal of Chemistry</i> , 2022, 46, 4395-4405.	1.4	6
12199	Investigation into the Pyrolysis Bond Dissociation Enthalpies (BDEs) of a Model Lignin Oligomer Using Density Functional Theory (DFT). <i>Energy & Fuels</i> , 2022, 36, 1565-1573.	2.5	4
12200	Mechanistic Insight into Hydroboration of Imines from Combined Computational and Experimental Studies. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	8
12201	A Theoretical Study on Non-Bridging Dimer Formation of a Cationic Platinum Complex with a Redox-Active Ligand. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0

#	ARTICLE	IF	CITATIONS
12202	Relevance of the electron transfer pathway in photodynamic activity of Ru(<i>ii</i>) polypyridyl complexes containing 4,7-diphenyl-1,10-phenanthroline ligands under normoxic and hypoxic conditions. Dalton Transactions, 2022, 51, 1888-1900.	1.6	7
12203	Density functional theory (DFT) investigation of the oxidative degradation of NaAsO ₂ via hydroxyl radical. Structural Chemistry, 2022, 33, 625-630.	1.0	1
12204	Unusual fluorescence behaviour of a heteroleptic Cu(<i>i</i>) complex featuring strong electron donating groups on a diimine ligand. New Journal of Chemistry, 2022, 46, 1693-1703.	1.4	4
12205	Sensitized and Self-Sensitized Photocatalytic Carbon Dioxide Reduction Under Visible Light with Ruthenium Catalysts Shows Enhancements with More Conjugated Pincer Ligands. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	5
12206	Low-Symmetry Phthalocyanines Bearing Carboxy-Groups: Synthesis, Spectroscopic and Quantum-Chemical Characterization. Molecules, 2022, 27, 524.	1.7	1
12207	Molecular insights into chirality transfer from double axially chiral phosphoric acid in a synergistic enantioselective intramolecular amination. Chemical Science, 2022, 13, 1323-1334.	3.7	6
12208	Automatic Approach to Explore the Multireaction Mechanism for Medium-Sized Bimolecular Reactions via Collision Dynamics Simulations and Transition State Searches. Journal of Chemical Theory and Computation, 2022, 18, 910-924.	2.3	6
12209	Organocatalytic insertion into C–B bonds by <i>in situ</i> generated carbene: mechanism, role of the catalyst, and origin of stereoselectivity. Catalysis Science and Technology, 2022, 12, 947-953.	2.1	18
12210	Roles of Small Molecules in the Stability and Sensitivity of CL-20-Based Host-Guest Explosives under Electric Fields: A Reactive Molecular Dynamics Study. Journal of Physical Chemistry A, 2022, 126, 286-295.	1.1	4
12211	Density functionals with asymptotic-potential corrections are required for the simulation of spectroscopic properties of materials. Chemical Science, 2022, 13, 1492-1503.	3.7	7
12212	Aromaticity-promoted CS ₂ activation by heterocycle-bridged P/N-FLPs: a comparative DFT study with CO ₂ capture. Physical Chemistry Chemical Physics, 2022, 24, 2521-2526.	1.3	6
12213	Computational predictions of adaptive aromaticity for the design of singlet fission materials. Inorganic Chemistry Frontiers, 2022, 9, 914-924.	3.0	13
12214	2-Acetamido-2-deoxy-d-glucono-1,5-lactone Sulfonylhydrazones: Synthesis and Evaluation as Inhibitors of Human OGA and HexB Enzymes. International Journal of Molecular Sciences, 2022, 23, 1037.	1.8	2
12215	Enantioselective Pd-catalyzed allylic substitution using phosphite-oxazoline PHOX-based ligands containing a methylene linker. European Journal of Inorganic Chemistry, 2022, .	1.0	2
12216	Electrostatic Perturbations in the Substrate-Binding Pocket of Taurine- β -Ketoglutarate Dioxygenase Determine its Selectivity. Chemistry - A European Journal, 2022, 28, .	1.7	32
12217	<i>N,O</i> -Bis(trimethylsilyl)trifluoroacetamide as an Effective Interface Film Additive on Lithium Anodes. ACS Applied Materials & Interfaces, 2022, 14, 5447-5458.	4.0	4
12218	Mechanistic Investigation of H ₂ O ₂ -dependent Chemiluminescence from Tetrabromo-1,4-Benzoquinone. ChemPhysChem, 2022, 23, e202100885.	1.0	3
12219	Unraveling the mechanism and substituent effects on the N-heterocyclic carbene-catalyzed transformation reaction of enals and imines. Molecular Catalysis, 2022, 519, 112122.	1.0	8

#	ARTICLE	IF	CITATIONS
12220	A correctly scaling rigorously spin-adapted and spin-complete open-shell CCSD implementation for arbitrary high-spin states. <i>Journal of Chemical Physics</i> , 2022, 156, 054111.	1.2	3
12221	<i>MAAT</i> Analysis of Aldofuranosyl Rings: Unbiased Modeling of Conformational Equilibria and Dynamics in Solution. <i>Biochemistry</i> , 2022, 61, 239-251.	1.2	6
12222	A computational study of polydimethylsiloxane derivatives as a semi-permeable membrane for in-field identification of naphthenic acids in water using portable mass spectrometry. <i>Journal of Molecular Liquids</i> , 2022, 351, 118657.	2.3	4
12223	DFT Study on Side Chain Detachment of Perfluorosulfonic Acid Ionomers by Radical-Assisted Nucleophilic Attack of Water. <i>Polymer Degradation and Stability</i> , 2022, 196, 109832.	2.7	4
12224	Adatom Defect Induced Spin Polarization of Asymmetric Structures. <i>ChemistryOpen</i> , 2022, 11, e202100208.	0.9	1
12225	Merging structural frameworks of imidazolium, pyridinium, and cholinium ionic liquids with cinnamic acid to tune solution state behavior and properties. <i>Journal of Molecular Liquids</i> , 2022, 352, 118673.	2.3	3
12226	Covalent organic frameworks based on electroactive naphthalenediimide as active electrocatalysts toward oxygen reduction reaction. <i>Applied Materials Today</i> , 2022, 26, 101384.	2.3	13
12227	Angle-resolved one and Two-Photon absorption spectrum in twisted bilayer graphene quantum dots. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 271, 120894.	2.0	6
12228	Succinylated isoniazid potential prodrug: Design of Experiments (DoE) for synthesis optimization and computational study of the reaction mechanism by DFT calculations. <i>Journal of Molecular Structure</i> , 2022, 1254, 132323.	1.8	1
12229	Reaction mechanisms of the initial steps for the oxidation of (0001 $\bar{1}$) C and (0001) Si faces of SiC with OH radicals. <i>Surface Science</i> , 2022, 719, 122031.	0.8	3
12230	Functionalized polyarylether-based COFs for rapid and selective extraction of uranium from aqueous solution. <i>Chemical Engineering Journal</i> , 2022, 434, 134623.	6.6	46
12231	Nonoxidative coupling of methane to olefins and aromatics over molten W-In bimetal catalyst. <i>Fuel</i> , 2022, 316, 123333.	3.4	2
12232	Regioselectivity of Pd-catalyzed o-Carborane Arylation: A Theoretical View. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	5
12233	Photoluminescence and electrochemiluminescence of thermally activated delayed fluorescence (TADF) emitters containing diphenylphosphine chalcogenide-substituted carbazole donors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4646-4667.	2.7	20
12234	Silaborative Assembly of Allenamides and Alkynes: Highly Regio- and Stereocontrolled Access to Bi- or Trimetallic Skipped Dienes. <i>Angewandte Chemie - International Edition</i> , 2022, , .	7.2	4
12235	A new approach exploiting thermally activated delayed fluorescence molecules to optimize solar thermal energy storage. <i>Nature Communications</i> , 2022, 13, 797.	5.8	18
12236	DFT Analysis of the Formation of a Titanium <i>n</i> -Butoxide Derivative $[\text{Ti}[\text{O}(\text{CH}_2)_3\text{CH}_3]_2\text{Cl}(\text{OH})_2]$ through OH Bridge Formation and Molecular Interactions between Butoxy Groups. <i>Chemistry Letters</i> , 2022, 51, 173-176.	0.7	0
12237	Functionalized Crystalline N-Trimethyltriindoles: Counterintuitive Influence of Peripheral Substituents on Their Semiconducting Properties. <i>Molecules</i> , 2022, 27, 1121.	1.7	2

#	ARTICLE	IF	CITATIONS
12238	Asymmetric Synthesis of Heterocyclic Chloroamines and Aziridines by Enantioselective Protonation of Catalytically Generated Enamines**. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4
12239	Drug delivery of carvedilol (cardiovascular drug) using phosphorene as a drug carrier: a DFT study. <i>Journal of Taibah University for Science</i> , 2022, 16, 31-46.	1.1	14
12240	Electrocatalytic Water Oxidation Activity of Molecular Copper Complexes: Effect of Redox-Active Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 3152-3165.	1.9	14
12241	Degradation of potassium alkyl xanthogenate in wet air oxidation: Enhancement method, degradation mechanism and structure impact. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 107349.	3.3	4
12242	Photoreactions of Sc ₃ N@C ₈₀ with Disilirane, Silirane, and Digermirane: A Photochemical Method to Separate 1h and D5h Isomers. <i>Photochem</i> , 2022, 2, 122-137.	1.3	1
12243	Role of High-Spin Species and Pendant Amines in Electrocatalytic Alcohol Oxidation by a Nickel Phosphine Complex. <i>ACS Catalysis</i> , 2022, 12, 2729-2740.	5.5	6
12244	The origin of enhanced O_2 production from photoionized CO ₂ clusters. <i>Communications Chemistry</i> , 2022, 5, .	2.0	3
12245	Key Piece in the Wolfe Cycle of Methanogenesis: The S–S Bond Dissociation Conducted by Noncubane [Fe ₄ S ₄] Cluster-Dependent Heterodisulfide Reductase. <i>ACS Catalysis</i> , 2022, 12, 2606-2622.	5.5	3
12246	Structural and Thermodynamic Effects on the Kinetics of C–H Oxidation by Multisite Proton-Coupled Electron Transfer in Fluorenyl Benzoates. <i>Journal of Organic Chemistry</i> , 2022, , .	1.7	3
12247	Lewis Acid–Lewis Base Interactions Promote Fast Interfacial Electron Transfers with a Pyridine-Based Donor Dye in Dye-Sensitized Solar Cells. <i>ACS Applied Energy Materials</i> , 2022, 5, 1516-1527.	2.5	6
12248	Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1382-1388.	2.1	12
12249	Sensitive fluorescent determination of indium (III) by a thiourea–quinoline-based chemosensor. <i>Instrumentation Science and Technology</i> , 2022, 50, 481-495.	0.9	2
12250	Spirovetivane- and Eudesmane-Type Sesquiterpenoids Isolated from the Culture Media of Two Cyanobacterial Strains. <i>Journal of Natural Products</i> , 2022, 85, 415-425.	1.5	2
12251	Silaborative Assembly of Allenamides and Alkynes: Highly Regio- and Stereocontrolled Access to Bi- or Trimetallic Skipped Dienes. <i>Angewandte Chemie</i> , 0, , .	1.6	1
12252	Levofloxacin degradation performance and mechanism in the novel electro-Fenton system constructed with vanadium oxide electrodes under neutral pH. <i>Chemical Engineering Journal</i> , 2022, 433, 133574.	6.6	19
12253	The pH dependence and role of fluorinated substituent of enoxacin binding to ferrihydrite. <i>Science of the Total Environment</i> , 2022, 823, 153707.	3.9	8
12254	Plasmonically Generated Tryptophan Radical Anion on Gold Nanoparticles Investigated by Combined Surface-Enhanced Raman Scattering and Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27596-27606.	1.5	4
12255	Investigation on micro-mechanism of palm oil as natural ester insulating oil for overheating thermal fault analysis of transformers. <i>High Voltage</i> , 2022, 7, 812-824.	2.7	20

#	ARTICLE	IF	CITATIONS
12256	Designing Potential Donor Materials Based on DRCN5T with Halogen Substitutions: A DFT/TDDFT Study. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13498.	1.8	2
12257	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
12258	Engineering Nanocomposite Metal-Phenolic Network Membranes with Hollow Mofs Via In-Situ Etching for High-Efficiency Organic Solvent Nanofiltration. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12259	Metal-free oxoammonium salt-mediated C(sp ³)â€“H oxidative Ugi-azide multicomponent reaction. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 2896-2908.	1.5	4
12260	Towards solvent regulated self-activation of N-terminal disulfide bond oxidoreductase-D. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7691-7699.	1.3	2
12261	Alkane Câ€“H activation and ligand exchange on silica supported d ⁰ metal alkylidenes: relevance to alkane metathesis. <i>Dalton Transactions</i> , 2022, , .	1.6	0
12262	Theoretical study for evaluating and discovering organic hydride compounds as novel trifluoromethylation reagents. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 2831-2842.	1.5	5
12263	An unprecedented C ₈₀ cage that violates the isolated pentagon rule. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2264-2270.	3.0	10
12264	Significance of density functional theory (DFT) calculations for electrocatalysis of N ₂ and CO ₂ reduction reactions. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8591-8603.	1.3	17
12265	Cyclo[18]carbon including zero-point motion: ground state, first singlet and triplet excitations, and hole transfer. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7779-7787.	1.3	4
12266	The DP5 probability, quantification and visualisation of structural uncertainty in single molecules. <i>Chemical Science</i> , 2022, 13, 3507-3518.	3.7	12
12267	Covalent organic framework-based materials as electrocatalysts for fuel cells. , 2022, , 229-250.		1
12268	Insight into the dual action mechanism of 3V-PPh ₃ polymers as carriers and ligands in the Rh/3V-PPh ₃ heterogeneous catalytic hydroformylation of ethylene to propionaldehyde. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 9673-9684.	1.3	4
12269	On the mechanism of electrochemical functionalization of carbon nanotubes with different structures with aminophenylphosphonic acid isomers: an experimental and computational approach. <i>Journal of Materials Chemistry A</i> , 2022, 10, 7271-7290.	5.2	4
12270	Remdesivir: Mechanism of Metabolic Conversion from Prodrug to Drug. <i>Current Drug Metabolism</i> , 2022, 23, 73-81.	0.7	1
12271	Mechanistic exploration of CO ₂ conversion to dimethoxymethane (DMM) using transition metal (Co, Ru) catalysts: an energy span model. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8387-8397.	1.3	9
12272	Global Analysis of Heme Proteins Elucidates the Correlation between Heme Distortion and the Heme-Binding Pocket. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 775-784.	2.5	10
12273	Isolation and biological evaluation 7-hydroxy flavone from <i>Avicennia officinalis</i> : insights from extensive <i>in vitro</i> , DFT, molecular docking and molecular dynamics simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 2848-2860.	2.0	5

#	ARTICLE	IF	CITATIONS
12274	Pyridinium salt-based covalent organic framework with well-defined nanochannels for efficient and selective capture of aqueous $^{99}\text{TcO}_4^-$. <i>Science Bulletin</i> , 2022, 67, 924-932.	4.3	87
12275	Free Energy and Stacking of Eumelanin Nanoaggregates. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1805-1818.	1.2	8
12276	Solvents and Ligands Matter: Structurally Variable Palladium and Nickel Clusters Assembled by Tridentate Selenium- and Tellurium-Containing Schiff Bases. <i>Inorganic Chemistry</i> , 2022, 61, 3785-3800.	1.9	1
12277	Analysis of the Geometric and Electronic Structure of Spin-Coupled Iron-Sulfur Dimers with Broken-Symmetry DFT: Implications for FeMoco. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1437-1457.	2.3	16
12278	Anion photoelectron spectroscopy and density functional theory studies of $\text{AuC}_{3n}\text{O}_{10}$ ($n=3$): Odd-even alternation in electron binding energies and structures. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 177-184.	0.6	1
12279	Cyclometalated Platinum(II) Complexes in a <i>Cis</i> - <i>N</i> , <i>N</i> Configuration: Photophysical Properties and Isomerization to <i>Trans</i> Isomers. <i>Inorganic Chemistry</i> , 2022, 61, 3420-3433.	1.9	11
12280	LModeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1821-1837.	2.3	16
12281	Dynamic Wetting of Photoresponsive Arylazopyrazole Monolayers is Controlled by the Molecular Kinetics of the Monolayer. <i>Journal of the American Chemical Society</i> , 2022, 144, 4026-4038.	6.6	12
12282	In Vitro and Computational Studies of Perezone and Perezone Angelate as Potential Anti-Glioblastoma Multiforme Agents. <i>Molecules</i> , 2022, 27, 1565.	1.7	2
12283	Perfluoroacenoacene for Solution Processed Distributed Feedback Laser: The Effect of 1,2-Oxaborine Doping. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	9
12284	Hierarchically Porous and Defective Carbon Fiber Cathode for Efficient Zn-Air Batteries and Microbial Fuel Cells. <i>Advanced Fiber Materials</i> , 2022, 4, 795-806.	7.9	26
12285	Subnanometer Ion Channel Anion Exchange Membranes Having a Rigid Benzimidazole Structure for Selective Anion Separation. <i>ACS Nano</i> , 2022, 16, 4629-4641.	7.3	33
12286	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1510-1524.	2.5	6
12287	Backbone Configuration and Electronic Property Tuning of Imide-Functionalized Ladder-Type Heteroarenes-Based Polymer Acceptors for Efficient All-Polymer Solar Cells. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	12
12288	Combined DFT and MD Simulation Protocol to Characterize Self-Healing Properties in Disulfide-Containing Materials: Polyurethanes and Polymethacrylates as Case Studies. <i>Frontiers in Materials</i> , 2022, 9, .	1.2	1
12289	Quinonoid versus Aromatic π -Conjugated Oligomers and Polymers and Their Diradical Characters. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5302-5310.	1.5	3
12290	The Two Hot Corinos of the SVS13-A Protostellar Binary System: Counterposed Siblings. <i>Astrophysical Journal Letters</i> , 2022, 928, L3.	3.0	15
12291	Catalytic Reduction of Dinitrogen to Ammonia and Hydrazine Using Iron-Dinitrogen Complexes Bearing Anionic Benzene-Based PCP-Type Pincer Ligands. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 683-692.	2.0	11

#	ARTICLE	IF	CITATIONS
12292	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. <i>Astrophysical Journal, Supplement Series</i> , 2022, 259, 39.	3.0	24
12293	Dehydrofluorination as a Residue-Free Selective Route to Câ€“C Bond Formation at Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6249-6257.	1.5	0
12294	Higher-order transition state approximation. <i>Journal of Chemical Physics</i> , 2022, 156, 114112.	1.2	6
12295	Increasing the kinetic stability of a gasâ€“phase contact ionâ€“pair through enhancement of the carbocation stability. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	2
12296	Benchmarking Semiempirical QM Methods for Calculating the Dipole Moment of Organic Molecules. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1905-1921.	1.1	8
12297	Tuning the Hydrolytic Behavior of Hydroxyquinoline Derivatives for Anticorrosion Applications. <i>Chemistry of Materials</i> , 2022, 34, 2842-2852.	3.2	5
12298	Vertical ionization potential benchmarks from Koopmans prediction of Kohnâ€“Sham theory with long-range corrected (LC) functional*. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 194001.	0.7	5
12299	Computational study of the transamination reaction in vinylogous acyls: Paving the way to design vitrimers with controlled exchange kinetics. <i>Journal of Polymer Science</i> , 2022, 60, 1988-1999.	2.0	6
12300	Precise recognition of palladium through interlaminal chelation in a covalent organic framework. <i>CheM</i> , 2022, 8, 1442-1459.	5.8	53
12301	Hydrogen-Bond Topology Is More Important Than Acid/Base Strength in Atmospheric Prenucleation Clusters. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1718-1728.	1.1	19
12302	Controlling the Formation of Two Concomitant Polymorphs in Hg(II) Coordination Polymers. <i>Inorganic Chemistry</i> , 2022, 61, 4965-4979.	1.9	7
12303	The effect of <sc>offâ€“center</sc> ĩfâ€“hole on the <sc>atomâ€“centered</sc> partial charges in halogenated molecules. <i>Journal of Computational Chemistry</i> , 2022, 43, 864-869.	1.5	0
12304	An orbital-based representation for accurate quantum machine learning. <i>Journal of Chemical Physics</i> , 2022, 156, 114101.	1.2	11
12305	Ni-Catalyzed Ligand-Controlled Selective 5-Exo and 6-Endo Cyclization/Cross-Couplings Involving an Unusual 1,2-Aryl Migration. <i>ACS Catalysis</i> , 2022, 12, 4131-4140.	5.5	7
12306	Acene-Extended Triptycenes: Synthesis, Characterization, and Singlet Exciton Fission Properties. <i>Journal of Organic Chemistry</i> , 2022, 87, 8841-8848.	1.7	4
12307	Protonation-Dependent Sequencing of 5-Formylcytidine in RNA. <i>Biochemistry</i> , 2022, 61, 535-544.	1.2	10
12308	Quadratic Unitary Coupled-Cluster Singles and Doubles Scheme: Efficient Implementation, Benchmark Study, and Formulation of an Extended Version. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2281-2291.	2.3	4
12309	Molybdenum bound nitrogenâ€“doped graphene catalyst for reduction of N ₂ to NH ₃ and NH ₂ NH ₂ , using FLP as a coâ€“catalyst: A DFT study. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	3

#	ARTICLE	IF	CITATIONS
12310	New Insights into the Redox Properties of Pyridinium Appended 1,2-Dithienylcyclopentenes. <i>ChemPhysChem</i> , 2022, , .	1.0	2
12311	Free and open source software for computational chemistry education. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, .	6.2	19
12312	Investigating the Ultrafast Dynamics and Long-Term Photostability of an Isomer Pair, Usujirene and Palythene, from the Mycosporine-like Amino Acid Family. <i>Molecules</i> , 2022, 27, 2272.	1.7	4
12313	Non-energetic Formation of Ethanol via CCH Reaction with Interstellar H ₂ O Ices. A Computational Chemistry Study. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 496-511.	1.2	19
12314	Experimental and theoretical investigation on the thermal isomerization reaction of triazolotriazines. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	1
12315	Mechanistic Investigations of the Synthesis of Lactic Acid from Glycerol Catalyzed by an Iridium-NHC Complex. <i>Processes</i> , 2022, 10, 626.	1.3	4
12316	A Case Study of the Glycoside Hydrolase Enzyme Mechanism Using an Automated QM-Cluster Model Building Toolkit. <i>Frontiers in Chemistry</i> , 2022, 10, 854318.	1.8	2
12317	4-Phenylcoumarin (4-PC) Glucoside from <i>Exostema caribaeum</i> as Corrosion Inhibitor in 3% NaCl Saturated with CO ₂ in AISI 1018 Steel: Experimental and Theoretical Study. <i>International Journal of Molecular Sciences</i> , 2022, 23, 3130.	1.8	2
12318	Density Functional Theory Study of Carbamoyl-Substituted Dihydroazulene/Vinylheptafulvene Derivatives and Solvent Effects. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4815-4825.	1.5	1
12319	On the Origins of Stereo- and Regio-Selectivities in the Formation of Fullerene-Fluorene Dyads. <i>Journal of Organic Chemistry</i> , 2022, 87, 4702-4711.	1.7	2
12320	Dinuclear Pt(II) Complexes with Red and NIR Emission Governed by Ligand Control of the Intramolecular Pt-Pt Distance. <i>Inorganic Chemistry</i> , 2022, 61, 5178-5183.	1.9	10
12321	Halogen Bonds Exist between Noncovalent Ligands and Natural Nucleic Acids. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 4424-4435.	2.9	11
12322	Fully conjugated azacorannulene dimer as large diaza[80]fullerene fragment. <i>Nature Communications</i> , 2022, 13, 1498.	5.8	16
12323	Physical Cross-Linkage Constructed Supramolecular Conductive Hydrogel as Sustainable and Remolded Epidermal Electronics. <i>ACS Applied Polymer Materials</i> , 2022, 4, 2585-2594.	2.0	6
12324	Twins of Minimalistic Carbon Dots: Uniform Emitting Units and Molecular Level Repeatable Photoluminescence. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	4
12325	Precise and controllable tandem strategy triggering boosted oxygen reduction activity. <i>Chinese Journal of Catalysis</i> , 2022, 43, 1042-1048.	6.9	10
12326	Selective Dimerization of Ethene to 2-Butene on Zn ²⁺ -Modified ZSM-5 Zeolite. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6570-6577.	1.5	8
12327	Structural and Biophysical Analysis of the Phytochelatin-Synthase-Like Enzyme from <i>Nostoc</i> sp. Shows That Its Protease Activity is Sensitive to the Redox State of the Substrate. <i>ACS Chemical Biology</i> , 2022, 17, 883-897.	1.6	3

#	ARTICLE	IF	CITATIONS
12328	Overlooked Effects of La-4f Orbitals in Endohedral Metallofullerenes. <i>Inorganic Chemistry</i> , 2022, 61, 5891-5902.	1.9	6
12329	Structural, spectroscopic and biological study of trifluoroethyl methansulfonate (methylsulfonyl), TFMSMS. <i>Journal of Molecular Structure</i> , 2022, , 133000.	1.8	0
12330	A theoretical investigation of a series of zinc ion responsive fluorescent probes based on 8-aminoquinoline. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113647.	1.1	2
12331	Insights into the Mechanism of Metal-Catalyzed Transformation of Oxime Esters: Metal-Bound Radical Pathway vs Free Radical Pathway. <i>Journal of Organic Chemistry</i> , 2022, 87, 6014-6024.	1.7	5
12332	Interpolating Moving Ridge Regression (IMRR): A machine learning algorithm to predict energy gradients for ab initio molecular dynamics simulations. <i>Chemical Physics</i> , 2022, 557, 111482.	0.9	2
12333	Investigations of tetramethyl glutaramide ligand in the formation of stable gas-phase tetrapositive complexes with metal tetracations. <i>International Journal of Mass Spectrometry</i> , 2022, 475, 116818.	0.7	0
12334	Linking azoles to isoniazid via hydrazone bridge: Synthesis, crystal structure determination, antitubercular evaluation and computational studies. <i>Journal of Molecular Liquids</i> , 2022, 354, 118873.	2.3	6
12335	Theoretical investigation of the influence of ĩ€-spacer on photovoltaic performances in carbazole-based dyes for dye-sensitized solar cells applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 428, 113870.	2.0	30
12336	Exploring the metal-free catalytic reduction of CO ₂ to methanol with saturated adamantane scaffolds of phosphine-borane frustrated Lewis pair: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108150.	1.3	4
12337	Functionalized graphene-based Quantum Dots: Promising adsorbents for CO, NO ₂ , SO ₂ , and NH ₃ Pollutant Gases. <i>Materials Today Communications</i> , 2022, 31, 103426.	0.9	3
12338	Engineering nanocomposite metal-phenolic network membranes with hollow MOFs via in-situ etching for High-efficiency organic solvent nanofiltration. <i>Chemical Engineering Journal</i> , 2022, 437, 135289.	6.6	33
12339	DFT studies of protonation and anion binding of Chatt type dinitrogen complex: Who is first?. <i>Inorganica Chimica Acta</i> , 2022, 536, 120899.	1.2	1
12340	Push-pull dyes based on Michler's aldehyde: Design and characterization of the optical and electrochemical properties. <i>Dyes and Pigments</i> , 2022, 202, 110278.	2.0	4
12341	Interactions of N-hydroxyamphetamine with an iron porphyrin: A unique intramolecular H-bond probed by DFT calculations. <i>Journal of Inorganic Biochemistry</i> , 2022, 231, 111779.	1.5	1
12342	An account of chronological computational investigations to ascertain the role of pĩ€-pĩ€ bonding in influencing the Lewis acidity of BX ₃ (X=ĀF, Cl, Br and I): Evolution of novel parameters and relegation of ĩ€-type back bonding concept. <i>Coordination Chemistry Reviews</i> , 2022, 463, 214519.	9.5	3
12343	Deep eutectic solvent-based polymer electrolyte for solid-state lithium metal batteries. <i>Journal of Energy Chemistry</i> , 2022, 70, 363-372.	7.1	32
12344	Substitution-inert polynuclear platinum complexes and Glycosaminoglycans: A molecular dynamics study of its non-covalent interactions. <i>Journal of Inorganic Biochemistry</i> , 2022, 232, 111811.	1.5	1
12345	Understanding the Photocatalytic Reduction of CO ₂ with Heterometallic Molybdenum(V) Phosphate Polyoxometalates in Aqueous Media. <i>ACS Catalysis</i> , 2022, 12, 453-464.	5.5	27

#	ARTICLE	IF	CITATIONS
12346	Kinetic and Computational Analysis of CO Substitution in a Dinuclear Osmium Carbonyl Complex: Intersection between Dissociative and Dissociative-Interchange Mechanisms. <i>Inorganic Chemistry</i> , 2022, 61, 246-253.	1.9	2
12347	Charge transfer excitations and constrained density functional theory. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	8
12348	Janus Cluster: Asymmetric Coverage of a Ag ₄₃ Cluster on the Symmetric Preyssler P ₅ W ₃₀ Polyoxometalate. <i>Chemistry of Materials</i> , 2021, 33, 9708-9714.	3.2	32
12349	Chelating the Alpha Therapy Radionuclides ²²⁵ Ac ³⁺ and ²¹³ Bi ³⁺ with 18-Membered Macrocyclic Ligands MacroDipa and Py-MacroDipa. <i>Inorganic Chemistry</i> , 2022, 61, 801-806.	1.9	15
12350	Deciphering the mechanism behind efficient enantioselective ethylation with thiazolidine-based amino alcohols. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	2
12351	Tropane-Based Dispirocyclic Oxiranes and Spirocyclic Ketones. <i>Synthesis</i> , 2022, 54, 723-731.	1.2	0
12352	Synthesis and structural analysis of cis-bis(1,10-phenanthroline)dicarbonyl ruthenium(II) 1.72-trifluoromethanesulfonate 0.28-hexafluoridophosphate. <i>European Journal of Chemistry</i> , 2021, 12, 389-393.	0.3	0
12353	Role of Coordination Geometry on the Magnetic Relaxation Dynamics of Isomeric Five-Coordinate Low-Spin Co(II) Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 317-327.	1.9	7
12354	A Benchmark Study of Quantum Mechanics and Quantum Mechanics-Molecular Mechanics Methods for Carbocation Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 167-178.	2.3	11
12355	Introducing Benzene-1,3,5-tri(dithiocarboxylate) as a Multidentate Linker in Coordination Chemistry. <i>Inorganic Chemistry</i> , 2021, 60, 19242-19252.	1.9	2
12356	Hydrosilylation of Aldehydes and Ketones Catalyzed by a 2-Iminopyrrolyl Alkyl-Manganese(II) Complex. <i>Inorganic Chemistry</i> , 2022, 61, 1195-1206.	1.9	10
12357	Hydroboration and Hydrosilylation of a Molybdenum Nitride Complex Bearing a PNP-Type Pincer Ligand. <i>Organometallics</i> , 2022, 41, 366-373.	1.1	5
12358	Boosting Palladium-Catalyzed Aryl Nitro Bond Activation Reaction by Understanding the Electronic, Electrostatic, and Polarization Effect: A Computational Study from a Basic Understanding to Ligand Design. <i>Journal of Organic Chemistry</i> , 2022, 87, 531-539.	1.7	2
12359	Computational Investigation of the Formation of Peroxide (ROOR) Accretion Products in the OH- and NO ₃ -Initiated Oxidation of \pm -Pinene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10632-10639.	1.1	13
12360	Molecular Structure of Nickel Octamethylporphyrin Rare Experimental Evidence of a Ruffling Effect in Gas Phase. <i>International Journal of Molecular Sciences</i> , 2022, 23, 320.	1.8	4
12361	A Lewis Base Nucleofugality Parameter, N_F^B , and Its Application in an Analysis of MIDA-Boronate Hydrolysis Kinetics. <i>Journal of Organic Chemistry</i> , 2022, 87, 721-729.	1.7	3
12362	N=N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. <i>Inorganic Chemistry</i> , 2022, 61, 474-485.	1.9	5
12363	Engineering an efficient and enantioselective enzyme for the Morita-Baylis-Hillman reaction. <i>Nature Chemistry</i> , 2022, 14, 313-320.	6.6	34

#	ARTICLE	IF	CITATIONS
12364	Modeling a unit cell: crystallographic refinement procedure using the biomolecular MD simulation platform <i>Amber</i> . <i>IUCr</i> , 2022, 9, 114-133.	1.0	4
12365	Tunable Spin Polarization of Zigzag-Zigzag Heterojunction Carbon Nanotubes. <i>Physica Status Solidi (B): Basic Research</i> , 2022, 259, 2100639.	0.7	0
12366	Protonation of Serine in Gas and Condensed and Microsolvated States in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2022, 126, 44-52.	1.1	0
12367	Synthesis of Redox-Active Photochromic Phenanthrene Derivatives. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	3
12368	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 151-166.	2.3	27
12369	Roles of Carbon Nanotube Confinement in Enhancing Second-Order Nonlinear Optical Properties of Triiodobenzene Aggregates. <i>Journal of Physical Chemistry C</i> , 2022, 126, 365-377.	1.5	4
12370	Fundamental Insights into Free-Radical Polymerization in the Presence of Catechols and Catechol-Functionalized Monomers. <i>Macromolecules</i> , 2022, 55, 49-64.	2.2	4
12371	A DFT study of NHC-catalyzed reactions between 2-bromo-2-enals and acylhydrazones: mechanisms, and chemo- and stereoselectivities. <i>New Journal of Chemistry</i> , 2022, 46, 9146-9154.	1.4	3
12372	Charge transfer complexes of a benzothienobenzothiophene derivative and their implementation as active layer in solution-processed thin film organic field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7319-7328.	2.7	11
12373	A theoretical approach for homogeneous CO ₂ reduction by Ni(cyclam): substituents with intra-molecular hydrogen transfer. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 2691-2696.	3.0	3
12374	Synthesis of an advanced metal-guided photochromic system for molecular keypad lock: detailed experimental findings and theoretical understanding. <i>New Journal of Chemistry</i> , 2022, 46, 8284-8302.	1.4	5
12375	Realizing high-rate aqueous zinc-ion batteries using organic cathode materials containing electron-withdrawing groups. <i>Sustainable Energy and Fuels</i> , 2022, 6, 2523-2531.	2.5	21
12376	Fundamental Study of the Optical and Vibrational Properties of Fx-AZB@MOF systems as Functions of Dye Substitution and the Loading Amount. <i>Langmuir</i> , 2022, 38, 4295-4309.	1.6	12
12377	The Lanthanide Contraction Is a Variable. <i>Inorganic Chemistry</i> , 2022, 61, 6120-6127.	1.9	6
12378	Impact of coordination ability of the selected anions on tuning the structure of Hg(II) complexes constructed from a neutral dithione ligand: Iodine uptake and DFT theoretical studies. <i>Inorganica Chimica Acta</i> , 2022, 538, 120969.	1.2	3
12379	Hydrogen Atom Transfer Driven Enantioselective Minisci Reaction of Alcohols. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	29
12380	Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase. <i>Journal of the American Chemical Society</i> , 2022, 144, 7208-7214.	6.6	14
12381	Theoretical insights into interaction energy, IR intensity and Raman activity enhancements of H ₂ O adsorbed on Mg containing Zn ₃ O ₃ nanoclusters: A computational study. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113708.	1.1	3

#	ARTICLE	IF	CITATIONS
12382	Theoretical Approach for the Luminescent Properties of Ir(III) Complexes to Produce Redâ€“Greenâ€“Blue LEC Devices. <i>Molecules</i> , 2022, 27, 2623.	1.7	1
12383	Intramolecular hydrogen bonding analysis. <i>Journal of Chemical Physics</i> , 2022, 156, 174302.	1.2	5
12384	Influence of the Nonprotein Amino Acid Mimosine in Peptide Conformational Propensities from Novel Amber Force Field Parameters. <i>Journal of Physical Chemistry B</i> , 2022, , .	1.2	0
12385	Poly (O-Aminophenol) Produced by Plasma Polymerization Has IR Spectrum Consistent with a Mixture of Quinoid & Keto Structures. <i>Plasma</i> , 2022, 5, 196-205.	0.7	0
12386	Hydrogen Atom Transfer Driven Enantioselective Minisci Reaction of Alcohols. <i>Angewandte Chemie</i> , 0, , .	1.6	1
12387	Cp ₂ TiCl ₂ : Synthesis, Characterization, Modeling and Catalysis. <i>Journal of Chemical Education</i> , 2022, 99, 2121-2128.	1.1	5
12388	Protonation of Borylated Carboxonium Derivative [2,6-B10H8O2CCH3] ⁺ : Theoretical and Experimental Investigation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4190.	1.8	8
12389	Review on applications of metalâ€“organic frameworks for CO2 capture and the performance enhancement mechanisms. <i>Renewable and Sustainable Energy Reviews</i> , 2022, 162, 112441.	8.2	35
12390	SO2 capture in a chemical stable Al(III) MOF: DUT-4 as an effective adsorbent to clean CH4. <i>Fuel</i> , 2022, 322, 124213.	3.4	17
12410	Regiochemistry of Donor Dendrons Controls the Performance of Thermally Activated Delayed Fluorescence Dendrimer Emitters for High Efficiency Solutionâ€“Processed Organic Lightâ€“Emitting Diodes. <i>Advanced Science</i> , 2022, 9, e2201470.	5.6	19
12411	Theoretical Study on Reaction Mechanisms of Dinitrogen Activation and Coupling by Carbeneâ€“Stabilized Borylenes in Comparison with Intramolecular Câ€“H Bond Activation. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	7
12412	On the use of a volume constraint to account for thermal expansion effects on the low-frequency vibrations of molecular crystals. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10408-10419.	1.3	6
12413	The effect of hydrogen bonding on the reactivity of OH radicals with prenol and isoprenol: a shock tube and multi-structural torsional variational transition state theory study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12601-12620.	1.3	6
12414	A straightforward method to quantify the electron-delocalizing ability of Î€-conjugated molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11486-11490.	1.3	3
12415	Computational Insight into Biotransformation Profiles of Organophosphorus Flame Retardants to Their Diester Metabolites by Cytochrome P450. <i>Molecules</i> , 2022, 27, 2799.	1.7	2
12416	The Sulfinylsulfonation of alkynes for Î²â€“Sulfinyl alkenylsulfone. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	12
12417	DFT Calculations of 31P NMR Chemical Shifts in Palladium Complexes. <i>Molecules</i> , 2022, 27, 2668.	1.7	7
12418	Covalent Organic Frameworks-based Nanocomposites for Oxygen reduction reaction. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2022, 102, 477-485.	0.9	2

#	ARTICLE	IF	CITATIONS
12419	Antioxidant activity of eugenol and its acetyl and nitroderivatives: the role of quinone intermediates—a DFT approach of DPPH test. <i>Journal of Molecular Modeling</i> , 2022, 28, 133.	0.8	3
12420	Raman Fingerprints of π -Electron Delocalization in Polythiophene-Based Insulated Molecular Wires. <i>Macromolecules</i> , 2022, 55, 3458-3468.	2.2	10
12421	Phosphine Ligand Binding and Catalytic Activity of Group 10–14 Heterobimetallic Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 6888-6897.	1.9	1
12422	Molecular docking assisted exploration on solubilization of poorly soluble drug remdesivir in sulfolbutyl ether-tycycloextrin. <i>AAPS Open</i> , 2022, 8, 9.	0.4	3
12423	Ho@C ₈₂ Metallofullerene: Calculated Isomeric Composition. <i>ECS Journal of Solid State Science and Technology</i> , 2022, 11, 053018.	0.9	4
12424	Quantum Chemical Approaches to the Calculation of NMR Parameters: From Fundamentals to Recent Advances. <i>Magnetochemistry</i> , 2022, 8, 50.	1.0	20
12425	Efficient removal of organophosphate esters by ligand functionalized MIL-101 (Fe): Modulated adsorption and DFT calculations. <i>Chemosphere</i> , 2022, 302, 134881.	4.2	21
12426	When Identification of the Reduction Sites in Mixed Molybdenum/Tungsten Keggin-Type Polyoxometalate Hybrids Turns Out Tricky. <i>Inorganic Chemistry</i> , 2022, 61, 7700-7709.	1.9	3
12427	Efficient Xe/Kr Separation Based on a Lanthanide–Organic Framework with One-Dimensional Local Positively Charged Rhomboid Channels. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22233-22241. Energy alignment manipulation at the C₆₀/TiO₂ interface using a blanket molecular dipole approach. <i>Surface Science</i>, 2022, 723, 122117.	4.0	18
12428	Efficient Xe/Kr Separation Based on a Lanthanide–Organic Framework with One-Dimensional Local Positively Charged Rhomboid Channels. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22233-22241. Energy alignment manipulation at the C₆₀/TiO₂ interface using a blanket molecular dipole approach. <i>Surface Science</i>, 2022, 723, 122117.	0.8	1
12429	Energy Decomposition Analysis of the Nature of Coordination Bonding at the Heme Iron Center in Cytochrome P450 Inhibition. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	4
12430	Structure and Electronic Properties of Neutral and Anionic X-Doped Medium-Sized Mg ₁₆ (X = Co, Fe, Ni) Clusters. <i>Journal of Cluster Science</i> , 0, , 1.	1.7	1
12431	High performance ambipolar semiconductor of pyridine-capped diketopyrrolopyrrole-porphyrin oligomers: Roles of thiophen substitution and oligomer length. <i>Materials Today Communications</i> , 2022, 31, 103636.	0.9	0
12432	Molecular dynamics and network analysis reveal the contrasting roles of polar solutes within organic phase amphiphile aggregation. <i>Journal of Molecular Liquids</i> , 2022, 359, 119226.	2.3	5
12433	Triptycene incorporated carbon nitride based donor-acceptor conjugated polymers with superior visible-light photocatalytic activities. <i>Journal of Colloid and Interface Science</i> , 2022, 622, 675-689.	5.0	8
12434	Dependence between luminescence properties of Cu(I) complexes and electronic/structural parameters derived from steric effects. <i>New Journal of Chemistry</i> , 2022, 46, 10584-10593.	1.4	2
12435	Polarizable Embedding Complex Polarization Propagator in Four- and Two-Component Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3671-3686.	2.3	6
12436	Highly regioselective tandem hydroformylation of substituted styrene using Iminophosphine rhodium complex immobilized on carbon. <i>Journal of Industrial and Engineering Chemistry</i> , 2022, 112, 218-232.	2.9	7

#	ARTICLE	IF	CITATIONS
12437	Contrasting solution-state properties within a family of amyloid-binding molecular tools. <i>Tetrahedron</i> , 2022, 116, 132817.	1.0	0
12438	Elucidating the molecular orbital dependence of the total electronic energy in multireference problems. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
12439	Structures and Bonding in Hexacarbonyl Diiron Polyenes: Cycloheptatriene and 1,3,5-Cyclooctatriene. <i>Chemistry</i> , 2022, 4, 447-453.	0.9	0
12440	Prototropic tautomerism of (E)-N-((4-((2-hydroxy-5-methoxybenzylidene)) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 627 Td (amin ions. <i>Polyhedron</i> , 2022, 222, 115909.	1.0	2
12441	Donor-acceptor interactions of gold(III) porphyrins with cobalt(II) phthalocyanine: chemical structure of products, their spectral characterization and DFT study. <i>Dalton Transactions</i> , 0, , .	1.6	0
12442	Homogeneous solution assembled Turing structures with near zero strain semi-coherence interface. <i>Nature Communications</i> , 2022, 13, .	5.8	13
12443	Catalytic Synthesis of Oxazolidinones from a Chitin-Derived Sugar Alcohol. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 1054-1059.	2.0	3
12444	Aging effect of Catechol Redox Polymer Nanoparticles for Hybrid Supercapacitors. <i>Batteries and Supercaps</i> , 0, , .	2.4	1
12445	9-((Diphenylphosphoryl)â€¦10-((phenylethynyl)anthracene Derivatives: Synthesis and Implications for the Substituent and Solvent Effects on the Lightâ€¦Emitting Properties. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	3
12446	Reactivity of 9-anilinoacridine Derivatives as Potent Anticancer Agents: A DFT Approach. <i>Current Physical Chemistry</i> , 2022, 12, 203-215.	0.1	0
12447	Conformational influence on the thermal rate constants and product distributions of 2-butanoneâ€¦+â€¦H abstraction reactions. <i>Chemical Physics Letters</i> , 2022, 801, 139723.	1.2	5
12448	Installing a molecular truss beam stabilizes MOF structures. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	3
12449	In vitro and in silico investigation of the photoprotective and antioxidant potential of Protium spruceanum leaves and its main flavonoids. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 431, 114037.	2.0	4
12450	Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N2O by Ru Pincer Complexes. <i>Inorganics</i> , 2022, 10, 69.	1.2	5
12451	P-functionalized carbon nanotubes promote highly stable electrocatalysts based on Fe-phthalocyanines for oxygen reduction: Experimental and computational studies. <i>Journal of Energy Chemistry</i> , 2022, 72, 276-290.	7.1	11
12452	A Computational approach toward organometallic ruthenium(II) compounds with tunable hydrolytic properties. <i>Chemical Physics</i> , 2022, 560, 111587.	0.9	1
12453	Computational investigation of substituent effects on the fluorescence wavelengths of oxyluciferin analogs. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 431, 114018.	2.0	1
12454	<i>N</i>-Hydroxyâ€¦<i>N</i>-oxide photoinduced tautomerization and excitation wavelength dependent luminescence of ESIPT-capable zinc (<sc>ii</sc>) complexes with a rationally designed 1-hydroxy-2,4-di(pyridin-2-yl)-1<i>H</i>-imidazole ESIPT-ligand. <i>Dalton Transactions</i> , 2022, 51, 9818-9835.	1.6	13

#	ARTICLE	IF	CITATIONS
12455	Antraquinone and its derivatives as sustainable materials for electrochemical applications – a joint experimental and theoretical investigation of the redox potential in solution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16207-16219.	1.3	11
12456	Mechanism of a cobalt-catalyzed hydroarylation reaction and origin of stereoselectivity. <i>Catalysis Science and Technology</i> , 2022, 12, 4380-4387.	2.1	11
12457	Alkene insertion reactivity of a <i>o</i> -carboranyl-substituted 9-borabluorene. <i>Chemical Science</i> , 2022, 13, 7492-7497.	3.7	10
12458	Inhibition of the Peroxygenase Lytic Polysaccharide Monooxygenase by Carboxylic Acids and Amino Acids. <i>Antioxidants</i> , 2022, 11, 1096.	2.2	4
12459	Synthesis of dielectric polystyrene via one-step nitration reaction for large-scale energy storage. <i>Chemical Engineering Journal</i> , 2022, 446, 137281.	6.6	38
12460	Evaluating the conformational space of the active site of D_{22} dopamine receptor. Scope and limitations of the standard docking methods. <i>Journal of Computational Chemistry</i> , 2022, 43, 1298-1312.	1.5	2
12461	Unveiling the mechanistic landscape of formic acid dehydrogenation catalyzed by Cp [*] -M(III) catalysts (M) Tj ETQq0 0 0 rgBT /Overlock <i>Journal of Hydrogen Energy</i> , 2022, 47, 21736-21744.	3.8	1
12462	Modelling the Radical Chemistry on Ice Surfaces: An Integrated Quantum Chemical and Experimental Approach. <i>Frontiers in Astronomy and Space Sciences</i> , 2022, 9, .	1.1	4
12463	Molecular Mechanism of Interaction of Curcumin with BSA, Surfactants and Live <i>E. Coli</i> Cell Membrane Revealed by Fluorescence Spectroscopy and Confocal Microscopy. <i>ChemPhysChem</i> , 2022, 23, .	1.0	4
12464	“Hidden” Nanoscale Catalysis in Alkyne Hydrogenation with Well-Defined Molecular Pd/NHC Complexes. <i>ACS Catalysis</i> , 2022, 12, 6980-6996.	5.5	8
12465	Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways. <i>ACS Physical Chemistry Au</i> , 2022, 2, 316-330.	1.9	5
12466	Interplay of Electronic and Geometric Structure Tunes Organic Biradical Character in Bimetallic Tetrathiafulvalene Tetrathiolate Complexes. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3329-3337.	1.1	4
12467	Unified Electrochemical Synthetic Strategy for [2 + 2 + 2] Cyclotrimerizations: Construction of 1,3,5- and 1,2,4-Trisubstituted Benzenes from Ni(I)-Mediated Reduction of Alkynes. <i>ACS Catalysis</i> , 2022, 12, 6874-6886.	5.5	10
12468	Coumarinolignans with Reactive Oxygen Species (ROS) and NF- κ B Inhibitory Activities from the Roots of <i>Waltheria indica</i> . <i>Molecules</i> , 2022, 27, 3270.	1.7	3
12469	Molecules with a TEMPO-based head group as high-performance organic friction modifiers. <i>Friction</i> , 2023, 11, 316-332.	3.4	6
12470	Ion Chemistry of Carbon Dioxide in Nonthermal Reaction with Molecular Hydrogen. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3463-3471.	1.1	2
12471	ESIPT-Active 8-Hydroxyquinoline-Based Fluorescence Sensor for Zn(II) Detection and Aggregation-Induced Emission of the Zn(II) Complex. <i>ACS Omega</i> , 2022, 7, 18017-18026.	1.6	17
12472	Primary- and secondary-sphere effects of amine substituent position on rhenium bipyridine electrocatalysts for CO ₂ reduction. <i>Polyhedron</i> , 2022, , 115933.	1.0	2

#	ARTICLE	IF	CITATIONS
12473	Does an Enol Pathway Preclude High Stereoselectivity in Iron-Catalyzed Indole C-H Functionalization via Carbene Insertion?. <i>Journal of Organic Chemistry</i> , 2022, 87, 7919-7933.	1.7	10
12474	Computational mechanistic studies on persulfate assisted α -phenylenediamine polymerization. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	2
12476	Comprehensive Study of the Chemistry behind the Stability of Carboxylic SWCNT Dispersions in the Development of a Transparent Electrode. <i>Nanomaterials</i> , 2022, 12, 1901.	1.9	3
12477	Molecular Simulation Analyses of Polymorphism Control Factors by the Example of Carbamazepine Forms I-IV: A Blueprint for Industrial Drug Formulation?. <i>Journal of Pharmaceutical Sciences</i> , 2022, 111, 2898-2906.	1.6	1
12478	Biphasic Behaviors of Nd ³⁺ Bound with Cyanex272, Cyanex301, and Cyanex302: A Molecular Dynamics Simulation Study. <i>Inorganic Chemistry</i> , 2022, 61, 8920-8929.	1.9	0
12479	On the formation enthalpies and bandgaps of linear, cyclic and cubic neutral sodium chloride clusters (NaCl) _n , n = 2, 3, 4, 5, 6, 10. <i>Materials Today Communications</i> , 2022, 31, 103733.	0.9	0
12480	Diffusion behavior of gas molecules in the one-dimensional channel of AlPO ₄ -5 molecular sieves. <i>Microporous and Mesoporous Materials</i> , 2022, 340, 112024.	2.2	4
12481	A DFT investigation of lithium adsorption on carbonaceous compounds as a potential anode material in lithium-ion batteries. <i>Journal of Molecular Structure</i> , 2022, 1265, 133384.	1.8	1
12485	Ab initio studies on the electronic structure of some substituted benzenes. <i>Proceedings of the Indian Academy of Sciences - Section A</i> , 1985, 95, 427-436.	0.2	2
12486	Enhanced luminescence in multivariate metal-organic frameworks through an isolated-ligand strategy. <i>Journal of Materials Chemistry C</i> , 2022, 10, 10473-10479.	2.7	7
12487	Highly transparent, self-healing and adhesive wearable ionogel as strain and temperature sensor. <i>Polymer Chemistry</i> , 2022, 13, 4064-4075.	1.9	8
12488	Nitrene-Mediated Multicomponent Couplings and Macrocyclization by CH-Functionalization. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
12489	Zn(II) complexes with thiazolylhydrazone: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity. <i>CrystEngComm</i> , 2022, 24, 5194-5214.	1.3	7
12490	N/O π -B dative bonds supplemented by N-H \cdots N/H \cdots C hydrogen bonds make BN-cages an attractive candidate for DNA-nucleobase adsorption - an MP2 prediction. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16862-16875.	1.3	3
12491	Symmetric Spirenes: Promising Building Blocks for New Generation Opto-Electronic Materials. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
12492	Copper(II) complexes supported by modified azo-based ligands: Nucleic acid binding and molecular docking studies. <i>Open Chemistry</i> , 2022, 20, 505-516.	1.0	0
12493	Comparative assessment of QM-based and MM-based models for prediction of protein-ligand binding affinity trends. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14525-14537.	1.3	5
12494	A transferable prediction model of molecular adsorption on metals based on adsorbate and substrate properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16545-16555.	1.3	3

#	ARTICLE	IF	CITATIONS
12495	Transition metal catalyzed cross-coupling and nitrogen reduction reactions: Lessons from computational studies. <i>Advances in Organometallic Chemistry</i> , 2022, , 35-78.	0.5	1
12496	Combined QM/MM, Machine Learning Path Integral Approach to Compute Free Energy Profiles and Kinetic Isotope Effects in RNA Cleavage Reactions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4304-4317.	2.3	17
12497	Spin-Orbit Couplings for Nonadiabatic Molecular Dynamics at the \hat{T} SCF Level. <i>Journal of Chemical Theory and Computation</i> , 0, , .	2.3	4
12498	Gas-Phase Peroxyl Radical Recombination Reactions: A Computational Study of Formation and Decomposition of Tetroxides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4046-4056.	1.1	9
12499	Sesquiterpene Lactones from <i>Vernonia tufnelliae</i> : Structural Characterization and Biological Evaluation. <i>Journal of Natural Products</i> , 2022, 85, 1681-1690.	1.5	3
12500	Bridging Plastic Recycling and Organic Catalysis: Photocatalytic Deconstruction of Polystyrene via a C-H Oxidation Pathway. <i>ACS Catalysis</i> , 2022, 12, 8155-8163.	5.5	57
12501	Rhodium-Catalyzed Ring Expansion Reactions for the Concise Construction of Densely Functionalized Oxathionines and Oxathiocines. <i>ACS Catalysis</i> , 2022, 12, 7524-7530.	5.5	5
12502	Many-fermion simulation from the contracted quantum eigensolver without fermionic encoding of the wave function. <i>Physical Review A</i> , 2022, 105, .	1.0	9
12503	2-Oxopurine Riboside: A Dual Fluorescent Analog and Photosensitizer for RNA/DNA Research. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4483-4490.	1.2	3
12504	Optical Characteristics of Spiropyran@MOF Composites as a Function of the Metal-Organic Framework Linker Substitution. <i>Journal of Physical Chemistry C</i> , 2022, 126, 10923-10931.	1.5	8
12505	Finding Valence Antibonding Levels while Avoiding Rydberg, Pseudo-continuum, and Dipole-Bound Orbitals. <i>Journal of the American Chemical Society</i> , 0, , .	6.6	3
12506	Stabilizing a 20-Electron Metallaazulyne by Aromaticity. <i>Inorganic Chemistry</i> , 2022, 61, 9073-9081.	1.9	3
12507	Quantum Revivals in Curved Graphene Nanoflakes. <i>Nanomaterials</i> , 2022, 12, 1953.	1.9	2
12508	Evaluation of Slight Changes in Aromaticity through Electronic and Density Functional Reactivity Theory-Based Descriptors. <i>ACS Omega</i> , 2022, 7, 21939-21945.	1.6	9
12509	New sp^2 ($n = 1, 2$) basis sets for quantum chemical calculations of the NMR chemical shifts of H, C, N, and O nuclei. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	6
12510	Band Edge Engineering of 2D Perovskite Structures through Spacer Cation Engineering for Solar Cell Applications. <i>Journal of Physical Chemistry C</i> , 2022, 126, 9937-9947.	1.5	6
12511	N -Acetyl Side-Chain Conformation in Saccharides: Solution Models Obtained from $MA^{\text{TM}}AT$ Analysis. <i>Journal of Organic Chemistry</i> , 2022, 87, 8368-8379.	1.7	5
12512	Theoretical insights into the possibility of removing CH_3Hg^+ using different adsorptive matrices: $g-C_3N_4$, cellulose xanthate, and vanillin-derived modified monomer. <i>Journal of Molecular Liquids</i> , 2022, 361, 119691.	2.3	1

#	ARTICLE	IF	CITATIONS
12513	In Silico Screening of Two-Photon Absorption Properties of a Large Set of Bis-Difluoroborate Dyes. ChemPhotoChem, 2022, 6, .	1.5	1
12514	DFT investigation on the effect of the permutation of some electron donating and accepting groups in Chemistry Accounts, 2022, 141, .	0.5	3
12515	Unveiling the Releasing Processes of Pt(II)-Based Anticancer Drugs from Oxidized Carbon Nanohorn: An In Silico Study. Journal of Physical Chemistry B, 2022, 126, 4246-4260.	1.2	4
12516	Describing Chemical Reactivity with Frontier Molecular Orbitals. JACS, 2022, 144, 1383-1394.	3.6	32
12517	Improvement of Fusel Alcohol Production by Engineering of the Yeast Branched-Chain Amino Acid Aminotransaminase. Applied and Environmental Microbiology, 2022, 88, .	1.4	1
12518	Elucidation of Metal Local Environments in Single-Atom Catalysts Based on Carbon Nitrides. Small, 2022, 18, .	5.2	15
12519	A mechanistic DFT study of Z-selective ring-opening metathesis polymerization by MAP catalysts. Molecular Catalysis, 2022, 527, 112418.	1.0	1
12520	Theoretical investigation on cobalt-catalyzed hydroacylation reaction: Mechanism and origin of stereoselectivity. Molecular Catalysis, 2022, 527, 112410.	1.0	7
12521	Should pyrolysis of diazotetranoic acid produce methylene ketene? A theoretical structural, thermochemical and kinetic study. Chemical Physics Letters, 2022, 802, 139770.	1.2	1
12522	Spectroscopic, XRD, Hirshfeld surface and density functional theory (DFT) studies of the non-covalent interactions in 2-hydroxy-3-iodo-5-nitroacetophenone. Journal of Molecular Structure, 2022, 1265, 133471.	1.8	9
12523	Flexible and free-standing bacterial cellulose derived cathode host and separator for lithium-sulfur batteries. Carbohydrate Polymers, 2022, 293, 119731.	5.1	22
12524	4-(1H-imidazo[4,5-f][1,10]phenanthroline-2-yl)benzaldehyde as a probe in pure solvents: Solvatochromism, electric dipole moment and pH influence. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 280, 121480.	2.0	3
12525	Characteristics of graphite oxide membranes with different thickness by low temperature thermal reduction for aqueous EDLC electrodes and hot activation phenomenon. Materials Research Bulletin, 2022, 154, 111927.	2.7	2
12526	Synthetic approach for the control of self-doping in luminescent organic semiconductors. Materials Chemistry Frontiers, 0, , .	3.2	0
12527	[<i>tert</i> -Butyl(diphenyl)silyl] trifluoromethanesulfonate acts as an effective additive for high-voltage lithium metal batteries. Materials Chemistry Frontiers, 0, , .	3.2	0
12528	Optimization of Chemical Synthesis with Heuristic Algorithms. SSRN Electronic Journal, 0, , .	0.4	0
12529	Effect of alkali metal cations on network rearrangement in polyisoprene ionomers. Physical Chemistry Chemical Physics, 2022, 24, 17042-17049.	1.3	5
12530	Synthesis, characterisation and reactivity of group 2 complexes with a thiopyridyl scorpionate ligand. Dalton Transactions, 2022, 51, 11922-11936.	1.6	2

#	ARTICLE	IF	CITATIONS
12531	Ab Initio Characterization of the Potential Energy Profiles for the Multi-Channel Reactions: H/Cl + Ch3oh. SSRN Electronic Journal, 0, , .	0.4	0
12533	From theory to computing: the Hartree-Fock model. , 2022, , 135-149.		0
12534	One-Electron Transfer during Dimerization of Phenoxy Radicals. Russian Journal of Organic Chemistry, 2022, 58, 637-647.	0.3	0
12535	Understanding the Regioselectivity of Ion-Pair-Assisted Meta-Selective C(sp ²)-H Activation in Conformationally Flexible Arylammonium Salts. Journal of Organic Chemistry, 2022, 87, 9222-9231.	1.7	2
12536	Colorectal Cancer Chemoprevention by S-Allyl Cysteine-Caffeic Acid Hybrids: In Vitro Biological Activity and In Silico Studies. Scientia Pharmaceutica, 2022, 90, 40.	0.7	3
12537	Self-Assembly Metal Chelate as Ultraviolet Filterable Interface Layer for Efficient Organic Solar Cells. Advanced Energy Materials, 2022, 12, .	10.2	7
12538	Delayed Fluorescence by Triplet-Triplet Annihilation from Columnar Liquid Crystal Films. ACS Applied Electronic Materials, 2022, 4, 3486-3494.	2.0	2
12539	Hydroxycarbonylation of Alkenes with Formic Acid Catalyzed by a Rhodium(III) Hydride Diiodide Complex Bearing a Bidentate Phosphine Ligand. Organometallics, 2022, 41, 1640-1648.	1.1	5
12540	Not That DDT: A Databank of Dynamics Trajectories for Organic Reactions. Journal of Chemical Education, 2022, 99, 2721-2725.	1.1	4
12541	Adsorptive capacity of a g-C ₃ N ₄ matrix for thiamethoxam removal: A DFT study. Computational and Theoretical Chemistry, 2022, 1215, 113816.	1.1	4
12542	Correspondence on "How Aromatic Are Molecular Nanorings? The Case of a Six-Porphyrin Nanoring". Angewandte Chemie - International Edition, 2022, 61, .	7.2	11
12543	Correspondence on "How Aromatic Are Molecular Nanorings? The Case of a Six-Porphyrin Nanoring". Angewandte Chemie, 0, , .	1.6	3
12544	Dual Reactivity of a Geometrically Constrained Phosphenium Cation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	18
12545	Reaction Mechanism Underlying Pd(II)-Catalyzed Oxidative Coupling of Ethylene and Benzene to Form Styrene: Identification of a Cyclic Mono-Pd ^{II} Bis-Cu ^{II} Complex as the Active Catalyst. Organometallics, 0, , .	1.1	4
12546	A Bond-Energy/Bond-Order and Populations Relationship. Journal of Chemical Theory and Computation, 2022, 18, 4774-4794.	2.3	5
12547	Nonconventional NMR Spin-Coupling Constants in Oligosaccharide Conformational Modeling: Structural Dependencies Determined from Density Functional Theory Calculations. ACS Omega, 2022, 7, 23950-23966.	1.6	4
12548	Origin of the Boosting Effect of Polyoxometalates in Photocatalysis: The Case of CO ₂ Reduction by a Rh-Containing Metal-Organic Framework. ACS Catalysis, 2022, 12, 9244-9255.	5.5	22
12549	Direct Benzene Hydroxylation with Dioxygen Induced by Copper Complexes: Uncovering the Active Species by DFT Calculations. Organometallics, 2022, 41, 1892-1904.	1.1	4

#	ARTICLE	IF	CITATIONS
12550	Rational Design of Synergistic Structure Between Single-Atoms and Nanoparticles for CO ₂ Hydrogenation to Formate Under Ambient Conditions. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	3
12551	Chemical Modifications Suppress Anharmonic Effects in the Lattice Dynamics of Organic Semiconductors. <i>ACS Materials Au</i> , 0, , .	2.6	4
12552	On the Dynamics of the Carbon–Bromine Bond Dissociation in the 1-Bromo-2-Methylnaphthalene Radical Anion. <i>Molecules</i> , 2022, 27, 4539.	1.7	1
12553	Synthesis and Optical Properties of 1,2,5,10-Tetraphenylanthra[2,3- <i>b</i>]phosphole Derivatives. <i>Journal of Organic Chemistry</i> , 2022, 87, 10493-10500.	1.7	1
12554	Oxo-Rhenium-Mediated Allylation of Furanoside Derivatives: A Computational Study on the Mechanism and the Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2022, 87, 9497-9506.	1.7	3
12555	Weakening the N–H Bonds of NH ₃ Ligands: Triple Hydrogen-Atom Abstraction to Form a Chromium(V) Nitride. <i>Inorganic Chemistry</i> , 2022, 61, 11165-11172.	1.9	6
12556	Discrimination of xylene isomers in a stacked coordination polymer. <i>Science</i> , 2022, 377, 335-339.	6.0	94
12557	The role of intramolecular interactions on the stability of the conformers of a spiropyran derivative. <i>Chemical Physics</i> , 2022, 562, 111654.	0.9	5
12558	Steric and Electronic Origins of Fluorescence in GFP and GFP-like Proteins. <i>Journal of the American Chemical Society</i> , 2022, 144, 12732-12746.	6.6	8
12559	Structural Investigation of Magnesium Complexes Supported by a Thiopyridyl Scorpionate Ligand. <i>Molecules</i> , 2022, 27, 4564.	1.7	0
12560	Geometric interpretation for coupled-cluster theory. A comparison of accuracy with the corresponding configuration interaction model. <i>Journal of Chemical Physics</i> , 0, , .	1.2	1
12561	Prenol as a Next-Generation Biofuel or Additive: A Comprehension of the Hydrogen Abstraction Reactions by a H Atom. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4791-4800.	1.1	1
12562	Dual Reactivity of a Geometrically Constrained Phosphenium Cation. <i>Angewandte Chemie</i> , 0, , .	1.6	0
12563	Highly Regioselective Synthesis of Bisadduct[C70] Additive toward the Enhanced Performance of Perovskite Solar Cells. <i>Nanomaterials</i> , 2022, 12, 2355.	1.9	2
12564	Conformational and functional changes of the native neuropeptide somatostatin occur in the presence of copper and amyloid- β . <i>Nature Chemistry</i> , 2022, 14, 1021-1030.	6.6	7
12565	Bioactive Ni(II), Cu(II) and Zn(II) complexes with an N3 functionalized Schiff base ligand: Synthesis, structural elucidation, thermodynamic and DFT calculation studies. <i>Inorganica Chimica Acta</i> , 2022, 541, 121083.	1.2	8
12566	Strain-Induced asymmetry and on-site dynamics of silicon defects in graphene. <i>Carbon Trends</i> , 2022, 9, 100189.	1.4	0
12567	Probing new DABCO-F based ionic liquids as catalyst in organic synthesis. <i>Journal of Molecular Structure</i> , 2022, 1268, 133638.	1.8	2

#	ARTICLE	IF	CITATIONS
12568	Experimental study and modified modeling on effect of SO ₂ on CO ₂ absorption using amine solution. <i>Chemical Engineering Journal</i> , 2022, 448, 137751.	6.6	14
12569	Location effect of triptycene on the photovoltaic performance of carbazole-based dyes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 433, 114132.	2.0	1
12570	Regularized CASPT2: an Intruder-State-Free Approach. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4814-4825.	2.3	17
12571	Revealing the Multifunctional Electrocatalysis of Indium-Modulated Phthalocyanine for High-Performance Lithium-Sulfur Batteries. <i>Energy and Environmental Materials</i> , 2024, 7, .	7.3	5
12572	Amino Acids Compete with Ammonia in Sulfuric Acid-Based Atmospheric Aerosol Prenucleation: The Case of Glycine and Serine. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5195-5206.	1.1	10
12573	Superionic Bifunctional Polymer Electrolytes for Solid-State Energy Storage and Conversion. <i>Advanced Materials</i> , 2023, 35, .	11.1	13
12574	Bis-polyethylene glycol-functionalized imidazolium ionic liquids: A multi-method approach towards bulk and surface properties. <i>Journal of Ionic Liquids</i> , 2022, 2, 100041.	1.0	9
12575	Mebendazole's Conformational Space and Its Predicted Binding to Human Heat-Shock Protein 90. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3604-3617.	2.5	1
12576	Mechanism of the phosphine-catalyzed [3+3] annulation with MBH carbonates as the potential dipoles. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	1
12577	Proton-coupled energy transfer in molecular triads. <i>Science</i> , 2022, 377, 742-747.	6.0	13
12578	A combined QTAIM/IRI topological analysis of the effect of axial/equatorial positions of NH ₂ and CN substituents in the [(PY5Me ₂)MoO] ⁺ complex. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108273.	1.3	3
12579	Dispersion Stabilizes Metal-Metal Bonds in the 1,8-Bis(silylamido)naphthalene Ligand Environment. <i>Organometallics</i> , 2022, 41, 2180-2187.	1.1	6
12580	Two Paths to Oxidative C-H Amination Under Basic Conditions: A Theoretical Case Study Reveals Hidden Opportunities Provided by Electron Upconversion**. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	7
12581	Unveiling the mechanism of the photocatalytic reduction of CO ₂ to formate promoted by porphyrinic Zr-based metal-organic frameworks. <i>Journal of Materials Chemistry A</i> , 2022, 10, 18103-18115.	5.2	21
12582	Angle distortion model for predicting enediyne activation towards Bergman cyclization: an alternate to the distance theory. <i>RSC Advances</i> , 2022, 12, 23552-23565.	1.7	2
12583	Insights into the Capture of CO ₂ by Nickel Hydride Complexes. <i>Catalysts</i> , 2022, 12, 790.	1.6	3
12584	Computation of NMR shieldings at the CASSCF level using gauge-including atomic orbitals and Cholesky decomposition. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	4
12585	New Phosphonite Ligands with High Steric Demand and Low Basicity: Synthesis, Structural Properties and Cyclometalated Complexes of Pt(II). <i>Inorganics</i> , 2022, 10, 109.	1.2	0

#	ARTICLE	IF	CITATIONS
12586	Fluoro Hydrogen Peroxide: A Plausible Molecular Form of Naturally-Occurring Fluorine. ACS Earth and Space Chemistry, 2022, 6, 2032-2040.	1.2	3
12587	Quantum mechanical study of interactions between sunscreen ingredients and nucleotide bases. Journal of Molecular Modeling, 2022, 28, .	0.8	0
12588	Intramolecular force field for carboxylate Pt(II)-complexes. Theoretical Chemistry Accounts, 2022, 141, .	0.5	1
12589	Chelating Rare-Earth Metals (Ln ³⁺) and ²²⁵ Ac ³⁺ with the Dual-Size-Selective Macrocyclic Ligand Py ₂ -MacroDipa. Inorganic Chemistry, 2022, 61, 12847-12855.	1.9	5
12590	Preparation and Reactivity of Rhenium ^{VI} -Nitride Complexes Bearing PNP-Type Pincer Ligands toward Nitrogen Fixation. Organometallics, 0, , .	1.1	2
12591	TD ^{SCF} modeling of electronic spectra of biliverdins in different environments. International Journal of Quantum Chemistry, 2022, 122, .	1.0	0
12592	Photocatalytic Isomerization of (E)-Anethole to (Z)-Anethole. Molecules, 2022, 27, 5342.	1.7	5
12593	Fisetin and Robinetin antiradical activity under solvent effect: density functional theory study. Journal of Molecular Modeling, 2022, 28, .	0.8	4
12594	Anion and radical anion products of flutamide studied by IR spectra and density functional calculations. Journal of Molecular Structure, 2023, 1271, 133927.	1.8	2
12595	Spectrochemistry of Firefly Bioluminescence. Chemical Reviews, 2022, 122, 13207-13234.	23.0	24
12596	External electric field-dependent photoinduced charge transfer in non-fullerene organic solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 284, 121763.	2.0	3
12597	Charge Transport in Twisted Organic Semiconductor Crystals of Modulated Pitch. Advanced Materials, 2022, 34, .	11.1	19
12598	The Speciation of Americium Cations in Neat Water Implicated from DFT Studies. Inorganic Chemistry, 2022, 61, 13858-13867.	1.9	1
12599	Design and Synthesis of RhodIndolizine Dyes with Improved Stability and Shortwave Infrared Emission up to 1250 nm. Journal of Organic Chemistry, 2022, 87, 11319-11328.	1.7	6
12600	Pyridine aldoxime ligation to iridium(III) centre: An innocent ancillary ligand in a series of organometallic complexes. Journal of Molecular Structure, 2022, , 133998.	1.8	1
12601	Unexpected role of two ortho-OH groups for the hydrogenation of CO ₂ to methanol catalyzed by Fe bipyridinol complexes. Molecular Catalysis, 2022, 529, 112559.	1.0	0
12602	Physical Mechanisms of Intermolecular Interactions and Cross-Space Charge Transfer in Two-Photon BDBT-TCNB Co-Crystals. Nanomaterials, 2022, 12, 2757.	1.9	3
12603	Dipicolylamine-Based Fluorescent Probes and Their Potential for the Quantification of Fe ³⁺ in Aqueous Solutions. ACS Omega, 2022, 7, 28342-28350.	1.6	4

#	ARTICLE	IF	CITATIONS
12604	Choice of computational protocol for carbon-13 nuclear magnetic resonance spin-spin coupling constants. <i>Magnetic Resonance in Chemistry</i> , 2022, 60, 985-995.	1.1	3
12605	Multiscale Strategy for Predicting Radiation Chemistry in Polymers. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5117-5124.	2.3	1
12606	Determination of the Rate Constant of the [4 + 2] Cycloaddition Between an Aryne Atropisomer and Furan in Solution. <i>Journal of Organic Chemistry</i> , 2022, 87, 11141-11147.	1.7	4
12608	Hardness of molecules and bandgap of solids from a generalized gradient approximation exchange energy functional. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	0
12609	Facile synthesis of $WCl_3(DME)_6$ and structural and electronic characterizations. <i>Journal of the Chinese Chemical Society</i> , 2022, 69, 1431-1437.	0.8	1
12610	Visualization of electron density changes along chemical reaction pathways. <i>Molecular Physics</i> , 0, , .	0.8	0
12611	Temperature, pressure, and adsorption-dependent redox potentials: I. Processes of CO_2 reduction to value-added compounds. <i>Energy Science and Engineering</i> , 2022, 10, 4520-4543.	1.9	3
12612	Adsorption ability of pristine C ₂₄ N ₂₄ nanocage promising as high hydrogen storage material: A DFT-D3 investigation. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 29896-29906.	3.8	8
12613	Cu(II)-Catalyzed Unsymmetrical Dioxidation of gem-Difluoroalkenes to Generate α,β -Difluorinated α -phenoxyketones. <i>Journal of Organic Chemistry</i> , 2022, 87, 10710-10725.	1.7	6
12614	Experimental and theoretical studies on prototropic tautomerism of 1-tetralone-2-carbothioamides and synthesis of regioselectively designed fused 2H-indazole derivatives. <i>Journal of Molecular Structure</i> , 2022, , 133976.	1.8	0
12615	Direct and Water-Mediated Adsorption of Stabilizers on SERS-Active Colloidal Bimetallic Plasmonic Nanomaterials: Insight into Citrate-AuAg Interactions from DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5236-5251.	1.1	3
12616	Phycocerythrin/phycoerythrin as efficient sensitizers of dye-sensitized solar cell. <i>Solar Energy</i> , 2022, 243, 494-499.	2.9	5
12617	In-depth analysis of the photophysics of BOPAHY dyes in solution, glass and film. <i>Dyes and Pigments</i> , 2022, 206, 110662.	2.0	6
12618	Antibacterial and antifungal activities in vitro of a novel silver(I) complex with sulfadoxine-salicylaldehyde Schiff base. <i>Polyhedron</i> , 2022, 225, 116073.	1.0	8
12619	Structural, vibrational characterization and DFT calculations of urea: DL-malic acid (1:1) co-crystal. <i>Journal of Molecular Structure</i> , 2022, 1270, 133930.	1.8	6
12620	Theoretical investigation on hydrolysis mechanism of cis-platin analogous Pt(II)/Pd(II) complex by DFT calculation and molecular docking approach for their interaction with DNA & HSA. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 117, 108314.	1.3	5
12621	Synthesis, in vitro, in silico and DFT studies of indole curcumin derivatives as potential anticancer agents. <i>Journal of Molecular Structure</i> , 2022, 1270, 133885.	1.8	9
12622	A combined QTAIM, DFT and molecular dynamics study on the nanoscale dynamical and structural organization of imidazolium-based dicationic ionic liquids. <i>Journal of Molecular Liquids</i> , 2022, 365, 120186.	2.3	4

#	ARTICLE	IF	CITATIONS
12623	Synthesis, crystal structures, spectroscopic characterization and in vitro evaluation of the 4-sulfonyl-3-methoxycinnamaldehydes as potential α -glucosidase and/or α -amylase inhibitors. <i>Journal of Molecular Structure</i> , 2023, 1271, 134119.	1.8	5
12624	Spin engineering of triangulenes and application for nano nonlinear optical materials design. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 18529-18542.	1.3	6
12625	DFT studies on rhodium(III)-catalyzed synthesis of indanones from <i>N</i> -methoxybenzamides via C^{H} activation reaction. <i>New Journal of Chemistry</i> , 2022, 46, 16576-16583.	1.4	0
12626	Searching for correlations between geometric and spectroscopic parameters of intramolecular hydrogen bonds in porphyrin-like macrocycles. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22319-22329.	1.3	0
12627	Tuning ESIPT-coupled luminescence by expanding π -conjugation of a proton acceptor moiety in ESIPT-capable zinc(II) complexes with 1-hydroxy-1 <i>H</i> -imidazole-based ligands. <i>Dalton Transactions</i> , 2022, 51, 15166-15188.	1.6	11
12628	Hydroboration of carbon dioxide with pinacolborane catalyzed by various aluminum hydrides: a comparative mechanistic study. <i>Catalysis Science and Technology</i> , 2022, 12, 6129-6141.	2.1	2
12629	Suppression of reversible photocyclization reaction induced fluorescence enhancement: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 25487-25494.	1.3	5
12630	A comparative study on the reactivity of ditantalum deuteride cluster anions $\text{Ta}_2\text{D}_2^{\text{--}}$ and $\text{Ta}_2\text{D}_4^{\text{--}}$ toward N_2 . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 24950-24958.	1.3	1
12631	Unveiling the origin of the chemoselectivity of bismacrocyclic-mediated C^{H} arylation of phenols: from mechanism concept to new coupling design. <i>Organic Chemistry Frontiers</i> , 2022, 9, 4890-4901.	2.3	0
12632	Mechanistic insight into $\text{Cp}^*\text{Rh}(\text{III})$ -catalyzed Lossen rearrangement vs C^{N} reductive elimination for the synthesis of pyridones. <i>New Journal of Chemistry</i> , 2022, 46, 16485-16494.	1.4	0
12633	The driving effects of common atmospheric molecules for formation of prenucleation clusters: the case of sulfuric acid, formic acid, nitric acid, ammonia, and dimethyl amine. <i>Environmental Science Atmospheres</i> , 2022, 2, 1469-1486.	0.9	5
12634	Donor-Acceptor naphthalimides and peryleneimides for all-solution-processed thin film lasers. <i>Journal of Materials Chemistry C</i> , 0, , .	2.7	0
12635	Porous Materials Formed by Four Self-construction Processes. <i>Organic and Biomolecular Chemistry</i> , 0, , .	1.5	0
12636	Theoretical insights into the mechanism and origin of chemoselectivity in the catalyst- and directing group-dependent oxidative cyclization of diynes with pyridine <i>N</i> -oxides. <i>Organic Chemistry Frontiers</i> , 2022, 9, 5168-5177.	2.3	2
12637	Structure and diffusive dynamics of aspartate α -decarboxylase (ADC) liganded with <i>D</i> -serine in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20336-20347.	1.3	1
12638	Stressing the differences in alizarin and purpurin dyes through UV-visible light absorption and $^1\text{H-NMR}$ spectroscopies. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 19452-19462.	1.3	3
12639	Degradation of the Neonicotinoid Thiamethoxam by the Solar-Fenton Process: Theoretical Insights and Ecotoxicological Evaluation. <i>SSRN Electronic Journal</i> , 0, , .	0.4	1
12640	Size-dependent properties and unusual reactivity of novel nonplanar heterocycloarenes. <i>Chemical Science</i> , 2022, 13, 11174-11182.	3.7	5

#	ARTICLE	IF	CITATIONS
12641	The DFT Approach to predict ¹³ C NMR chemical shifts of hydrocarbon species adsorbed on Zn-modified zeolites. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 22241-22249.	1.3	2
12642	Alkyne-alkenyl coupling at a diruthenium complex. <i>Dalton Transactions</i> , 2022, 51, 15703-15715.	1.6	9
12643	Utilization of sym-tetrazines as guanidine delivery cycloaddition reagents. An experimental and computational study. <i>Journal of Molecular Structure</i> , 2023, 1272, 134207.	1.8	3
12644	Green synthesis of gold nanoparticles using quercetin biomolecule from mangrove plant, Ceriops tagal: Assessment of antiproliferative properties, cellular uptake and DFT studies. <i>Journal of Molecular Structure</i> , 2023, 1272, 134167.	1.8	6
12645	A P450 Harboring Manganese Protoporphyrin IX Generates a Manganese Analogue of Compound I by Activating Dioxigen. <i>ACS Catalysis</i> , 2022, 12, 11108-11117.	5.5	6
12646	Bright, Modular, and Switchable Near-Infrared II Emission from Compact Tetrathiafulvalene-Based Diradicaloid Complexes. <i>Journal of the American Chemical Society</i> , 2022, 144, 16447-16455.	6.6	9
12647	Managing the Redox Potential of PCET in Grothuss-Type Proton Wires. <i>Journal of the American Chemical Society</i> , 2022, 144, 15672-15679.	6.6	9
12648	Dual Fluorescence of Octatetraene Hints at a Novel Type of Singlet-to-Singlet Thermally Activated Delayed Fluorescence Process. <i>Journal of Physical Chemistry C</i> , 2022, 126, 14976-14985.	1.5	8
12649	Understanding the Nature and Strength of Noncovalent Face-to-Face Arene-Fullerene Interactions. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	1
12650	Prediction of correlation energies using variational subspace valence bond. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	1
12651	Microbial biofilms as living photoconductors due to ultrafast electron transfer in cytochrome OmcS nanowires. <i>Nature Communications</i> , 2022, 13, .	5.8	24
12652	Unraveling origin of chemoselectivity and regioselectivity of iridium-catalyzed B(4)H functionalization of <i>o</i> -carborane by alkyne. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	0
12653	Machine learning the frontier orbital energies of SubPc based triads. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	3
12654	Design of Molecules with Low Hole and Electron Reorganization Energy Using DFT Calculations and Bayesian Optimization. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6336-6347.	1.1	7
12655	Halogen-atom and group transfer reactivity enabled by hydrogen tunneling. <i>Science</i> , 2022, 377, 1323-1328.	6.0	46
12656	New Methods for Preparation of the Monofluorosubstituted Derivative of the closo-Borate Anion [2-B10H9F]2-, Its Properties, and Analysis of Its Reactivity. <i>Russian Journal of Inorganic Chemistry</i> , 2022, 67, 1583-1590.	0.3	7
12657	Iridium Complexes with a Naphthyridine-Based <i>Si</i> , <i>N</i> -Ligand: Synthesis and Catalytic Activity toward Olefin Hydrogenation. <i>Organometallics</i> , 2022, 41, 2612-2621.	1.1	3
12658	Oligonucleotides Featuring a Covalently Mercurated 6-Phenylcarbazole Residue as High-Affinity Hybridization Probes for Thiopyrimidine-Containing Sequences. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4

#	ARTICLE	IF	CITATIONS
12659	Trajectory surface hopping molecular dynamics on Chemiluminescence of cyclic peroxides. Journal of the Chinese Chemical Society, 2023, 70, 269-286.	0.8	1
12660	A DFT study of the interaction of aspirin, paracetamol and caffeine with one water molecule. Journal of Molecular Modeling, 2022, 28, .	0.8	5
12661	Enhancement of Thermally Activated Delayed Fluorescence (TADF) in Multi-Resonant Emitters via Control of Chalcogen Atom Embedding. Chemistry of Materials, 2022, 34, 8022-8030.	3.2	15
12662	Theoretical Rovibrational Characterization of Si ₃ O ₃ and Mg ₃ O ₃ : Intermediates between Small Molecules and Nanocrystals. ACS Earth and Space Chemistry, 2022, 6, 2471-2480.	1.2	2
12663	Novel Multipotent Amantadine-M30D Hybrids with Highly Selective Butyrylcholinesterase Inhibition and Neuroprotective Effects as Effective Anti-Alzheimer's Agents. ACS Chemical Neuroscience, 2022, 13, 2681-2698.	1.7	1
12664	Inorganic Bases Enhanced Organocatalysis for Aerobic α -Hydroxylation of Aliphatic Cycloketones. Asian Journal of Organic Chemistry, 0, , .	1.3	1
12665	Binaphthyl-Proline Hybrid Chiral Ligands: Modular Design, Synthesis, and Enantioswitching in Cu(II)-Catalyzed Enantioselective Henry Reactions. Journal of Organic Chemistry, 2023, 88, 7651-7659.	1.7	8
12666	Rationalizing the Substituent Effects in Diels-Alder Reactions of Triazolinediones with Anthracene. Journal of Physical Chemistry A, 2022, 126, 6657-6667.	1.1	2
12667	NO Bond Cleavage on Gas-Phase Ir _n ⁺ Clusters Investigated by Infrared Multiple Photon Dissociation Spectroscopy. Journal of Physical Chemistry A, 2022, 126, 6668-6677.	1.1	5
12668	Deciphering the role of (anti)aromaticity in cofacial excimers of linear acenes. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	4
12669	Elongation of a Trigonal-Prismatic Copper Cluster by Diphosphine Ligands with Longer Spacers. Inorganic Chemistry, 2022, 61, 15144-15151.	1.9	5
12670	Structure and Reactivity of [Ru-Al] and [Ru-Sn] Heterobimetallic PPh ₃ -Based Complexes. Organometallics, 2022, 41, 2716-2730.	1.1	3
12672	Cost-Effective Implementation of Multiconformer Transition State Theory for Alkoxy Radical Unimolecular Reactions. Journal of Physical Chemistry A, 2022, 126, 6483-6494.	1.1	4
12673	Reaction Pathways of Diplatinum Complexes Bearing a Phenylpropene-Derived η^5 -Chelator with Weak/Strong σ -Donor Neutral Ligands. ChemistrySelect, 2022, 7, .	0.7	1
12674	Understanding the Nature and Strength of Noncovalent Face-to-Face Arene-Fullerene Interactions. Angewandte Chemie - International Edition, 2022, 61, .	7.2	2
12675	Explaining the High Catalytic Activity in Bis(indenyl) Methyl Zirconium Cation Using Combined EDA-NOCV/QTAIM Approach. ChemPhysChem, 0, , .	1.0	1
12676	Can armchair nanotubes host organic color centers?. Journal of Physics Condensed Matter, 2022, 34, 464004.	0.7	0
12677	σ -Holes in Iodonium Ylides: Halogen-Bond Activation of Carboxylic Acids, Phenols and Thiophenols May Enable Their X-H Insertion Reactions. Chemistry - A European Journal, 0, , .	1.7	2

#	ARTICLE	IF	CITATIONS
12678	Quantum chemistry calculation and experimental research on the component proportion of black disperse dye. <i>Textile Reseach Journal</i> , 2023, 93, 750-761.	1.1	1
12679	Robust Nonspiro-Based Hole Conductors for High-Efficiency Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	11
12680	Mycobacterium Time-Series Genome Analysis Identifies AAC2 as a Potential Drug Target with Naloxone Showing Potential Bait Drug Synergism. <i>Molecules</i> , 2022, 27, 6150.	1.7	7
12681	From Gas Phase Observations to Solid State Reality: The Identification and Isolation of Trinuclear Salicylaldoximate Copper Complexes. <i>Molecules</i> , 2022, 27, 6421.	1.7	0
12682	Dissecting the mechanisms of environment sensitivity of smart probes for quantitative assessment of membrane properties. <i>Open Biology</i> , 2022, 12, .	1.5	8
12683	Filling the Gaps in the Challenging Asymmetric Hydrogenation of Exocyclic Benzofused Alkenes with Ir ^{III} P,N Catalysts. <i>Advanced Synthesis and Catalysis</i> , 2023, 365, 167-177.	2.1	4
12684	Detailed Density Functional Theory Study of the Cationic Zirconocene Compound [Cp(C ₅ H ₄ CMe ₂ C ₆ H ₄ F)ZrMe] ⁺ . <i>ACS Omega</i> , 2022, 7, 35136-35152.	1.6	1
12685	Applying the quantum chemical simulation to describe electrical conductivity in silicate-based materials. <i>Vestnik MGSU</i> , 2022, , 1175-1186.	0.2	0
12686	Creating enzyme-mimicking nanopockets in metal-organic frameworks for catalysis. <i>Science Advances</i> , 2022, 8, .	4.7	24
12687	Rapid calculation of internal conversion and intersystem crossing rate for organic materials discovery. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	5
12688	Energy Transfer Mechanism and Quantitative Modeling of Rate from an Antenna to a Lanthanide Ion. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7418-7431.	1.1	11
12689	Noncovalent Stabilization of Radical Intermediates in the Enantioselective Hydroamination of Alkenes with Sulfonamides. <i>Journal of the American Chemical Society</i> , 2022, 144, 18948-18958.	6.6	11
12691	Benchmarking the semi-stochastic CC(<i>P</i> ; <i>Q</i>) approach for singlet-triplet gaps in biradicals. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
12692	Eu@C ₈₈ Isomers: Calculated Relative Populations. <i>ECS Journal of Solid State Science and Technology</i> , 2022, 11, 101008.	0.9	1
12693	Adaptive Aromaticity in Osmapentalene and Osmapyridinium Complexes with Carbene Ligands. <i>Journal of Physical Organic Chemistry</i> , 0, , .	0.9	2
12694	Ab initio characterization of the potential energy profiles for the multi-channel reactions: H/Cl ⁺ +CH ₃ OH. <i>Computational and Theoretical Chemistry</i> , 2022, 1217, 113906.	1.1	1
12695	Sensitivity of coupled cluster electronic properties on the reference determinant: Can Kohn-Sham orbitals be more beneficial than Hartree-Fock orbitals?. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	4
12696	Experimental and DFT studies of selenium decorated graphene oxide: Redox stability, cytotoxicity, and corrosion inhibition of AZ13 Mg alloy. <i>Materials Chemistry and Physics</i> , 2022, 292, 126870.	2.0	0

#	ARTICLE	IF	CITATIONS
12697	Exploring the Fe doped borazine system as a promising CFC adsorbent: A DFT study. Computational and Theoretical Chemistry, 2022, 1217, 113903.	1.1	1
12698	Improving the accuracy of GIPAW chemical shielding calculations with cluster and fragment corrections. Solid State Nuclear Magnetic Resonance, 2022, 122, 101832.	1.5	7
12699	Mechanistic insight highlights the key steps and significance of metal in Ir(κ^3)-catalysed C=C-H activated chromones generation. Organic and Biomolecular Chemistry, 2022, 20, 9703-9721.	1.5	1
12700	Si ₅ -pentagonal rings and Y-shaped Si ₄ building blocks in Li ₃₂ Si ₁₈ system: similarities with the crystalline Zintl phase Li ₁₂ Si ₇ . Molecular Systems Design and Engineering, 0, , .	1.7	0
12701	Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study. New Journal of Chemistry, 0, , .	1.4	0
12702	Improving IDP theoretical chemical shift accuracy and efficiency through a combined MD/ADMA/DFT and machine learning approach. Physical Chemistry Chemical Physics, 2022, 24, 27678-27692.	1.3	1
12703	Computational mining of endohedral C ₇₀ electrides: tri-metal alkali and alkaline-earth encapsulation. Dalton Transactions, 2022, 51, 16836-16844.	1.6	1
12704	PM-IRRAS and DFT investigation of the surface orientation of new Ir piano-stool complexes attached to Au(111). Dalton Transactions, 2022, 51, 17688-17699.	1.6	1
12705	First 1-hydroxy-1H-imidazole-based ESIPT emitter with an O-H \cdots O intramolecular hydrogen bond: ESIPT-triggered TICT and speciation in solution. New Journal of Chemistry, 0, , .	1.4	3
12706	Electronic absorption spectral analysis of chlorin-based dyad sensitizers by TD-DFT calculations. Journal Physics D: Applied Physics, 2022, 55, 504001.	1.3	0
12707	Redox-tunable Lewis bases for electrochemical carbon dioxide capture. Nature Energy, 2022, 7, 1065-1075.	19.8	30
12708	The Influence of the Electron Density in Acyl Protecting Groups on the Selectivity of Galactose Formation. Journal of the American Chemical Society, 2022, 144, 20258-20266.	6.6	12
12709	Modeling Singlet Oxygen-Induced Degradation Pathways Including Environmental Effects of 1,2-Dimethoxyethane in Li ₂ O Batteries through Density Functional Theory. Journal of Physical Chemistry A, 2022, 126, 7997-8006.	1.1	4
12710	Electronically controlled regioselective hydroarylation of gem-difluoroallenes. Cell Reports Physical Science, 2022, 3, 101117.	2.8	7
12711	Reorganization Energies for Interfacial Proton-Coupled Electron Transfer to a Water Oxidation Catalyst. Journal of the American Chemical Society, 2022, 144, 20514-20524.	6.6	7
12712	An Ab Initio Investigation on Relevant Oligomerization Reactions of Toluene Diisocyanate (TDI). Polymers, 2022, 14, 4183.	2.0	1
12713	Efficient synthesis of new azo-sulfonamide derivatives and investigation of their molecular docking and cytotoxicity results. Arabian Journal of Chemistry, 2022, 15, 104383.	2.3	7
12714	Synthesis, Conformational Analysis and Evaluation of the 2-aryl-4-(4-bromo-2-hydroxyphenyl)benzo[1,5]thiazepines as Potential \pm -Glucosidase and/or \pm -Amylase Inhibitors. Molecules, 2022, 27, 6935.	1.7	2

#	ARTICLE	IF	CITATIONS
12715	Applying Generalized Variational Principles to Excited-State-Specific Complete Active Space Self-consistent Field Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6608-6621.	2.3	7
12716	Cooperative Intrinsic Basicity and Hydrogen Bonding Render Sml ₂ More Azaphilic than Oxophilic. <i>ACS Omega</i> , 0, .	1.6	0
12717	Anti-Symmetric Electromagnetic Interactionsâ€™ Response in Electron Circular Dichroism and Chiral Origin of Periodic, Complementary Twisted Angle in Twisted Bilayer Graphene. <i>Molecules</i> , 2022, 27, 6525.	1.7	1
12718	Base-Free Catalytic Hydrogen Production from Formic Acid Mediated by a Cubane-Type Mo ₃ S ₄ Cluster Hydride. <i>Inorganic Chemistry</i> , 2022, 61, 16730-16739.	1.9	2
12719	Microbial Denitrification: Active Site and Reaction Path Models Predict New Isotopic Fingerprints. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 2582-2594.	1.2	1
12720	Impacts of polarizable continuum models on the SCF convergence and DFT delocalization error of large molecules. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	2
12721	Molecular Tuning in Diaryl-Capped Pyrrolo[2,3-d:5,4-dâ€™]bisthiazoles: Effects of Terminal Aryl Unit and Comparison to Dithieno[3,2-b:2â€™,3â€™-d]pyrrole Analogues. <i>Molecules</i> , 2022, 27, 6638.	1.7	0
12722	[CMMIM][BF ₄ ⁻] Ionic Liquid-Catalyzed Facile, One-Pot Synthesis of Chromeno[4,3-d<i>pyrido[1,2-a<i>pyrimidin-6-ones: Evaluation of Their Photophysical Properties and Theoretical Calculations. <i>ACS Omega</i> , 2022, 7, 39147-39158.	1.6	8
12723	Electrocatalytic Conversion of CO ₂ to Formate at Low Overpotential by Electrolyte Engineering in Model Molecular Catalysis. <i>ChemSusChem</i> , 2022, 15, .	3.6	6
12724	Nano-crystalline precursor formation, stability, and transformation to mullite-type visible-light photocatalysts. <i>Journal of Materials Science</i> , 2022, 57, 19280-19299.	1.7	3
12725	Application of Halfâ€™ Sandwich Metalâ€™ Phosphinite Compounds to Biological Activities: Determine the energies of the HOMO and LUMO levels. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2023, 649, .	0.6	1
12726	Tools for Understanding and Predicting the Affinity of Per- and Polyfluoroalkyl Substances for Anion-Exchange Sorbents. <i>Environmental Science & Technology</i> , 2022, 56, 15470-15477.	4.6	9
12727	Hydrolytically Stable and Cytotoxic [ONO<i>N<i>Ti(IV)-Type Octahedral Complexes. <i>Inorganic Chemistry</i> , 2022, 61, 17653-17661.	1.9	6
12728	Electrochemical Strategy for Proton Relay Installation Enhances the Activity of a Hydrogen Evolution Electrocatalyst. <i>Journal of the American Chemical Society</i> , 2022, 144, 20267-20277.	6.6	8
12729	Polarizable MD and QM/MM investigation of acrylamide-based leads to target the main protease of SARS-CoV-2. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	3
12730	Theoretical Insight into Bâ€™C Chemical Bonding in Closo-Borate [BnHnâ€™1CH3]2â€™ (n = 6, 10, 12) and Monocarborane [CBnHnCH3]â€™ (n = 5, 9, 11) Anions. <i>Inorganics</i> , 2022, 10, 186.	1.2	2
12731	Fineâ€™ Tuning the Photophysics of Donorâ€™ Acceptor (Dâ€™A₃) Thermally Activated Delayed Fluorescence Emitters Using Isomerisation. <i>ChemPhotoChem</i> , 2023, 7, .	1.5	1
12732	Dinuclear silver(I)â€™ and gold(I)â€™N heterocyclic carbene complexes; Synthesis, structural characterizations, photoluminescence and theoretical studies. <i>Journal of Molecular Structure</i> , 2023, 1274, 134430.	1.8	1

#	ARTICLE	IF	CITATIONS
12733	Benchmarking Density Functionals, Basis Sets, and Solvent Models in Predicting Thermodynamic Hydricities of Organic Hydrides. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7566-7577.	1.1	0
12734	Modeling Charge Transfer Reactions by Hopping between Electronic Ground State Minima: Application to Hole Transfer between DNA Bases. <i>Molecules</i> , 2022, 27, 7408.	1.7	3
12735	Effects of Heterogeneous Protein Environment on Excitation Energy Transfer Dynamics in the Fenna-Matthews-Olson Complex. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9271-9287.	1.2	3
12736	A strategy to construct low temperature curable copolyimides with pyrimidine based diamine. <i>Polymer</i> , 2022, 261, 125418.	1.8	3
12737	Reactivities of silane coupling agents in the silica/rubber composites: Theoretical insights into the relationships between energy barriers and electronic characteristics. <i>Journal of Computational Chemistry</i> , 2023, 44, 581-593.	1.5	1
12738	A versatile artificial metalloenzyme scaffold enabling direct bioelectrocatalysis in solution. <i>Science Advances</i> , 2022, 8, .	4.7	2
12739	Oxygenation Induced Electronic Structure Changes in Anionic Platinum(II) Complex Bearing 2-Phenylpyridine and Benzene-1,2-dithiolate Ligands: Theoretical Study. <i>Russian Journal of Inorganic Chemistry</i> , 0, , .	0.3	0
12740	Synthesis, spectral characterization, DFT and in silico ADME studies of the novel pyrido[1,2-a]benzimidazoles and pyrazolo[3,4-b]pyridines. <i>Journal of Molecular Structure</i> , 2023, 1274, 134454.	1.8	8
12741	Corrosion inhibitory potential of selected flavonoid derivatives: Electrochemical, molecular dynamics and quantum chemical approaches. <i>Results in Engineering</i> , 2022, 16, 100694.	2.2	5
12742	DFT Insights into the mechanism of Ru(II) Catalyzed C7-selective amidation of N-pivaloylindole. <i>Journal of Organometallic Chemistry</i> , 2022, 982, 122534.	0.8	1
12743	Insights into the reactivity properties, docking, DFT and MD simulations of orphenadrinium dihydrogen citrate in different solvents. <i>Journal of Molecular Liquids</i> , 2022, 367, 120583.	2.3	15
12744	Non-covalent Cl \cdots X interactions in several silver compounds based on [B12Cl12]2 $^{+}$ clusters: 35Cl NQR and X-ray diffraction. <i>Inorganica Chimica Acta</i> , 2023, 544, 121231.	1.2	1
12745	Carbazole based D- π -A dyes for DSSC applications: DFT/TDDFT study of the influence of π -spacers on the photovoltaic performance. <i>Chemical Physics</i> , 2023, 565, 111738.	0.9	5
12746	Mechanistic insights into the self-esterification of lactic acid under neutral and acidic conditions. <i>Journal of Molecular Structure</i> , 2023, 1273, 134336.	1.8	1
12747	Supramolecular architecture and SHG activity of organic crystals formed between the amidinothiourea and nicotinic acid. <i>Journal of Molecular Structure</i> , 2023, 1273, 134385.	1.8	3
12748	Lithium sensors based on photophysical changes of 1-aza-12-crown-4 naphthalene derivatives synthesized via Buchwald-Hartwig amination. <i>RSC Advances</i> , 2022, 12, 31976-31984.	1.7	2
12749	Insights into the mechanism and selectivity of the Rh-catalyzed cycloisomerization reaction of benzylallene-alkynes involving C-H bond activation. <i>Organic Chemistry Frontiers</i> , 2022, 10, 115-126.	2.3	2
12750	Facile C=O bond cleavage on polynuclear vanadium nitride clusters V ₄ N ₅ . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 29765-29771.	1.3	1

#	ARTICLE	IF	CITATIONS
12751	Comparative oxidative ability of mononuclear and dinuclear high-valent iron ^{oxo} species towards the activation of methane: does the axial/bridge atom modulate the reactivity?. Dalton Transactions, 2023, 52, 308-325.	1.6	3
12752	<i>cis</i> → <i>trans</i> isomerization of dimethyl 2,3-dibromofumarate. RSC Advances, 2022, 12, 32471-32474.	1.7	0
12753	DFT insights into the mechanism of O ₂ activation catalyzed by a structural and functional model of cysteine dioxygenase with tris(2-pyridyl)methane-based ligand architecture. Journal of Inorganic Biochemistry, 2023, 238, 112066.	1.5	2
12754	Synthesis, characterization, theoretical studies and antioxidant and cytotoxic evaluation of a series of Tetrahydrocurcumin (THC)-benzylated derivatives. Journal of Molecular Structure, 2023, 1273, 134355.	1.8	2
12756	Copper(I)-Catalyzed Syntheses of Benzo[<i>b</i>]fluorenes by the Cascade Reactions of 2-Alkynylbenzaldehyde <i>N</i> -Tosylhydrazones and Aromatic Terminal Alkynes. Journal of Organic Chemistry, 2022, 87, 16011-16018.	1.7	3
12757	Revisiting the Fluorescence of Benzothiadiazole Derivatives: Anti-Kasha Emission or Not?. ChemPhotoChem, 0, .	1.5	0
12758	Catalytic Nitrous Oxide Reduction with H ₂ Mediated by Pincer Ir Complexes. Inorganic Chemistry, 2022, 61, 18590-18600.	1.9	6
12759	Group 6 (Cr, Mo, W) and Group 7 (Mn, Re) bipyridyl tetracarbonyl complex for electrochemical CO ₂ conversion: DFT and DLPNO-CCSD(T) study for effects of the central metal on redox potential, thermodynamics, and kinetics. Chemical Physics, 2023, 565, 111758.	0.9	2
12760	Mechanistic Studies of the Electrocatalytic Carbon-Bromine Cleavage and the Hydrogen Atom Incorporation from 1,1,1,3,3,3-Hexafluoroisopropanol. Journal of the Electrochemical Society, 2022, 169, 115502.	1.3	3
12761	Synthesis of coplanar quaternary ammonium salts with excellent electrochemical properties based on an anthraquinone skeleton and their application in copper plating. Electrochimica Acta, 2023, 437, 141541.	2.6	2
12762	One-Bond ¹³ C→ ¹ H and ¹³ C→ ¹³ C Spin-Coupling Constants as Constraints in <i>MA</i> ™AT Analysis of Saccharide Conformation. Journal of Physical Chemistry B, 2022, 126, 9506-9515.	1.2	4
12763	Application of Multiconfiguration Pair-Density Functional Theory to the Diels-Alder Reaction. Journal of Physical Chemistry A, 2022, 126, 8834-8843.	1.1	1
12764	Speciation and Structures in Pt Surface Sites Stabilized by N-Heterocyclic Carbene Ligands Revealed by Dynamic Nuclear Polarization Enhanced Indirectly Detected ¹⁹⁵ Pt NMR Spectroscopic Signatures and Fingerprint Analysis. Journal of the American Chemical Society, 2022, 144, 21530-21543.	6.6	11
12765	Theoretical investigation of structural parameters, reactivity behavior, and thermodynamic properties of Anderson polyoxometalate (POM). Structural Chemistry, 2023, 34, 1231-1240.	1.0	4
12766	Tailoring Donor-Acceptor Emitters to Minimise Localisation Induced Quenching of Thermally Activated Delayed Fluorescence. ChemPhotoChem, 2023, 7, .	1.5	1
12767	Synthesis and Characterisation of Novel Bis(diphenylphosphane oxide)methanidoytterbium(III) Complexes. Molecules, 2022, 27, 7704.	1.7	1
12768	Reliability of Computing van der Waals Bond Lengths of Some Rare Gas Diatomics. International Journal of Molecular Sciences, 2022, 23, 13944.	1.8	0
12769	New Local Explorations of the Unitary Coupled Cluster Energy Landscape. Journal of Chemical Theory and Computation, 2022, 18, 7350-7358.	2.3	1

#	ARTICLE	IF	CITATIONS
12770	Extended π -Conjugated Ligands Tune Excited-State Energies of Iron(II) Polypyridine Dyes. <i>Inorganic Chemistry</i> , 2022, 61, 18850-18860.	1.9	2
12771	A Materials Acceleration Platform for Organic Laser Discovery. <i>Advanced Materials</i> , 2023, 35, .	11.1	10
12772	Inverse kinetic isotope effects in the oxygen reduction reaction at platinum single crystals. <i>Nature Chemistry</i> , 2023, 15, 271-277.	6.6	27
12773	Theoretical Investigation of the Electronic Spectra of Cadmium Chalcogenide 2D Nanoplatelets. <i>Journal of Physical Chemistry A</i> , 2022, 126, 8818-8825.	1.1	0
12774	Electronic Substitution Effect on the Ground and Excited State Properties of Indole Chromophore: A Computational Study**. <i>ChemPhysChem</i> , 2023, 24, .	1.0	3
12775	Electrocatalytic CO ₂ reduction with a binuclear bis π -terpyridine pyrazole π -bridged cobalt complex. <i>Chemistry - A European Journal</i> , 0, , .	1.7	2
12776	Evaluating the predictive character of the method of constrained geometries simulate external force with density functional theory. <i>Forces in Mechanics</i> , 2022, 9, 100143.	1.3	4
12777	Pyridine coordination enabled stepwise PT/ET N-H transfer and metal-independent C-C cleavage mechanism for Cu-mediated dehydroacylation of unstrained ketones. <i>Dalton Transactions</i> , 2022, 51, 18409-18415.	1.6	1
12778	A General Twisted Intramolecular Charge Transfer Triggering Strategy by Protonation for Zero-Background Fluorescent Turn-On Sensing. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10871-10881.	2.1	3
12779	Catalytic Mechanisms of Transfer Hydrogenation of Azobenzene with Ammonia Borane by Pincer Bismuth Complex: Crucial Role of C=N Functional Group on the Pincer Ligand. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	3
12780	Halogenation of the 3-position of pyridines through Zincke imine intermediates. <i>Science</i> , 2022, 378, 773-779.	6.0	35
12781	DMPO Spin Trapping Study of the Photolysis of 2-(4-Nitrophenyl)-1 <i>H</i> -indolyl-3-methyl Derivatives. <i>Chemistry Letters</i> , 2023, 52, 10-12.	0.7	1
12783	Locating the hydrogen atoms in endohedral clusterfullerenes by density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2451-2461.	1.3	2
12784	Improving the kinetic resolution of rac-2-(diphenylthiophosphinoferrocene) methanol catalyzed by <i>Thermomyces lanuginosus</i> lipase immobilized on imobead-150. <i>Molecular Catalysis</i> , 2023, 535, 112867.	1.0	0
12785	Palladium-catalyzed generation of CO from formic acid for alkoxycarbonylation of internal alkenes involves a PTSA-assisted NH π -Pd mechanism: a DFT mechanistic study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 2294-2303.	1.3	2
12786	Design, synthesis, theoretical study, antioxidant, and anticholinesterase activities of new pyrazolo-fused phenanthrolines. <i>RSC Advances</i> , 2022, 12, 33032-33048.	1.7	2
12787	A theoretical study of the ligand-controlled palladium-catalysed regiodivergent synthesis of dibenzosilepin derivatives. <i>Dalton Transactions</i> , 2023, 52, 737-746.	1.6	3
12788	A TD-DFT study of a class of D π - π -A fluorescent probes for detection of typical oxidants. <i>Organic and Biomolecular Chemistry</i> , 2023, 21, 315-322.	1.5	2

#	ARTICLE	IF	CITATIONS
12789	An ultra-thin polymer electrolyte for 4.5ÅV high voltage LiCoO ₂ quasi-solid-state battery. <i>Chemical Engineering Journal</i> , 2023, 455, 140846.	6.6	11
12790	Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1349-1362.	1.3	2
12791	Theoretical investigation of borane compounds mimicking transition metals for N ₂ fixation and activation. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
12792	“Optimized route”™ to synthesize isoelectronic and isostructural Au(III)- and Pt(II)-NHC complexes: synthesis, structure, spectral properties, electrochemistry, and molecular docking studies. <i>New Journal of Chemistry</i> , 2022, 47, 284-296.	1.4	2
12793	Chemically induced crosslinked enhanced emission of carbon polymer dots discerning healthy and cancer cells through pH-dependent tunable photoluminescence. <i>Journal of Materials Chemistry B</i> , 0, , .	2.9	3
12794	The scavenging mechanism of aminopyrines towards hydroxyl radical: A computational mechanistic and kinetics investigation. <i>Computational and Theoretical Chemistry</i> , 2023, 1219, 113973.	1.1	1
12795	Adsorption of a water molecule on the surface of neutral and charged titanium clusters: Ti-H ₂ O, Ti+1-H ₂ O, Ti _n -1-H ₂ O, n=9. <i>Journal of Molecular Liquids</i> , 2023, 369, 120953.	2.3	2
12796	A comprehensive benchmark investigation of quantum chemical methods for carbocations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1903-1922.	1.3	3
12797	Mechanism of formic acid dehydrogenation catalysed by Cp*Co(III) and Cp*Rh(III) complexes with N,N'-bidentate imidazoline-based ligands: A DFT exploration. <i>Molecular Catalysis</i> , 2023, 535, 112860.	1.0	0
12798	Bio-inspired Cu(II) amido-quinoline complexes as catalysts for aromatic C-H bond hydroxylation. <i>Dalton Transactions</i> , 2023, 52, 540-545.	1.6	3
12799	Photodegradation of bisphenol A by ZnS combined with H ₂ O ₂ : Evaluation of photocatalytic activity, reaction parameters, and DFT calculations. <i>Journal of Molecular Liquids</i> , 2023, 371, 121096.	2.3	7
12800	Distinct binding pattern of nor-NOHA inhibitor to liver arginase in aqueous solution “ Perspectives from molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2023, 371, 121014.	2.3	0
12801	Effective removal of Hg ²⁺ and Cd ²⁺ in aqueous systems by Fe-Mn oxide modified biochar: A combined experimental and DFT calculation. <i>Desalination</i> , 2023, 549, 116306.	4.0	14
12802	Host-guest complexation of cucurbit[7]uril and cucurbit[8]uril with the antimuscarinic drugs tropicamide and atropine. <i>Journal of Molecular Graphics and Modelling</i> , 2023, 119, 108380.	1.3	4
12803	Intensification of NO ₂ removal in sulfite solutions with reusable copper chloride: Mechanism and process parameters. <i>Separation and Purification Technology</i> , 2023, 308, 122996.	3.9	0
12804	Effect of azomethine group containing compounds on gene profiles in Wnt and MAPK signal patterns in lung cancer cell line: In silico and in vitro analyses. <i>Journal of Molecular Structure</i> , 2023, 1275, 134619.	1.8	3
12805	Hydrogermylation initiated by trialkylborohydrides: a living anionic mechanism. <i>Chemical Communications</i> , 2022, 58, 13979-13982.	2.2	5
12806	Influence of the metal-support and metal-metal interactions on Pd nucleation and NO adsorption in a Pd ₄ /Al ₂ O ₃ (110D) model. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	1

#	ARTICLE	IF	CITATIONS
12807	Comment on "Multiple locations of boron atoms in the exohedral and endohedral C ₆₀ fullerene". Physical Review A, 2022, 106, .	1.0	3
12808	Water-Soluble Salts Based on Benzofuroxan Derivatives" Synthesis and Biological Activity. International Journal of Molecular Sciences, 2022, 23, 14902.	1.8	2
12809	Diastereoselective Synthesis of Novel Spiro-Phosphacoumarins and Evaluation of Their Anti-Cancer Activity. International Journal of Molecular Sciences, 2022, 23, 14348.	1.8	2
12810	Density Functional Theory Study on the H ₂ -Acceptorless Dehydrogenative Boration of Alkenes Catalyzed by a Zirconium Complex. Journal of Organic Chemistry, 2022, 87, 16632-16643.	1.7	1
12811	Correlation between Electronic Descriptor and Proton-Coupled Electron Transfer Thermodynamics in Doped Graphite-Conjugated Catalysts. Journal of Physical Chemistry Letters, 2022, 13, 11216-11222.	2.1	4
12812	Self-Assembled Monolayers of Molecular Conductors with Terpyridine-Metal Redox Switching Elements: A Combined AFM, STM and Electrochemical Study. Molecules, 2022, 27, 8320.	1.7	0
12813	Trapping the Transition State in a [2,3]-Sigmatropic Rearrangement by Applying Pressure. ACS Omega, 2022, 7, 45208-45214.	1.6	3
12814	Evaluation of Photocatalytic Performance of Nano-Sized Sr _{0.9} La _{0.1} TiO ₃ and Sr _{0.25} Ca _{0.25} Na _{0.25} Pr _{0.25} TiO ₃ Ceramic Powders for Water Purification. Nanomaterials, 2022, 12, 4193.	1.9	1
12815	Mechanism of Photocatalytic CO ₂ Reduction by Iron Spin-Crossover Complex with Copper Photosensitizer. Organometallics, 2022, 41, 3568-3580.	1.1	1
12816	Into the Role of Unsaturated Trinuclear Metal Carbonyls in the Formation of [M ₃ (2,3-bpp)(CO) ₁₀] with M=Ru, Os: A DFT Stability Analysis and Electronic Structure. Journal of Cluster Science, 0, , .	1.7	0
12817	Rare Earth Complexes of Europium(II) and Substituted Bis(pyrazolyl)borates with High Photoluminescence Efficiency. Molecules, 2022, 27, 8053.	1.7	0
12818	The Origin of Stereoselectivity in the Hydrogenation of Oximes Catalyzed by Iridium Complexes: A DFT Mechanistic Study. Molecules, 2022, 27, 8349.	1.7	2
12819	[3 + 2]-Cycloadditions with Porphyrin π^2 -Bonds: Theoretical Basis of the Counterintuitive <i>meso</i> -Aryl Group Influence on the Rates of Reaction. Journal of Organic Chemistry, 2022, 87, 16473-16482.	1.7	1
12820	Phosphine Modulation for Enhanced CO ₂ Capture: Quantum Mechanics Predictions of New Materials. Journal of Physical Chemistry Letters, 2022, 13, 11183-11190.	2.1	2
12821	Duplex DNA Retains the Conformational Features of Single Strands: Perspectives from MD Simulations and Quantum Chemical Computations. International Journal of Molecular Sciences, 2022, 23, 14452.	1.8	2
12822	Substrate-Assisted Reductive Elimination Determining the Catalytic Cycle: A Theoretical Study on the Ni-Catalyzed 2,3-Disubstituted Benzofuran Synthesis via C=O Bond Activation. Organometallics, 2022, 41, 3581-3588.	1.1	3
12823	Magnet-Free Time-Resolved Magnetic Circular Dichroism with Pulsed Vector Beams. Journal of Physical Chemistry Letters, 2022, 13, 11300-11306.	2.1	5
12824	Temperature, pressure, and adsorption-dependent redox potentials: \dots . Processes of CH ₄ oxidation to value-added compounds. Energy Science and Engineering, 0, , .	1.9	0

#	ARTICLE	IF	CITATIONS
12825	Development of accurate potentials for the physisorption of water on graphene. <i>Journal of Chemical Physics</i> , 0, , .	1.2	0
12826	Benchmark accuracy of predicted NMR observables for quadrupolar ¹⁴ N and ¹⁷ O nuclei in molecular crystals. <i>Magnetic Resonance in Chemistry</i> , 2023, 61, 253-267.	1.1	4
12827	Block Effective Hamiltonian Theory and Its Application. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 61-70.	2.3	1
12828	Covalently Confined Sulfur Composite with Carbonized Bacterial Cellulose as an Efficient Cathode Matrix for High-Performance Potassium-Sulfur Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 16634-16646.	3.2	5
12829	One-dimensional nanospace confinement effects on the chemical properties of organic molecules in carbon nanotubes: Quantum chemical calculation analyses. , 2022, 1, 175-187.		0
12830	Can the Fluxionality in Borospherene Influence the Confinement-Induced Bonding between Two Noble Gas Atoms?. <i>Molecules</i> , 2022, 27, 8683.	1.7	1
12831	Bridges and Vertices in Heteroboranes. <i>Molecules</i> , 2023, 28, 190.	1.7	0
12832	An Efficient Approach to Large-Scale Ab Initio Conformational Energy Profiles of Small Molecules. <i>Molecules</i> , 2022, 27, 8567.	1.7	2
12833	Metal-Free Carbon-Based Covalent Organic Frameworks with Heteroatom-Free Units Boost Efficient Oxygen Reduction. <i>Advanced Materials</i> , 2023, 35, .	11.1	41
12834	Solvation Structure and Ion-Solvent Hydrogen Bonding of Hydrated Fluoride, Chloride and Bromide-A Comparative QM/MM MD Simulation Study. <i>Liquids</i> , 2022, 2, 445-464.	0.8	1
12835	Transition-metal-catalyzed synthesis of organophosphate-appended cyclobutanofullerenes from C60 and secondary propargylic phosphates. <i>Tetrahedron Letters</i> , 2023, 115, 154299.	0.7	1
12836	Non-innocent Role of the Halide Ligand in the Copper-Catalyzed Olefin Aziridination Reaction. <i>ACS Catalysis</i> , 2023, 13, 706-713.	5.5	4
12837	Molecular dynamics simulations of fluoroethylene carbonate and vinylene carbonate as electrolyte additives for Li-ion batteries. <i>Molecular Simulation</i> , 2023, 49, 271-283.	0.9	0
12838	Ethylenediamine control of the supramolecular chemistry of magnesium phthalocyanine. <i>Inorganica Chimica Acta</i> , 2023, 548, 121362.	1.2	1
12839	Mechanosynthesis of Triazolyl-bis(indolyl)methane Pharmacophores via Gold Catalysis: A Prelude to Molecular Electronic Properties and Biological Potency. <i>ChemMedChem</i> , 0, , .	1.6	3
12840	Experimental and density functional theoretical analyses on degradation of acid orange 7 via UV irradiation and ultrasound enhanced by fenton process. <i>Journal of Molecular Structure</i> , 2023, 1277, 134833.	1.8	5
12841	Organic Heterocyclic Strategy for Precisely Regulating Electronic State of Palladium Interface to Boost Alcohol Oxidation. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	12
12842	Synthesis of Chrysoporphyryns and a Related Benzopyrene-Fused System. <i>Journal of Organic Chemistry</i> , 2022, 87, 16276-16296.	1.7	3

#	ARTICLE	IF	CITATIONS
12843	Benchmark Ab Initio Determination of the Conformers, Proton Affinities, and Gas-Phase Basicities of Cysteine. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9667-9679.	1.1	3
12844	Evolving a high-performance bio-imaging tool derived from a compact fluorophore as well as creating a reaction-based fluorescent probe for precise determination of Ag ⁺ . <i>Chemical Engineering Journal</i> , 2023, 455, 140756.	6.6	2
12845	Luminescent cyclometalated platinum compounds with N, P, and O [^] O ligands: Density-functional theory studies and analysis of the anticancer potential. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	2
12846	Simulation Reveals the Chameleonic Behavior of Macrocycles. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 138-146.	2.5	5
12847	A Biologically Active Chromone from <i>Bomarea setacea</i> (<i>alstroemeriaceae</i>): Leishmanicidal, Antioxidant and Multilevel Computational Studies. <i>ChemistrySelect</i> , 2022, 7, .	0.7	2
12848	Structural Investigation of DHICA Eumelanin Using Density Functional Theory and Classical Molecular Dynamics Simulations. <i>Molecules</i> , 2022, 27, 8417.	1.7	0
12849	Nonoxidative Couplings of Methane to Form Ethylene Catalyzed by Coinage Metal-Containing ZSM-5 Zeolites: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2022, 126, 20903-20919.	1.5	0
12850	SOMAS: a platform for data-driven material discovery in redox flow battery development. <i>Scientific Data</i> , 2022, 9, .	2.4	4
12851	Identification of potential inhibitors of omicron variant of SARS-Cov-2 RBD based virtual screening, MD simulation, and DFT. <i>Frontiers in Chemistry</i> , 0, 10, .	1.8	1
12852	A multi-fidelity machine learning approach to high throughput materials screening. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	8
12853	Experimental and Computational Studies of Ruthenium Complexes Bearing <i>Z</i> -Acceptor Aluminum-Based Phosphine Pincer Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 20690-20698.	1.9	2
12854	Effects of ancillary ligands in acceptorless benzyl alcohol dehydrogenation mediated by phosphine-free cobalt complexes. <i>Frontiers of Chemical Science and Engineering</i> , 0, , .	2.3	1
12855	Insight into Stereocontrol in the Asymmetric Intramolecular Allylation with a <i>tert</i> -Butylsulfonamide Nucleophile: Application in the Synthesis of Chiral Isoindoline-1-Carboxylic Acid Esters. <i>Journal of Organic Chemistry</i> , 2023, 88, 613-625.	1.7	2
12856	Enantioselective Copper-Catalyzed Borylative Amidation of Allenes. <i>Journal of the American Chemical Society</i> , 2022, 144, 22850-22857.	6.6	12
12857	Effects of Encapsulating Tube and Encapsulated Molecular Chain Length on the Second-Order Nonlinear Optical Responses of Carbon Nanotubes Filled with Head-To-Tail Polar Molecules. <i>Journal of Physical Chemistry C</i> , 2022, 126, 21328-21337.	1.5	1
12858	Synthesis of TSF Donors Substituted with the <i>meso</i> -Dimethylethylenedithio Group: Structures and Conducting Properties of (<i>meso</i> -DM-BETS) ₂ X (X ⁺ = PF ₆ ⁻ and AsF ₆ ⁻). <i>Bulletin of the Chemical Society of Japan</i> , 2023, 96, 35-41.	2.0	0
12859	Sustainable synthesis of hierarchically grown chloramphenicol-imprinted poly(caffeic acid) nanostructured films. <i>Journal of Applied Polymer Science</i> , 2023, 140, .	1.3	2
12860	A Thermodynamic Cycle-Based Electrochemical Windows Database of 308 Electrolyte Solvents for Rechargeable Batteries. <i>Advanced Functional Materials</i> , 2023, 33, .	7.8	16

#	ARTICLE	IF	CITATIONS
12861	Thiosemicarbazonecopper/Halido Systems: Structure and DFT Analysis of the Magnetic Coupling. <i>Inorganics</i> , 2023, 11, 31.	1.2	1
12862	Solvent Phase Optimizations Improve Correlations with Experimental Stability Constants for Aqueous Lanthanide Complexes. <i>Solvent Extraction and Ion Exchange</i> , 2023, 41, 241-251.	0.8	2
12863	Variational Subspace Valence Bond. , 2024, , 424-440.		0
12864	Electronic properties of carbazole/biphenylamino functionalized sulfone-based host materials. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	1
12865	Optimization of chemical synthesis with heuristic algorithms. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4323-4331.	1.3	1
12866	<i>i>N</i>-Electron Valence Perturbation Theory with Reference Wave Functions from Quantum Computing: Application to the Relative Stability of Hydroxide Anion and Hydroxyl Radical. <i>Journal of Physical Chemistry A</i>, 2023, 127, 817-827.</i>	1.1	9
12867	[ReH ₃ (PPh ₃) ₄] - A Key Compound in the Rhenium Hydride Chemistry. <i>Chemistry - A European Journal</i> , 0, , .	1.7	0
12868	Disentangling global and local ring currents. <i>Chemical Science</i> , 2023, 14, 1762-1768.	3.7	4
12869	Degradation by hydrolysis of three triphenylmethane dyes: DFT and TD-DFT study. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	1
12870	New photoinitiators derived from PET waste: Molecular simulations and photocatalytic efficiency. <i>Journal of Polymer Research</i> , 2023, 30, .	1.2	3
12871	Non-ergodic fragmentation upon collision-induced activation of cysteine-water cluster cations. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
12872	Electrostatics and Chemical Reactivity at the Air-water Interface. <i>Journal of the American Chemical Society</i> , 2023, 145, 1400-1406.	6.6	21
12873	Rational design of cooperative chelating sites on covalent organic frameworks for highly selective uranium extraction from seawater. <i>Cell Reports Physical Science</i> , 2023, 4, 101220.	2.8	11
12874	Mechanistic Insights into Multisilver-Mediated Synergistic Activation of Terminal Alkynes. <i>Inorganic Chemistry</i> , 2023, 62, 1414-1422.	1.9	0
12875	Chiral explosives: A theoretical investigation of structure and chiroptical properties of triacetone triperoxide and hexamethylene triperoxide diamine. <i>Chirality</i> , 0, , .	1.3	0
12876	Sub-system self-consistency in coupled cluster theory. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	3
12877	Benchmarking computational chemistry approaches on iminodiacetic acid. <i>Journal of the Indian Chemical Society</i> , 2023, 100, 100895.	1.3	3
12878	Stable fast-charging sodium-ion batteries achieved by a carbomethoxy-modified disodium organic material. <i>Cell Reports Physical Science</i> , 2023, , 101240.	2.8	2

#	ARTICLE	IF	CITATIONS
12879	Tracking the Delocalized Proton in Concerted Proton Transfer in Bulk Water. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 448-459.	2.3	3
12880	High-level ab initio mapping of the multiple H-abstraction pathways of the OH + glycine reaction. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
12881	Projection-Based Density Matrix Renormalization Group in Density Functional Theory Embedding. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 716-722.	2.1	3
12882	Symmetry dependent optical properties of zeolites: A quantum mechanical study. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	0
12883	Effect of intermacrocyclic interactions: Modulation of metal spin-state in oxo/hydroxo/fluoro-bridged diiron(III)/dimanganese(III) porphyrin dimers. <i>Advances in Inorganic Chemistry</i> , 2023, , 95-184.	0.4	1
12884	Dinitrogen reduction using ruthenium coordinated by nitrogen-doped graphene and cobalt complex coordinated by anionic PNP pincer ligand as catalysts and Frustrated Lewis Pair as a co-catalyst: Density Functional Theory studies. <i>Applied Organometallic Chemistry</i> , 2023, 37, .	1.7	2
12885	Temperature, pressure, and adsorption dependent redox potentials: III. Processes of CO conversion to value-added compounds. <i>Energy Science and Engineering</i> , 2024, 12, 362-393.	1.9	0
12886	A theoretical analysis of the reduction and lithiation of pillar[6]quinone. <i>Journal of Electroanalytical Chemistry</i> , 2023, 930, 117170.	1.9	0
12887	Computational Study of the Inhibition of RgpB Gingipain, a Promising Target for the Treatment of Alzheimer's Disease. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 950-958.	2.5	0
12888	Is there a better way of representing stationary wave functions than basis expansion?. <i>International Journal of Quantum Chemistry</i> , 0, , .	1.0	0
12889	QM-cluster Model Study of CO ₂ Hydration Mechanisms in Metal-substituted Human Carbonic Anhydrase II. <i>Electronic Structure</i> , 0, , .	1.0	1
12890	Multifunctional Electrolyte Additive Enables Highly Reversible Anodes and Enhanced Stable Cathodes for Aqueous Zinc-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 4152-4165.	4.0	8
12891	NHC-catalyzed N-H functionalization/cycloaddition reaction of indole aldehyde and ketone: A DFT perspective. <i>Computational and Theoretical Chemistry</i> , 2023, 1220, 114007.	1.1	5
12892	Adsorption, sensing and catalytic properties of the pristine C ₂₄ N ₂₄ nanocage to small gas molecules: A DFT-D3 investigation. <i>Vacuum</i> , 2023, 209, 111798.	1.6	4
12893	High-performance fluorescent and colorimetric dual-mode nitrite sensor boosted by a versatile coumarin probe equipped with diazotization-coupling reaction-sites. <i>Sensors and Actuators B: Chemical</i> , 2023, 379, 133261.	4.0	9
12894	Single-Hydroxide Bridged Dimers of U and Np Actinyls: A Density Functional Study on Their Existence and Structure in Aqueous Solution. <i>Inorganic Chemistry</i> , 2023, 62, 830-840.	1.9	2
12895	Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 147-156.	2.3	7
12896	Molecular and Aggregate Structural, Thermal, Mechanical and Photophysical Properties of Long-Chain Amide Gelators Containing an α,β -Diketo Group in the Presence or Absence of a Tertiary Amine Group. <i>Gels</i> , 2023, 9, 36.	2.1	0

#	ARTICLE	IF	CITATIONS
12897	The effect of immediate environment on bond strength of different bond types—A valence bond study. <i>Journal of Chemical Physics</i> , 2022, 157, 244301.	1.2	0
12898	Advances in Parallel Heat Bath Configuration Interaction. <i>Journal of Physical Chemistry A</i> , 2023, 127, 400-411.	1.1	5
12899	A Guide to In Silico Drug Design. <i>Pharmaceutics</i> , 2023, 15, 49.	2.0	22
12900	Tunable Photochromism of Spirooxazine in the Solid State: A New Design Strategy Based on the Hypochromic Effect. <i>Advanced Materials</i> , 2023, 35, .	11.1	20
12901	In-Silico Device Performance Prediction of Cosensitizer Dye Pairs for Dye-Sensitized Solar Cells. <i>Advanced Energy Materials</i> , 2023, 13, .	10.2	1
12902	Impact of counteranions on N-heterocyclic carbene gold(ⁱ)-catalyzed cyclization of propargylic amide. <i>RSC Advances</i> , 2023, 13, 2896-2902.	1.7	0
12903	Accurate Spin-Orbit Coupling by Relativistic Mixed-Reference Spin-Flip-TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 953-964.	2.3	4
12904	Mechanistic Study of Chemoselectivity for Carbon Radical Hydroxylation versus Chlorination with Fe ^{III} (OH)(Cl) Complexes. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	1
12905	Lithium, Tin(II), and Zinc Amino-Boryloxy Complexes: Synthesis and Characterization. <i>Inorganic Chemistry</i> , 2023, 62, 2576-2591.	1.9	0
12906	A PLS study on the psychotropic activity for a series of cannabinoid compounds. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	3
12907	Predicting the structures and vibrational spectra of molecular crystals containing large molecules with the generalized energy-based fragmentation approach. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	6
12908	Understanding the role of ring strain in $\hat{1}^2$ -alkyl migration at Mg and Zn centres. <i>Chemical Science</i> , 2023, 14, 1590-1597.	3.7	2
12909	Application of statistical learning and mechanistic modelling towards mapping the substrate electronic space in a Cu-catalyzed Suzuki–Miyaura coupling. <i>Catalysis Science and Technology</i> , 0, .	2.1	0
12910	Mechanism-Guided Design of Robust Palladium Catalysts for Selective Aerobic Oxidation of Polyols. <i>Journal of the American Chemical Society</i> , 2023, 145, 2282-2293.	6.6	3
12911	A Deep Understanding on the Effective Generation of Twisted Intramolecular Charge Transfer by Protonation in Thiazolo[5,4- <i>d</i>]thiazole Derivatives. <i>Journal of Physical Chemistry A</i> , 2023, 127, 902-912.	1.1	2
12912	Ir ^I ($\hat{1}^4$ -diene) precatalyst activation by strong bases: formation of an anionic Ir ^{III} tetrahydride. <i>Dalton Transactions</i> , 0, .	1.6	0
12913	Acid-Triggered Switchable Near-Infrared/Shortwave Infrared Absorption and Emission of Indolizine-BODIPY Dyes. <i>Molecules</i> , 2023, 28, 1287.	1.7	2
12914	New palladium(ⁱⁱ) and platinum(ⁱⁱ) complexes with an ONS donor azo-thioether pincer ligand: synthesis, characterization, protein binding study and <i>in vitro</i> cytotoxicity. <i>New Journal of Chemistry</i> , 2023, 47, 4931-4943.	1.4	5

#	ARTICLE	IF	CITATIONS
12915	The core ionization energies calculated by delta SCF and Slater's transition state theory. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	5
12916	Mind the GAP: quantifying the breakdown of the linear vibronic coupling Hamiltonian. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7195-7204.	1.3	4
12917	Tuning the competition between photoisomerization and phototherapy in biomimetic cyclocurcumin analogues. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 439, 114583.	2.0	0
12918	First Planar Binuclear Phthalocyanines Sharing a Common Carbazole Linkage: Synthesis, Optical and Photochemical Properties. <i>Bulletin of the Chemical Society of Japan</i> , 2023, 96, 226-240.	2.0	0
12919	Effect of Charge State on the Equilibrium and Kinetic Properties of Mechanically Interlocked [5]Rotaxane: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2023, 127, 1254-1263.	1.2	1
12920	Linear, Electron-Rich, Homoleptic Rare Earth Metallocene and Its Redox Activity. <i>Inorganic Chemistry</i> , 2023, 62, 2095-2104.	1.9	3
12921	Hydrogen physisorption on the (BeO) _n , B ₂ H ₄ (Be,Ti), and B ₆ Ti ₃ metal clusters: a computational study of energies and atomic charges. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0
12922	Modification of 6,7-Dichloro-5,8-Quinolinedione at C2 Position: Synthesis, Quantum Chemical Properties, and Activity against DT-Diaphorase Enzyme. <i>Applied Sciences (Switzerland)</i> , 2023, 13, 1530.	1.3	1
12923	Electronic structure and density functional theory. , 2023, , 3-35.		0
12924	Advances in the homogeneous catalyzed alcohols homologation: The mild side of the Guerbet reaction. A mini-review. <i>Catalysis Today</i> , 2023, 423, 114003.	2.2	5
12925	The effects of conformation and intermolecular hydrogen bonding on the structure and IR spectra of flutamide; a study based on the matrix isolation technique, ab initio and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 292, 122417.	2.0	2
12926	Phenolic compounds extraction from propolis using imidazole-based ionic liquids: A theoretical and experimental study. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	0.9	4
12927	Mechanistic insights into the electroreduction of CO ₂ by a phosphine-nitrogen-coordinated manganese carbonyl complex for CO ₂ -to-CO conversion over H ₂ formation. <i>Inorganica Chimica Acta</i> , 2023, 549, 121419.	1.2	2
12928	Using Stationary Points on Potential Energy Surfaces to Model Intermolecular Interactions and Retention in Gas Chromatography. <i>Chromatographia</i> , 2004, 59, 329-334.	0.7	1
12929	Protonation of serine: conformers, proton affinities and gas-phase basicities at the "gold standard" and beyond. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8891-8902.	1.3	0
12930	Electrochemical sensing of NADH using 4-nitrobenzenediazonium tetrafluoroborate salt functionalized multiwalled carbon nanotubes. <i>Dalton Transactions</i> , 0, , .	1.6	1
12931	Design, synthesis, and application of covalent organic frameworks as catalysts. <i>New Journal of Chemistry</i> , 2023, 47, 6765-6788.	1.4	4
12932	Synthesis and Reactivity of Redox-Active Cerium(IV) Aryloxide Complexes. <i>Organometallics</i> , 2023, 42, 1094-1105.	1.1	0

#	ARTICLE	IF	CITATIONS
12933	Synthesis and Optical Properties of a Series of Push-Pull Dyes Based on Pyrene as the Electron Donor. <i>Molecules</i> , 2023, 28, 1489.	1.7	1
12934	Metabolite-induced in vivo fabrication of substrate-free organic bioelectronics. <i>Science</i> , 2023, 379, 795-802.	6.0	36
12935	Molecular modification effects on the electrochromic and photochromic properties of diarylethene with intramolecular isomerization behavior. <i>Journal of Chemical Physics</i> , 2023, 158, 114701.	1.2	1
12936	A study of the valence photoelectron spectrum of uracil and mixed water-uracil clusters. <i>Journal of Chemical Physics</i> , 2023, 158, 114301.	1.2	2
12937	Microwave measurements, calculations, and analysis for the gas phase ammonia-formic acid dimer. <i>Journal of Molecular Spectroscopy</i> , 2023, 393, 111772.	0.4	4
12938	Photoinduced Perfluoroalkylation Mediated by Cobalt Complexes Supported by Naphthyridine Ligands. <i>Organometallics</i> , 2023, 42, 2632-2643.	1.1	1
12939	Tetraquinoxalinoporphyrazine π -extended NIR-absorbing photosensitizer with improved photostability. <i>Dyes and Pigments</i> , 2023, 216, 111326.	2.0	3
12940	Theoretical exploration of the mechanisms on the iron complexes catalyzed ammonia borane dehydrogenation and polyaminoborane formation. <i>International Journal of Hydrogen Energy</i> , 2023, 48, 23633-23644.	3.8	1
12941	Taming the Lewis Superacid $\text{Al}(\text{ORF})_3$ ($\text{RF}=\text{C}(\text{CF}_3)_3$): DFT Guided Identification of the "Stable yet Reactive" Adduct $\text{S}(\text{Pr})_2\text{Al}(\text{ORF})_3$; Its Use as ORF-Abstractor from a $\text{Ni}(\text{ORF})_6$ complex. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	0
12942	Tuning the Photophysical Properties of Ru(II) Photosensitizers for PDT by Protonation and Metallation: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3625-3635.	1.1	1
12943	Chemo- and regioselectivities of the TBAF-catalyzed C F bond allylation of trifluoromethylalkenes: A theoretical view. <i>Molecular Catalysis</i> , 2023, 542, 113111.	1.0	0
12944	Tandem coordinative chain transfer polymerization for long chain branched Polyethylene: The role of chain displacement. <i>European Polymer Journal</i> , 2023, 190, 112008.	2.6	3
12945	Theoretical study of C6F5-corrole molecules functionalized with aromatic groups for Photodynamic Therapy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 293, 122500.	2.0	2
12946	Physicochemical insight into the metal atom effect on magnetocaloric behavior of paramagnetic metalloporphyrins. <i>Polyhedron</i> , 2023, 236, 116384.	1.0	2
12947	A bioinspired cobalt catalyst based on a tripodal imidazole/pyridine platform capable of water reduction and oxidation. <i>Journal of Inorganic Biochemistry</i> , 2023, 242, 112162.	1.5	0
12948	In silico evaluation of geroprotective phytochemicals as potential sirtuin 1 interactors. <i>Biomedicine and Pharmacotherapy</i> , 2023, 161, 114425.	2.5	2
12949	Silk fibroin-based biopolymer composite binders with gradient binding energy and strong adhesion force for high-performance micro-sized silicon anodes. <i>Journal of Energy Chemistry</i> , 2023, 80, 442-451.	7.1	5
12950	A combined DFT and molecular docking study on novel tricarbonylrhenium(I) complexes bearing mono- and bivalent benzenesulfonamide scaffolds as human carbonic anhydrase IX and XII inhibitors. <i>Journal of Molecular Structure</i> , 2023, 1282, 135211.	1.8	3

#	ARTICLE	IF	CITATIONS
12951	Optimized <i>Baccharis dracunculifolia</i> extract as photoprotective and antioxidant: In vitro and in silico assessment. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 440, 114654.	2.0	0
12952	Exploring a new family of designer copper(II) complexes of anthracene-appended polyfunctional organic assembly displaying potential anticancer activity via cytochrome c mediated mitochondrial apoptotic pathway. <i>Journal of Inorganic Biochemistry</i> , 2023, 243, 112182.	1.5	5
12953	Direct observation on argon tagging nitrobenzene radical anion in gas phase: Infrared photodissociation spectroscopy and theoretical calculation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122482.	2.0	2
12954	Theoretical insights into the synthesis reaction mechanism of HMX based on TAT nitration reaction. <i>Chemical Physics Letters</i> , 2023, 820, 140448.	1.2	2
12955	<i>Lippia javanica</i> leaf extract as an effective anti-corrosion agent against mild steel corrosion in 1 M HCl and its characterization by UHPLC/Q-TOF-MS spectroscopy and quantum chemical evaluation of its adsorption process on Fe(110). <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2023, 667, 131405.	2.3	7
12956	Enhanced Sampling for Free Energy Profiles with Post-Transition-State Bifurcations. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2735-2743.	2.3	1
12957	An advanced organic cathode for non-aqueous and aqueous calcium-based dual ion batteries. <i>Journal of Power Sources</i> , 2023, 569, 232995.	4.0	8
12958	Efficient full dechlorination of chlorinated ethenes on single enzyme-like Co ^{N4} sites in nitrogen-doped carbons. <i>Applied Catalysis B: Environmental</i> , 2023, 328, 122459.	10.8	4
12959	Projected Hybrid Density Functionals: Method and Application to Core Electron Ionization. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 837-847.	2.3	3
12960	Polyaromatic hydrocarbon antennas as tools for tuning properties of push-pull difluoroborates. <i>Dyes and Pigments</i> , 2023, 212, 111112.	2.0	0
12961	Evaluating the active site-substrate interplay between x-ray crystal structure and molecular dynamics in chorismate mutase. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
12962	Insights into the CO ₂ Capture Capacity of Covalent Organic Frameworks. <i>ChemPhysChem</i> , 2023, 24, .	1.0	2
12963	Controlling Near-Infrared Photoluminescence Properties of Single-Walled Carbon Nanotubes by Substituent Effect in Stepwise Chemical Functionalization. <i>Journal of Physical Chemistry C</i> , 2023, 127, 2360-2370.	1.5	5
12964	Synthesis, spectroscopic characterization, antibacterial activity and antiproliferative profile of a new silver(I) complex of 5-fluorocytosine. <i>Journal of Fluorine Chemistry</i> , 2023, 266, 110096.	0.9	0
12965	New Dual Inhibitors of SARS-CoV-2 Based on Metal Complexes with Schiff-Base 4-Chloro-3-Methyl Phenyl Hydrazine: Synthesis, DFT, Antibacterial Properties and Molecular Docking Studies. <i>Inorganics</i> , 2023, 11, 63.	1.2	7
12966	Towards Cross-Platform Portability of Coupled-Cluster Methods with Perturbative Triples using SYCL. , 2022, , .		2
12967	Bis(1-naphthylimino)acenaphthene: Redox Properties and One-Electron Reduction. <i>Doklady Physical Chemistry</i> , 2022, 505, 89-94.	0.2	0
12968	Sc-HOPO: A Potential Construct for Use in Radioscandium-Based Radiopharmaceuticals. <i>Inorganic Chemistry</i> , 2023, 62, 20567-20581.	1.9	5

#	ARTICLE	IF	CITATIONS
12969	Exploring Coumarin-Based Boron Emissive Complexes as Temperature Thermometers in Polymer-Supported Materials. <i>Sensors</i> , 2023, 23, 1689.	2.1	3
12970	Linear Conjugated Coordination Polymers for Electrocatalytic Oxygen Evolution Reaction. <i>Small</i> , 2023, 19, .	5.2	2
12971	HOAX: a hyperparameter optimisation algorithm explorer for neural networks. <i>Molecular Physics</i> , 0, , .	0.8	0
12972	A New Motif in Halogen Bonding: Cooperative Intermolecular Sâ”Brâ”â”O, Oâ”â”F, and Fâ”â”F Associations in the Crystal Packing of Î±,Î±-Di(sulfonyl bromide) Perfluoroalkanes. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	0
12973	Nearly-freestanding supramolecular assembly with tunable structural properties. <i>Scientific Reports</i> , 2023, 13, .	1.6	2
12974	Distal Mutations in the Î²-Clamp of DNA Polymerase III* Disrupt DNA Orientation and Affect Exonuclease Activity. <i>Journal of the American Chemical Society</i> , 2023, 145, 3478-3490.	6.6	2
12975	Dodging the Conventional Reactivity of <i>o</i> -Alkynylanilines under Gold Catalysis for Distal 7-endo Cyclization. <i>Journal of Organic Chemistry</i> , 2023, 88, 2260-2287.	1.7	3
12976	Vibrational frequency Analysis, DFT and <i>in Vitro</i> Fungicidal Activity Studies of Biphenyl-4-Carboxylic Acid, 2,4-Difluorobiphenyl and 4-Acetylbiphenyl- A Comparative Study. <i>Polycyclic Aromatic Compounds</i> , 2024, 44, 129-161.	1.4	0
12977	Employing Long-Range Inductive Effects to Modulate Metal-to-Ligand Charge Transfer Photoluminescence in Homoleptic Cu(I) Complexes. <i>Inorganic Chemistry</i> , 2023, 62, 3248-3259.	1.9	12
12978	Mechanistic View on the Orderâ”Disorder Phase Transition in Amphidynamic Crystals. <i>Journal of Physical Chemistry Letters</i> , 2023, 14, 1570-1577.	2.1	2
12979	Physical Chemistry in Context: Using Quantum Mechanics to Understand the Greenhouse Effect. <i>Journal of Chemical Education</i> , 2023, 100, 1333-1342.	1.1	0
12980	Anti-inflammatory Quinoline Alkaloids from the Roots of <i>Waltheria indica</i> . <i>Journal of Natural Products</i> , 2023, 86, 276-289.	1.5	1
12981	A catastrophe theory-based model for optimal control of chemical reactions by means of oriented electric fields. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	2
12982	[2,1,3]-Benzothiadiazole-Spaced Co-Porphyrin-Based Covalent Organic Frameworks for O ₂ Reduction. <i>ACS Nano</i> , 2023, 17, 3492-3505.	7.3	13
12983	Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1715-1735.	1.1	19
12984	A Single-Atom Upgrade to Polydicyclopentadiene. <i>Macromolecules</i> , 2023, 56, 1592-1600.	2.2	1
12985	Theoretical simulations on metal nanocluster systems. , 2023, , 201-231.		0
12986	Computational Investigation of Substituent Effects on the Alcohol + Carbonyl Channel of Peroxy Radical Self- and Cross-Reactions. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1686-1696.	1.1	2

#	ARTICLE	IF	CITATIONS
12987	Small, Electron-Donating Substituents Give CO ₂ Activation by Permethylpentalene Zirconium Amido Complexes the Upper Hand: A DFT Study of Distortion and Interaction. <i>Inorganic Chemistry</i> , 2023, 62, 3000-3006.	1.9	0
12988	Benchmarking two-photon absorption strengths of rhodopsin chromophore models with CC3 and CCSD methodologies: An assessment of popular density functional approximations. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	2
12989	Atomistic simulations for investigation of substrate effects on lipid in-source fragmentation in secondary ion mass spectrometry. <i>Biointerphases</i> , 2023, 18, .	0.6	2
12990	A Combined Experimental and Theoretical Study of ESR Hyperfine Coupling Constants for N,N,Nâ€™,Nâ€™-Tetrasubstituted p-Phenylenediamine Radical Cations. <i>International Journal of Molecular Sciences</i> , 2023, 24, 3447.	1.8	0
12991	Computational Evidence of the Incipient Oxocarbenium Ion as a “Hidden Intermediate” During the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition. <i>Chemistry - A European Journal</i> , 0, .	1.7	0
12992	Vibronic Relaxation Pathways in Molecular Spin Qubit Na ₉ [Ho(W ₅ O ₁₈) ₂]·35H ₂ O under Pressure. <i>Magnetochemistry</i> , 2023, 9, 53.	1.0	0
12993	Excellent Static and dynamic hyperpolarizabilities of TM@C ₆ O ₆ Li ₆ (TM = Sc, Ti, V, Cr and Mn) complexes to prove their NLO applications. <i>Optik</i> , 2023, 276, 170660.	1.4	6
12994	Alkyl Sulfonyl Fluorides Incorporating Geminal Dithioesters as SuFEx Click Hubs via Water-Accelerated Organosuperbase Catalysis. <i>Organic Letters</i> , 2023, 25, 1056-1060.	2.4	3
12995	Cross-assembly confined bifunctional catalysis via non-covalent interactions for asymmetric halogenation. <i>CheM</i> , 2023, 9, 1255-1269.	5.8	6
12996	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. <i>Polymer Reviews</i> , 2024, 64, 80-118.	5.3	3
12997	A Bifunctional Fluorine-Free Electrolyte Additive for Realizing Dendrite-Free Lithium Anodes. <i>ChemSusChem</i> , 2023, 16, .	3.6	2
12998	Mechanistic insights into the Cu(II)/DBU-catalyzed incorporation of CO ₂ into homopropargylic amines. <i>New Journal of Chemistry</i> , 2023, 47, 5691-5700.	1.4	0
12999	Computational Evolution Of New Catalysts For The Morita-Baylis-Hillman Reaction**. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	5
13000	ESIPT-Capable 4-(2-Hydroxyphenyl)-2-(Pyridin-2-yl)-1H-Imidazoles with Single and Double Proton Transfer: Synthesis, Selective Reduction of the Imidazolic OH Group and Luminescence. <i>Molecules</i> , 2023, 28, 1793.	1.7	6
13001	Computational Evolution Of New Catalysts For The Morita-Baylis-Hillman Reaction**. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	1
13002	Theoretical Study on the Copper-Catalyzed ortho-Selective C-H Functionalization of Naphthols with Î±-Phenyl-Î±-Diazoesters. <i>Molecules</i> , 2023, 28, 1767.	1.7	1
13003	Synthesis and Optoelectronic Features of Rhodamine-Triazole Dyads as Metallochromic Probes for Copper-Selective Chemosensing. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	1
13004	A hydrophilic fully conjugated covalent organic framework for photocatalytic CO ₂ reduction to CO nearly 100% using pure water. <i>Journal of Materials Chemistry A</i> , 2023, 11, 5627-5635.	5.2	1

#	ARTICLE	IF	CITATIONS
13005	Phosphite Bearing [(1/4-ADT)^RFe₂(CO)₆] (ADT = Azadithiolate) Moieties: A Tool for the Building of Multimetallic [FeFe]-Hydrogenase Mimics. <i>Organometallics</i> , 2023, 42, 316-326.	1.1	2
13006	Asymmetric [2+1] cycloaddition of difluoroalkyl-substituted carbenes with alkenes under rhodium catalysis: Synthesis of chiral difluoroalkyl-substituted cyclopropanes. <i>IScience</i> , 2023, 26, 105896.	1.9	3
13007	Quasiclassical Trajectory Simulation as a Protocol to Build Locally Accurate Machine Learning Potentials. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1133-1142.	2.5	1
13008	Theoretical understanding of stability of mechanically interlocked carbon nanotubes and their precursors. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 7527-7539.	1.3	2
13009	2D-block geminals: A non 1-orthogonal and non 0-seniority model with reduced computational complexity. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	3
13010	1,3-Diaza-Claisen Rearrangements of Vinyl Pyrrolidines Tethered to In Situ Generated Carbodiimides Afford Ring-Expanded [9,5]- and [9,6]-Bicyclic Guanidines. <i>Journal of Organic Chemistry</i> , 2023, 88, 2851-2868.	1.7	1
13011	Unraveling the Steric Link to Copper Precursor Decomposition: A Multi-Faceted Study for the Printing of Flexible Electronics. <i>Small Methods</i> , 2023, 7, .	4.6	1
13012	Computational Exploration of Dirhodium Complex-Catalyzed Selective Intermolecular Amination of Tertiary vs. Benzylic C-H Bonds. <i>Molecules</i> , 2023, 28, 1928.	1.7	1
13013	Direct Proton-Coupled Electron Transfer between Interfacial Tyrosines in Ribonucleotide Reductase. <i>Journal of the American Chemical Society</i> , 2023, 145, 4784-4790.	6.6	2
13014	Kinetic Properties Study of H Atom Abstraction by CH₃E Radicals from Fuel Molecules with Different Functional Groups. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1960-1974.	1.1	4
13015	Oxidopyridinium Cycloadditions Revisited: A Combined Computational and Experimental Study on the Reactivity of 1-(2-Pyrimidyl)-3-oxidopyridinium Betaine. <i>Journal of Organic Chemistry</i> , 2023, 88, 3193-3207.	1.7	3
13016	Inverse Electron-Demanding Diels-Alder Reactions in the Chemical Synthesis of Prenylated Indole Alkaloids Containing a Bicycle[2.2.2]diazaoctane Moiety: A Theoretical Study. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	0
13017	Investigation of the thermal deconstruction of Î² and 4-O-5 linkages in lignin model oligomers by density functional theory (DFT). <i>RSC Advances</i> , 2023, 13, 6181-6190.	1.7	1
13018	Carbonized Bacterial Cellulose-Derived Binder-Free, Flexible, and Free-Standing Cathode Host for High-Performance Stable Potassium-Sulfur Batteries. <i>ACS Applied Energy Materials</i> , 2023, 6, 3042-3051.	2.5	7
13019	Computational Design of Frustrated Lewis Pairs as a Strategy for Catalytic Hydrogen Activation and Hydrogenation Catalyst. <i>ACS Omega</i> , 2023, 8, 8488-8496.	1.6	0
13020	Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. <i>Journal of Physical Chemistry B</i> , 2023, 127, 2052-2065.	1.2	0
13021	Efficient Construction of Involuntary Linear Combinations of Anticommuting Pauli Generators for Large-Scale Iterative Qubit Coupled Cluster Calculations. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1722-1733.	2.3	1
13022	What is the Optimal Dipole Moment for Nonpolarizable Models of Liquids?. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 1790-1804.	2.3	5

#	ARTICLE	IF	CITATIONS
13023	Effect of Substituent Location on the Relationship between the Transition Dipole Moments, Difference Static Dipole, and Hydrophobicity in Squaraine Dyes for Quantum Information Devices. <i>Molecules</i> , 2023, 28, 2163.	1.7	1
13024	Modelling Complex Bimolecular Reactions in a Condensed Phase: The Case of Phosphodiester Hydrolysis. <i>Molecules</i> , 2023, 28, 2152.	1.7	1
13025	Surface Reaction of Methyl Mercaptan (CH ₃ SH) with Hydrogen Atoms on Amorphous Solid Water. <i>Astrophysical Journal</i> , 2023, 944, 219.	1.6	3
13026	Adaptive, problem-tailored variational quantum eigensolver mitigates rough parameter landscapes and barren plateaus. <i>Npj Quantum Information</i> , 2023, 9, .	2.8	14
13027	Mechanism Investigation on Direct Conversion of Methane over a Mononuclear Rh-ZSM-5 Catalyst: Multiple Roles of CO. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4887-4895.	1.5	0
13028	Spectroscopy, molecular structure, and electropolymerization of Ni(II) and Cu(II) complexes containing a thiophene-appending fluorinated Schiff base ligand. <i>Dalton Transactions</i> , 2023, 52, 4224-4236.	1.6	3
13029	Mechanistic insights into H ₃ B-NMeH ₂ dehydrogenation by Co-based complexes: a DFT perspective. <i>New Journal of Chemistry</i> , 2023, 47, 6661-6672.	1.4	1
13030	Perchlorate-induced structural diversity in thiosemicarbazone copper(II) complexes provides insights to understand the reactivity in acidic and basic media. <i>CrystEngComm</i> , 2023, 25, 2213-2226.	1.3	2
13031	Mechanism of Silylation of Vinyl Arenes by Hydrodisiloxanes Driven by Stoichiometric Amounts of Sodium Triethylborohydride—A Combined DFT and Experimental Study. <i>International Journal of Molecular Sciences</i> , 2023, 24, 4924.	1.8	0
13032	Fueling the search for light dark matter-electron scattering with spherical proportional counters. <i>Physical Review D</i> , 2023, 107, .	1.6	4
13033	Mechanism and origins of ligand-controlled regioselectivity of copper-catalyzed borocarbonylation of imines with B ₂ pin ₂ and alkyl iodides: a computational study. <i>Organic Chemistry Frontiers</i> , 2023, 10, 2024-2032.	2.3	0
13034	Palladium-Catalyzed Cyclization of a Poryne Precursor to Higher Pyrenylenes. <i>Angewandte Chemie - International Edition</i> , 2023, 62, .	7.2	9
13035	Palladium-Catalyzed Cyclization of a Poryne Precursor to Higher Pyrenylenes. <i>Angewandte Chemie</i> , 2023, 135, .	1.6	0
13036	Heteronuclear Dual Single-Atom Catalysts for Ambient Conversion of CO ₂ from Air to Formate. <i>ACS Catalysis</i> , 2023, 13, 3915-3924.	5.5	12
13037	Probing solvation electrostatics at the air-water interface. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	0.5	6
13038	Oxidation of norbornadiene: Theoretical investigation on H-atom abstraction and related radical decomposition reactions. <i>Propulsion and Power Research</i> , 2023, 12, 104-113.	2.0	1
13039	Additive-Assisted Perylene Polymorphism Controlled via Secondary Bonding Interactions. <i>Crystal Growth and Design</i> , 2023, 23, 2710-2720.	1.4	1
13040	Multifunctional Triggering by Solid-Phase Molecular Motion: Relaxor Ferroelectricity, Modulation of Magnetic Exchange Interactions, and Enhancement of Negative Thermal Expansion. <i>Chemistry of Materials</i> , 2023, 35, 2421-2428.	3.2	3

#	ARTICLE	IF	CITATIONS
13041	Penta-coordinated or -valent: the nature of the chemical bond of some Tiâ€Câ€Al compounds. Dalton Transactions, 2023, 52, 4494-4500.	1.6	0
13042	A comparative study of the potential of [Os{(NHCH ₂ CH ₂) ₃ X}] catalysts (X = 3/4N, P) for the reduction of dinitrogen to ammonia and hydrazine using FLPâ€H ₂ as a coâ€catalyst by density functional theory. Applied Organometallic Chemistry, 2023, 37, .	1.7	0
13043	DELTA50: A Highly Accurate Database of Experimental 1H and 13C NMR Chemical Shifts Applied to DFT Benchmarking. Molecules, 2023, 28, 2449.	1.7	6
13044	Enantioselective Rhodiumâ€Catalyzed Pausonâ€Khand Reactions of 1,6â€Chloroenynes with 1,1â€Disubstituted Olefins. Angewandte Chemie, 0, , .	1.6	0
13045	Enantioselective Rhodiumâ€Catalyzed Pausonâ€Khand Reactions of 1,6â€Chloroenynes with 1,1â€Disubstituted Olefins. Angewandte Chemie - International Edition, 0, , .	7.2	0
13046	Biphenyl Au(III) Complexes with Phosphine Ancillary Ligands: Synthesis, Optical Properties, and Electroluminescence in Light-Emitting Electrochemical Cells. Inorganic Chemistry, 2023, 62, 4903-4921.	1.9	4
13047	Nonadiabatic Coupling in Trajectory Surface Hopping: How Approximations Impact Excited-State Reaction Dynamics. Journal of Chemical Theory and Computation, 2023, 19, 1827-1842.	2.3	9
13048	Oxidation State Tuning of Room Temperature Phosphorescence and Delayed Fluorescence in Phenothiazine and Phenothiazineâ€5,5â€dioxide Dimers. Chemistry - A European Journal, 2023, 29, .	1.7	3
13049	Insights into How NH ₄ ⁺ Ions Enhance the Activity of Dimeric G-Quadruplex/Hemin DNAzyme. ACS Catalysis, 2023, 13, 4330-4338.	5.5	5
13050	Co-Catalyzed Asymmetric Hydrogenation. The Same Enantioselection Pattern for Different Mechanisms. International Journal of Molecular Sciences, 2023, 24, 5568.	1.8	2
13051	Fusing Thiadiazole and Terephthalate: A Concept to Promote the Electrochemical Performance of Conjugated Dicarboxylates. ChemSusChem, 2023, 16, .	3.6	2
13052	Direct Synthesis of 1-Butanol with High Faradaic Efficiency from CO ₂ Utilizing Cascade Catalysis at a Ni-Enhanced (Cr ₂ O ₃) ₃ Ga ₂ O ₃ Electrocatalyst. Journal of the American Chemical Society, 2023, 145, 6762-6772.	6.6	9
13053	The Origin of Anionâ€ Autocatalysis. JACS Au, 2023, 3, 1039-1051.	3.6	5
13054	Electrophilicity and nucleophilicity scales at different DFT computational levels. Journal of Physical Organic Chemistry, 2023, 36, .	0.9	12
13055	Caffeine Biodegradation by Cytochrome P450 1A2. What Determines the Product Distributions?. Chemistry - A European Journal, 2023, 29, .	1.7	7
13056	Stereochemistry of the Reactions between Palladacycle Complexes and Primary Alkyl Iodides. Organometallics, 2023, 42, 606-614.	1.1	0
13057	A systematic mechanistic survey on the reactions between OH radical and CH ₃ OH on ice. Faraday Discussions, 0, 245, 508-518.	1.6	1
13058	Structure Performance Correlation of N-Heterocyclic Oligomer Leveler for Acid Copper Plating of Advanced Interconnects. Molecules, 2023, 28, 2783.	1.7	4

#	ARTICLE	IF	CITATIONS
13059	Computational evaluation of bioactive compounds from <i>Viscum album</i> (mistletoe) as inhibitors of p63 for pancreatic cancer treatment. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-15.	2.0	1
13060	Deep transfer learning for predicting frontier orbital energies of organic materials using small data and its application to porphyrin photocatalysts. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10536-10549.	1.3	4
13061	Unraveling two distinct polymorph transition mechanisms in one n-type single crystal for dynamic electronics. <i>Nature Communications</i> , 2023, 14, .	5.8	2
13062	Simulating optical linear absorption for mesoscale molecular aggregates: An adaptive hierarchy of pure states approach. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
13063	Size-Reduced Basis Set Calculation of Accurate Isotropic Nuclear Magnetic Shieldings Using CTOCD-GRRO and GPRO Methods in Amino Acids and Oligopeptides. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3036-3047.	1.1	0
13064	Energy Storage Application of Conducting Polymers Featuring Dual Acceptors: Exploring Conjugation and Flexible Chain Length Effects. <i>Small</i> , 2023, 19, .	5.2	5
13065	Interpreting vibrational circular dichroism spectra: the Cai factor for absolute configuration with confidence. <i>Journal of Cheminformatics</i> , 2023, 15, .	2.8	0
13066	Mechanistic Insights Into the Rhodium-Catalyzed C-H Alkenylation/Directing Group Migration and [3+2] Annulation: A DFT Study. <i>Journal of Organic Chemistry</i> , 2023, 88, 4494-4503.	1.7	0
13067	Ligand Control in Co-Catalyzed Regio- and Enantioselective Hydroboration: Homoallyl Secondary Boronates via Uncommon 4,3-Hydroboration of 1,3-Dienes. <i>Journal of the American Chemical Society</i> , 2023, 145, 7462-7481.	6.6	5
13068	Photoluminescence Properties of Single-Walled Carbon Nanotubes Influenced by the Tether Length of Reagents with Two Reactive Sites. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	4
13069	Improved Elastic Image Pair Method for Finding Transition States. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2410-2417.	2.3	5
13070	Design and Synthesis of 3-(¹² -d-Glucopyranosyl)-4-amino/4-guanidino Pyrazole Derivatives and Analysis of Their Glycogen Phosphorylase Inhibitory Potential. <i>Molecules</i> , 2023, 28, 3005.	1.7	2
13071	Oxidized Bridged Carbenoids as Viable Intermediates in a Fe(III) Catalyzed C-H Insertion Reaction. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	2
13073	A host-dye complex for sensitive fluorescence detection and clearing of spermine in cells. <i>Sensors and Actuators B: Chemical</i> , 2023, 386, 133757.	4.0	7
13075	Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation vs. substituent. <i>Nanoscale</i> , 0, , .	2.8	0
13077	Photoelectrocatalytic Dioxygen Reduction Based on a Novel Thiophene-Functionalized Tricarbonylchloro(1,10-phenanthroline)rhenium(I). <i>Molecules</i> , 2023, 28, 3229.	1.7	0
13078	Insights into the Fluxional Processes of Monomethylcyclohexenyl Manganese Tricarbonyl. <i>Molecules</i> , 2023, 28, 3232.	1.7	1
13079	Crystallographic evidence for the stereoselective substitution of equatorial pyridyl ligands in ruthenium(III) complexes. <i>Heliyon</i> , 2023, 9, e14876.	1.4	0

#	ARTICLE	IF	CITATIONS
13080	On the axial chirality of leucoindigo. <i>Journal of Computational Chemistry</i> , 2023, 44, 1578-1586.	1.5	0
13081	Influence of Cysteine 440 on the Active Site Properties of 3-Deoxy- <i>Arabino-Heptulosonate</i> 7-Phosphate Synthase in <i>Mycobacterium tuberculosis</i> (DAHPS). <i>ACS Omega</i> , 0, , .	1.6	0
13082	Stepâ€Economic Mechanosynthesis of Hybrid Azoles: Deciphering their Î€â€Orbital and Pharmacological Characteristics. <i>ChemMedChem</i> , 0, , .	1.6	0
13083	Mechanism of metalated pyrrole-singlet oxygen chemiluminescent reaction. <i>Polyhedron</i> , 2023, 238, 116421.	1.0	0
13084	A novel calculation strategy for optimized prediction of the reduction of electrochemical window at anode. <i>Chinese Physics B</i> , 0, , .	0.7	1
13085	An unprecedented route to achieve persistent 1H-azirine. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	1
13086	Ruthenium (II) Complexes of CNC Pincers and Bipyridine in the Photocatalytic CO ₂ Reduction Reaction to CO Using Visible Light: Catalysis, Kinetics, and Computational Insights. <i>ACS Catalysis</i> , 2023, 13, 5986-5999.	5.5	3
13087	Population analysis and the effects of Gaussian basis set quality and quantum mechanical approach: main group through heavy element species. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	0
13088	Structural and Dynamic Characterization of Liâ€Ionic Liquid Electrolyte Solutions for Application in Li-Ion Batteries: A Molecular Dynamics Approach. <i>Batteries</i> , 2023, 9, 234.	2.1	1
13089	Molecular modeling and DFT studies on the antioxidant activity of <i>Centaurea scoparia</i> flavonoids and molecular dynamics simulation of their interaction with Î²-lactoglobulin. <i>RSC Advances</i> , 2023, 13, 12361-12374.	1.7	5
13090	<i>Vitis vinifera</i> Red Globe grape: In natura investigations on skin pigmentation using phase-resolved photoacoustic and TDDFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, , 122761.	2.0	0
13091	A Nâ€Heterocyclic Carbeneâ€Supported Zinc Catalyst for the 1,2â€Regioselective Hydroboration of Nâ€Heteroarenes. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	7
13092	Synthesis of Bis(amino acids) Containing the Styryl-cyclobutane Core by Photosensitized [2+2]-Cross-cycloaddition of Allylidene-5(4H)-oxazolones. <i>International Journal of Molecular Sciences</i> , 2023, 24, 7583.	1.8	0
13151	Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93.		0
13250	PAQR: Pivoting Avoiding QR factorization. , 2023, , .		0
13309	Electronic current densities and origin-independent property densities induced by optical fields. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
13322	Nonlinear optical response of anthracene as a D-Î€-A conjugated system: Quantum computation study. <i>AIP Conference Proceedings</i> , 2023, , .	0.3	0
13398	Basis Set Functions. <i>Scientific Computation</i> , 2023, , 31-54.	0.2	0

#	ARTICLE	IF	CITATIONS
13528	High throughput anharmonic vibrational and rotational spectral computations. Annual Reports in Computational Chemistry, 2023, , 65-85.	0.9	1
13657	Density functional theory methods applied to homogeneous and heterogeneous catalysis: a short review and a practical user guide. Physical Chemistry Chemical Physics, 2024, 26, 7950-7970.	1.3	0