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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

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1444	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2005</b> , 1, 415-32	6.4	799
1443	Theoretical investigation of the hydrogen abstraction reaction of the OH radical with CH3CHF2 (HFC152-a): a dual level direct density functional theory dynamics study. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 8158-67	2.8	25
1442	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. <b>2005</b> , 123, 124107		297
1441	Benchmarking approximate density functional theory. I. s/d excitation energies in 3d transition metal cations. <b>2005</b> , 26, 1505-18		51
1440	Assessment of various density functionals and basis sets for the calculation of molecular anharmonic force fields. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 104, 830-845	2.1	64
1439	Correlation energy functionals dependent on an effective number of electrons: charged species and equilibrium geometries. <b>2005</b> , 123, 144111		
1438	SIX-DIMENSIONAL DYNAMICS OF DISSOCIATIVE CHEMISORPTION OF H2 ON METAL SURFACES. <b>2005</b> , 04, 493-581		76

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1436	Linear Response Properties Required to Simulate Vibrational Spectra of Biomolecules in Various Media: (R)-Phenyloxirane (A Comparative Theoretical and Spectroscopic Vibrational Study). <b>2005</b> , 91-124	4	11
1435	Vibrational spectra and structure of CH3Cl:NO complex: IR matrix isolation and DFT study. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 10880-5	2.8	2
1434	A New Algorithm for Efficient Direct Dynamics Calculations of Large-Curvature Tunneling and Its Application to Radical Reactions with 9-15 Atoms. <i>Journal of Chemical Theory and Computation</i> , <b>2005</b> , 1, 1063-78	6.4	29
1433	Combustion Chamber Fluid Dynamics and Hypergolic Gel Propellant Chemistry Simulations for Selectable Thrust Rocket Engines.		О
1432	How well can density functional methods describe hydrogen bonds to pi acceptors?. <b>2005</b> , 109, 19046-5	1	158
1431	Benchmark calculations of reaction energies, barrier heights, and transition-state geometries for hydrogen abstraction from methanol by a hydrogen atom. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 773-8	2.8	49
1430	Databases for transition element bonding: metal-metal bond energies and bond lengths and their use to test hybrid, hybrid meta, and meta density functionals and generalized gradient approximations. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 4388-403	2.8	185
1429	Design of density functionals that are broadly accurate for thermochemistry, thermochemical kinetics, and nonbonded interactions. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 5656-67	2.8	1172
1428	Bond dissociation energies and radical stabilization energies associated with model peptide-backbone radicals. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 6318-25	2.8	67
1427	Multicoefficient extrapolated density functional theory studies of pipi interactions: the benzene dimer. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 4209-12	2.8	98
1426	Benchmark database of barrier heights for heavy atom transfer, nucleophilic substitution, association, and unimolecular reactions and its use to test theoretical methods. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 2012-8	2.8	68o
1425	How well can new-generation density functional methods describe stacking interactions in biological systems?. <i>Physical Chemistry Chemical Physics</i> , <b>2005</b> , 7, 2701-5	3.6	238
1424	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. <b>2005</b> , 123, 161103		877
1423	Infinite-basis calculations of binding energies for the hydrogen bonded and stacked tetramers of formic acid and formamide and their use for validation of hybrid DFT and ab initio methods. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 6624-7	2.8	87
1422	Quantum chemical and master equation studies of the methyl vinyl carbonyl oxides formed in isoprene ozonolysis. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 10710-25	2.8	52
1421	Origin of tight binding of a near-perfect transition-state analogue by cytidine deaminase: implications for enzyme catalysis. <b>2005</b> , 127, 3191-7		37
1420	A comparative study of the catalytic mechanisms of the zinc and cadmium containing carbonic anhydrase. <b>2005</b> , 127, 4242-53		69

1419	Computational strategies for evaluating barrier heights for gas-phase reactions of lithium enolates. Journal of Organic Chemistry, <b>2005</b> , 70, 4279-83	4.2	35
1418	Thermochemistry is not a lower bound to the activation energy of endothermic reactions: a kinetic study of the gas-phase reaction of atomic chlorine with ammonia. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 6844-50	2.8	32
1417	Characterization of Hydrogen Bonding: From van der Waals Interactions to Covalency. <b>2006</b> , 1-50		11
1416	The Ni2+O2 reaction: the IR spectrum and structure of Ni2O2. A combined IR matrix isolation and theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2006</b> , 8, 3715-25	3.6	24
1415	An extended hindered-rotor model with incorporation of Coriolis and vibrational-rotational coupling for calculating partition functions and derived quantities. <b>2006</b> , 124, 044314		82
1414	Comparative assessment of density functional methods for 3d transition-metal chemistry. <b>2006</b> , 124, 224105		169
1413	QM/MM modelling of the TS-1 catalyst using HPCx. <b>2006</b> , 16, 1919		42
1412	Scaling dynamical correlation energy from density functional theory correlation functionals. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 396-403	2.8	4
1411	Regio- and stereospecific ring opening of 1,1-dialkyl-2-(aryloxymethyl)aziridinium salts by bromide. <b>2006</b> , 1554-6		52
1410	Combustion Chamber Fluid Dynamics and Hypergolic Gel Propellant Chemistry Simulations for Selectable Thrust Rocket Engines. <b>2006</b> ,		O
1409	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 364-82	6.4	2934
1408	A density functional that accounts for medium-range correlation energies in organic chemistry. <b>2006</b> , 8, 5753-5		172
1407	Comparative DFT study of van der Waals complexes: rare-gas dimers, alkaline-earth dimers, zinc dimer, and zinc-rare-gas dimers. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 5121-9	2.8	628
1406	H2, Ne, and N2 Energies of Encapsulation into C60 Evaluated with the MPWB1K Functional. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 782-5	6.4	87
1405	Catecholamine-induced release of nitric oxide from N-nitrosotryptophan derivatives: a non-enzymatic method for catecholamine oxidation. <b>2006</b> , 4, 257-67		10
1404	Benchmark study of DFT functionals for late-transition-metal reactions. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 709-16	2.8	193
1403	Systematic errors in computed alkane energies using B3LYP and other popular DFT functionals. <b>2006</b> , 8, 3631-4		363
1402	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. <b>2006</b> , 104, 777-794		11

1401	Variational transition-state theory study of the dimethyl sulfoxide (DMSO) and OH reaction. Journal of Physical Chemistry A, <b>2006</b> , 110, 798-808	2.8	21
1400	Dissociation mechanism of a stable intermediate: perfluorohydroxylamine. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 10880-9	2.8	
1399	Hybrid density functional theory with specific reaction parameter: hydrogen abstraction reaction of fluoromethane by the hydroxyl radical. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 7663-71	2.8	14
1398	Reaction-path dynamics and theoretical rate constants for the CH(n)F(4-n) + O3> HOOO + CH(n-1)F(4-n) (n = 2,3) reactions. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 11113-9	2.8	7
1397	H-Atom abstraction from CH(3)NHNH(2) by NO(2): CCSD(T)/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p) and CCSD(T)/6-311+G(2df,p)//CCSD/6-31+G(d,p) calculations. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 6129-38	2.8	20
1396	Computational Improvements to Quantum Wave Packet ab Initio Molecular Dynamics Using a Potential-Adapted, Time-Dependent Deterministic Sampling Technique. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 1203-19	6.4	30
1395	Assessment of several hybrid DFT functionals for the evaluation of bond length alternation of increasingly long oligomers. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 5952-9	2.8	71
1394	Assessment of density functionals for pi systems: Energy differences between cumulenes and poly-ynes; proton affinities, bond length alternation, and torsional potentials of conjugated polyenes; and proton affinities of conjugated Shiff bases. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 10	2.8 <b>478-8</b> 6	182 5
1393	Tautomerism in the guanyl radical. <b>2006</b> , 128, 13796-805		68
1392	Rozen's epoxidation reagent, CH3CN.HOF: a theoretical study of its structure, vibrational spectroscopy, and reaction mechanism. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 8275-81	2.8	8
1391	Reliable low-cost theoretical procedures for studying addition-fragmentation in RAFT polymerization. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 2486-92	2.8	78
1390	Multiconfiguration Molecular Mechanics Based on Combined Quantum Mechanical and Molecular Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 1237-54	6.4	37
1389	Theoretical study of the antioxidant properties of pyridoxine. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 13068-72	2.8	63
1388	Assessment of Model Chemistries for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2006</b> , 2, 1009-18	6.4	203
1387	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. <b>2006</b> , 328, 307-317		8
1386	Theoretical studies on the reactions X+CHBrF2 (X=F, Br). Chemical Physics Letters, 2006, 432, 6-10	2.5	1
1385	Computations of the Energetics of C60F36 Isomers. <b>2006</b> , 14, 57-65		1
1384	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. <b>2006</b> , 125, 194101		3551

1383	An assessment of theoretical procedures for predicting the thermochemistry and kinetics of hydrogen abstraction by methyl radical from benzene. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 8942-51.8	67
1382	Modeling the kinetics of bimolecular reactions. <b>2006</b> , 106, 4518-84	464
1381	Theoretical study of host-guest interaction and its manifestations in the properties of model endohedral fullerenes with small covalent molecules inside the C n and C n H m cages. <b>2006</b> , 51, S1-S27	8
1380	Ab initio dynamics with wave-packets and density matrices. <b>2006</b> , 116, 326-337	26
1379	Accurate ab initio prediction of propagation rate coefficients in free-radical polymerization: Acrylonitrile and vinyl chloride. <b>2006</b> , 324, 96-110	125
1378	Characterization of synthetic oxomanganese complexes and the inorganic core of the O2-evolving complex in photosystem II: evaluation of the DFT/B3LYP level of theory. <b>2006</b> , 100, 786-800	94
1377	Formation of heteroatom active sites in zeolites by hydrolysis and inversion. <b>2006</b> , 45, 1633-8	23
1376	Dispersion and repulsion contributions to the solvation free energy: comparison of quantum mechanical and classical approaches in the polarizable continuum model. <b>2006</b> , 27, 1769-80	44
1375	Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer. <b>2006</b> , 89, 2254-2272	35
1374	Formation of Heteroatom Active Sites in Zeolites by Hydrolysis and Inversion. <b>2006</b> , 118, 1663-1668	2
1373	Conceptual, Qualitative, and Quantitative Theories of 1,3-Dipolar and DielsAlder Cycloadditions Used in Synthesis. <b>2006</b> , 348, 2337-2361	259
1372	Hydrogen BondingNew Insights. <b>2006</b> ,	350
1371	Effects of ionization on N-glycylglycine peptide: influence of intramolecular hydrogen bonds. <b>2006</b> , 124, 154306	24
1370	Quantum Mechanics for Organic Chemistry. 1-41	1
1369	Solution-Phase Organic Chemistry. 349-411	
1368	Electrochemical properties of the polypyrrole films doped with benzenesulfonate. <b>2007</b> , 157, 66-73	29
1367	Application of quantum-chemical approximations to environmental problems: Prediction of physical and chemical properties of TNT and related species. <b>2007</b> , 69, 1144-50	19
1366	Reinvestigating the role of multiple hydrogen transfers in Baeyer-Villiger reactions. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 6580-3	23

1365	General performance of density functionals. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10439-52	2.8	810
1364	Assessment of long-range corrected functionals performance for n>pi* transitions in organic dyes. <b>2007</b> , 127, 094102		112
1363	Carbon-Hydrogen Bond Activation in Hydridotris(pyrazolyl)borate Platinum(IV) Complexes: Comparison of Density Functionals, Basis Sets, and Bonding Patterns. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 2268-81	6.4	14
1362	How accurate are DFT treatments of organic energies?. <b>2007</b> , 9, 1851-4		245
1361	Density functional theory with dispersion corrections for supramolecular structures, aggregates, and complexes of (bio)organic molecules. <b>2007</b> , 5, 741-58		636
1360	A computational study on the stacking interaction in quinhydrone. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 1998-2001	2.8	40
1359	How well can new-generation density functionals describe protonated epoxides where older functionals fail?. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 295-8	4.2	40
1358	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. <b>2007</b> , 126, 144105		264
1357	Long-range corrected density functional calculations of chemical reactions: redetermination of parameter. <b>2007</b> , 126, 154105		258
1356	Chlorinebenzene complexesthe reliability of density functionals for non-covalent radical complexes. <i>Physical Chemistry Chemical Physics</i> , <b>2007</b> , 9, 5649-55	3.6	13
1355	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. Journal of Chemical Theory and Computation, <b>2007</b> , 3, 2210-20	6.4	39
1354	Bond dissociation energies and radical stabilization energies: an assessment of contemporary theoretical procedures. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 13638-44	2.8	91
1353	Theoretical investigation of the hydrogen abstraction reaction of the OH radical with CH2FCH2F (HFC-152): a dual-level direct dynamics study. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 8095-103	2.8	10
1352	Density Functional and Semiempirical Molecular Orbital Methods Including Dispersion Corrections for the Accurate Description of Noncovalent Interactions Involving Sulfur-Containing Molecules. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 1656-64	6.4	70
1351	Comparison of ab initio and DFT electronic structure methods for peptides containing an aromatic ring: effect of dispersion and BSSE. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 13272-7	2.8	71
1350	Computational chemistry of polyatomic reaction kinetics and dynamics: the quest for an accurate CH5 potential energy surface. <b>2007</b> , 107, 5101-32		55
1349	Hydrogenation of simple aromatic molecules: a computational study of the mechanism. <b>2007</b> , 129, 924-	.33	40
1348	Intramolecular hydrogen bond energy in polyhydroxy systems: a critical comparison of molecular tailoring and isodesmic approaches. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 6472-80	2.8	52

1347	Dual cation and anion acceptor molecules. The case of the (eta6-C6H6)(eta6C6F6)Cr0 complex. Journal of Physical Chemistry A, 2007, 111, 3137-42	2.8	28
1346	The origins of femtomolar protein-ligand binding: hydrogen-bond cooperativity and desolvation energetics in the biotin-(strept)avidin binding site. <b>2007</b> , 129, 5419-29		141
1345	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: benchmarks approaching the complete basis set limit. <b>2007</b> , 127, 184104		195
1344	Atom-Centered Density Matrix Propagation Calculations on the Methyl Transfer from CH3Cl to NH3: Gas-Phase and Continuum-Solvated Trajectories. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 336-43	6.4	11
1343	Vibrational overtone induced elimination reactions within hydrogen-bonded molecular clusters: the dynamics of water catalyzed reactions in CH2FOH.H2On. <i>Physical Chemistry Chemical Physics</i> , <b>2007</b> , 9, 3864-71	3.6	44
1342	Tunneling in green tea: understanding the antioxidant activity of catechol-containing compounds. A variational transition-state theory study. <b>2007</b> , 129, 5846-54		80
1341	Four-membered heterocycles with a carbon-heteroatom exocyclic double bond at the 3-position: puckering potential and thermodynamic properties. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 2797-80	3 <sup>2.8</sup>	22
1340	Comparative assessment of theoretical methods for the determination of geometrical properties in biological zinc complexes. <b>2007</b> , 111, 9146-52		31
1339	Ab initio, density functional theory, and continuum solvation model prediction of the product ratio in the S(N)2 reaction of NO2(-) with CH3CH2Cl and CH3CH2Br in DMSO solution. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10068-74	2.8	20
1338	Novel synthesis of 3,4-diaminobutanenitriles and 4-amino-2-butenenitriles from 2-(cyanomethyl)aziridines through intermediate aziridinium salts: an experimental and theoretical approach. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 4733-40	4.2	28
1337	*H atom and *OH radical reactions with 5-methylcytosine. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 8968-72	2.8	22
1336	Scaled density functional theory correlation functionals. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 103	9 <b><u>9</u>.<del>S</del></b>	
1335	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 569-82	6.4	193
1334	The experimental and calculational thermochemistry of 1,2,4,5-benzenetetracarboxylic dianhydride: is this 10 pi multiring species aromatic?. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 7181-8	2.8	14
1333	Global DFT-Based Reactivity Indicators: An Assessment of Theoretical Procedures in Zeolite Catalysis. <b>2007</b> , 111, 3028-3037		13
1332	O-H bond dissociation enthalpies of oximes: a theoretical assessment and experimental implications. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 13112-25	2.8	30
1331	Global Potential Energy Surfaces with Correct Permutation Symmetry by Multiconfiguration Molecular Mechanics. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 938-48	6.4	14
1330	Thermochemical and kinetic analysis of the thermal decomposition of monomethylhydrazine: an elementary reaction mechanism. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 3748-60	2.8	25

#### (2007-2007)

1329	Direct-dynamics VIST study of the [1,7] hydrogen shift in 7-methylocta-1,3(2),5(2)-triene. A model system for the hydrogen transfer reaction in previtamin D3. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 719-25	2.8	14	
1328	Calorimetric and computational study of indanones. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 11153-9	2.8	17	
1327	Theoretical study of the fragmentation pathways of norbornane in its doubly ionized ground state. Journal of Physical Chemistry A, 2007, 111, 10834-48	2.8	13	
1326	Explanation of the unusual temperature dependence of the atmospherically important OH + H(2)S> H(2)O + HS reaction and prediction of the rate constant at combustion temperatures. <b>2007</b> , 129, 127	765-71	43	
1325	Theoretical modeling of hydroxyl-radical-induced lipid peroxidation reactions. <b>2007</b> , 111, 5684-93		40	
1324	Theoretical Investigations of Isolated Mo(VI) and Mo(IV) Centers of a MolybdenaBilica Catalyst for Olefin Metathesis. <b>2007</b> , 111, 9337-9348		30	
1323	Thermochemical kinetics of hydrogen-atom transfers between methyl, methane, ethynyl, ethyne, and hydrogen. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 4632-42	2.8	54	
1322	Formation of Active Sites in TS-1 by Hydrolysis and Inversion. <b>2007</b> , 111, 14720-14731		21	
1321	Association patterns in (HF)(m)(H2O)(n) (m + n = 2-8) clusters. Journal of Physical Chemistry A, 2007, 111, 7940-56	2.8	17	
1320	Significance of ammonia in growth of atmospheric nanoclusters. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10671-4	2.8	60	
1319	Uncatalyzed transfer hydrogenation of quinones and related systems: a theoretical mechanistic study. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 6456-67	2.8	16	
1318	Should contemporary density functional theory methods be used to study the thermodynamics of radical reactions?. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 10754-68	2.8	131	
1317	Computational study of CO2 reduction by amines. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 3719-26	2.8	18	
1316	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 1830-6	6.4	8	
1315	How to compute isomerization energies of organic molecules with quantum chemical methods. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 2118-26	4.2	210	
1314	The mechanism of the Baeyer-Villiger rearrangement: quantum chemistry and TST study supported by experimental kinetic data. <b>2007</b> , 5, 3682-9		87	
1313	An evaluation of harmonic vibrational frequency scale factors. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 11683-700	2.8	1987	
1312	Density Functionals for Noncovalent Interaction Energies of Biological Importance. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 289-300	6.4	528	

1311	Reactions of hydrogen atom with hydrogen peroxide. <i>Journal of Physical Chemistry A</i> , <b>2007</b> , 111, 13554-668	39
1310	Computational Requirements for Simulating the Structures and Proton Activity of Silicaceous Materials. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 593-604	17
1309	Structure and stability of VO2+ in aqueous solution: a Car-Parrinello and static ab initio study. <b>2007</b> , 46, 4835-43	37
1308	A kinetic and thermodynamic study of the glycosidic bond cleavage in deoxyuridine. <b>2007</b> , 111, 3800-12	32
1307	Structure and stability of the (001) alpha-quartz surface. <i>Physical Chemistry Chemical Physics</i> , <b>2007</b> , 9, 2146-52	164
1306	CH/pi interactions in DNA and proteins. A theoretical study. <b>2007</b> , 111, 9372-9	51
1305	Remote position substituents as modulators of conformational and reactive properties of quinones. Relevance of the pi/pi intramolecular interaction. <i>Journal of Organic Chemistry</i> , <b>2007</b> , 72, 1883 <sup>4</sup> 9 <sup>4</sup>	17
1304	. 2007,	105
1303	Methyl vinyl ketone+OH and methacrolein+OH oxidation reactions: a master equation analysis of the pressure- and temperature-dependent rate constants. <b>2007</b> , 13, 1180-90	8
1302	Unusual bond formation in aspartic protease inhibitors: a theoretical study. <b>2007</b> , 13, 5388-93	25
1301	Ring opening of the cyclobutane in a thymine dimer radical anion. <b>2007</b> , 13, 8979-84	23
1300	DFT and ab initio calculations on two reactions between hydrogen atoms and the fire suppressants 2-H heptafluoropropane and CF3Br. <b>2007</b> , 28, 1582-1592	12
1299	Endohedral stannaspherenes Mn@Sn12 and its dimer: ferromagnetic or antiferromagnetic?. <b>2007</b> , 8, 2096-9	21
1298	Efficient singlet-state deactivation of cyano-substituted indolines in protic solvents via CNHO hydrogen bonds. <b>2007</b> , 8, 2627-35	13
1297	Triflic-Acid-Mediated Polycondensation of Carbonyl Compounds with Aromatic Hydrocarbons IA Theoretical Study. <b>2007</b> , 16, 227-239	19
1296	Metal complexation of protocatechuic acid and its derivatives: Determination of the optimal computational conditions for the simulation of electronic spectra. <b>2007</b> , 806, 131-140	8
1295	The H2-hydrogenation of ketones catalysed by ruthenium(II) complexes: A density functional theory study. <b>2007</b> , 812, 39-49	32
1294	Uncatalyzed 1,4-hydrogenation of polycyclic aromatic hydrocarbons: A computational study. <b>2007</b> , 811, 13-17	10

Reactions of NO2 with CH3NHNH and CH3NNH2: A direct molecular dynamics study. <b>2007</b> , 818, 119-1	24	17
1292 Electronic structure and luminescence of [AuS2PPh(OCH2CHCH2)]2 complex. <b>2007</b> , 820, 141-147		25
A reparametrization of a meta-GGA exchange-correlation functional with improved descriptions of van der Waals interactions. <i>Chemical Physics Letters</i> , <b>2007</b> , 436, 394-399	2.5	6
Performance of DFT/MPWB1K for stacking and H-bonding interactions. <i>Chemical Physics Letters</i> , <b>2007</b> , 439, 35-39	2.5	67
Accurate multi-level electronic structure methods (MLSE-DFT) for atomization energies and reaction energy barriers. <i>Chemical Physics Letters</i> , <b>2007</b> , 442, 220-223	2.5	7
A density functional theory study of the hydrogen bond interactions in glycine dimers. <i>Chemical Physics Letters</i> , <b>2007</b> , 445, 117-124	2.5	21
Performance of hybrid density functional theory methods toward oxygen electroreduction over platinum. <b>2007</b> , 52, 3149-3159		7
Experimental and computational study on photophysical properties of substituted o-hydroxy acetophenone derivatives: Intramolecular proton transfer and solvent effect. <b>2007</b> , 342, 309-317		18
Quantum chemical investigation of linear hydrogen bonding in ONCCNIEHX (X = F, Cl, Br) dimers.  International Journal of Quantum Chemistry, 2007, 107, 1194-1204	2.1	2
Reaction-path dynamics and theoretical rate constants for the reaction CH4 + O3 -> HOOO + CH3.  International Journal of Quantum Chemistry, 2007, 107, 1999-2005	2.1	13
Initiation of petroleum formation and antioxidant function <b>a</b> DFT study of sulfur?sulfur bond dissociation enthalpies. <b>2007</b> , 20, 754-763		4
$_{12}8_{2}$ Evidences for a new Ultraviolet Absorption Band of the FSO3 Radical. <b>2007</b> , 221, 897-909		2
Long-range corrected density functional study on weakly bound systems: balanced descriptions of various types of molecular interactions. <b>2007</b> , 126, 234114		133
Hybrid density functional theory with a specific reaction parameter: hydrogen abstraction reaction of trifluoromethane by the hydroxyl radical. <b>2007</b> , 117, 383-395		11
Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. <b>2007</b> , 118, 589-595		9
Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with <b>1</b> correlation. <b>2007</b> , 118, 693-707		19
Hybrid density functional theory with a specific reaction parameter: hydrogen abstraction reaction of difluoromethane by the hydroxyl radical. <i>Journal of Molecular Modeling</i> , <b>2007</b> , 13, 1109-21	2	4
1276 Chemical reactivity analysis of the CO+OH and CO+HO2 reactions. <b>2008</b> , 862, 138-147		9

1275	Application of Density Functional Theory for evaluation of standard two-electron reduction potentials in some quinone derivatives. <b>2008</b> , 870, 10-14		15
1274	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. <b>2008</b> , 120, 215-241		19079
1273	On the mechanism of the OH initiated oxidation of acetylene in the presence of O2 and NO x. <b>2008</b> , 121, 219-225		11
1272	Hydrogen-bonding properties of galanthamine: an investigation through crystallographic database observations and computational chemistry. <b>2008</b> , 64, 338-47		3
1271	The role of noninnocent solvent molecules in organocatalyzed asymmetric Michael addition reactions. <b>2008</b> , 14, 10472-85		49
1270	Reaction mechanism of molybdoenzyme formate dehydrogenase. <b>2008</b> , 14, 8674-81		43
1269	Stereoconversion of amino acids and peptides in uryl-pendant binol schiff bases. <b>2008</b> , 14, 9935-42		31
1268	Theoretical investigation of the OH*-initiated oxidation of benzaldehyde in the troposphere. <b>2008</b> , 9, 1453-9		17
1267	Direct dynamics study on the reaction of acetaldehyde with ozone. <b>2008</b> , 29, 247-55		10
1266	Calculation of weakly polar interaction energies in polypeptides using density functional and local MIler-Plesset perturbation theory. <b>2008</b> , 29, 1344-52		30
1265	Mechanistic studies on the formation of glycosidase-substrate and glycosidase-inhibitor covalent intermediates. <b>2008</b> , 29, 2565-74		35
1264	Isostructural Potassium and Thallium Salts of Sterically Crowded Thio- and Selenophenols: A Structural and Computational Study. <b>2008</b> , 2008, 5609-5616		5
1263	Functionalized 2,5-Dipyridinylpyrroles by Electrochemical Reduction of 3,6-Dipyridinylpyridazine Precursors. <i>European Journal of Organic Chemistry</i> , <b>2008</b> , 2008, 2156-2166	3.2	25
1262	Synthesis of Enantiopure Highly Functionalized Pyrrolizines and Indolizines from Natural ⊞-Amino Acids: An Ex⊡perimental and Theoretical Investigation. <i>European Journal of Organic Chemistry</i> , <b>2008</b> , 2008, 2808-2816	3.2	20
1261	Reactions of Carbenes with Ethers: The Role of Noncovalent Interactions. <i>European Journal of Organic Chemistry</i> , <b>2008</b> , 2008, 3363-3368	3.2	11
1260	Sources of error in DFT computations of C-C bond formation thermochemistries: pi>sigma transformations and error cancellation by DFT methods. <b>2008</b> , 47, 7746-9		148
1259	Sources of Error in DFT Computations of C?C Bond Formation Thermochemistries: ₽□ Transformations and Error Cancellation by DFT Methods. <b>2008</b> , 120, 7860-7863		22
1258	Study of the factors determining the mobility of ions in the polypyrrole films doped with aromatic sulfonate anions. <b>2008</b> , 53, 3828-3835		50

#### (2008-2008)

1257	Efficient and accurate ab initio prediction of thermodynamic parameters for intermolecular complexes. <i>Chemical Physics Letters</i> , <b>2008</b> , 451, 147-152	2.5	7
1256	Quantum chemical and RRKM/master equation studies of isoprene ozonolysis: Methacrolein and methacrolein oxide. <i>Chemical Physics Letters</i> , <b>2008</b> , 451, 186-191	2.5	31
1255	How the site of ionisation influences side-chain fragmentation in histidine radical cation. <i>Chemical Physics Letters</i> , <b>2008</b> , 451, 276-281	2.5	14
1254	Hydroxyl radical <b>T</b> hymine adduct induced DNA damages. <i>Chemical Physics Letters</i> , <b>2008</b> , 458, 186-189	2.5	17
1253	Stacking interaction of cytosine with carbon nanotubes: MP2, DFT and Raman spectroscopy study. <i>Chemical Physics Letters</i> , <b>2008</b> , 459, 153-158	2.5	52
1252	A commentary on Density functional calculation of hydrogen-filled C60 moleculesDby C-K. Yang [Carbon 2007;45(12):2451🖪3]. <b>2008</b> , 46, 704-705		13
1251	Reply to the Commentary on <b>D</b> ensity functional calculation of hydrogen-filled C60 molecules <b>2008</b> , 46, 705		6
1250	Comparative study of calix[4]arene derivatives: implications for ligand design. 2008, 49, 2393-2396		12
1249	Theoretical investigation of the gas phase oxidation mechanism of dimethyl sulfoxide by OH radical. <b>2008</b> , 851, 1-14		9
1248	Molecular tweezers as receptors for anions: An energetic and topological study. <b>2008</b> , 854, 1-9		12
1247	Assessment of Density Functionals, Semiempirical Methods, and SCC-DFTB for Protonated Creatinine Geometries. <b>2008</b> , 861, 68-73		10
1246	Assessment of density functionals for the investigation of iridium(III) complexes. 2008, 861, 97-102		17
1245	Theoretical study of inosine tetrad and octamer interacting with alkali metal ions. 2008, 869, 94-97		6
1244	New organic FET-like photoactive device, experiments and DFT modeling. 2008, 25, 299-307		20
1243	Density functionals with broad applicability in chemistry. <b>2008</b> , 41, 157-67		5345
1242	Orbital-dependent density functionals: Theory and applications. <b>2008</b> , 80, 3-60		941
1241	Radical coupling reaction of paramagnetic endohedral metallofullerene La@C82. 2008, 130, 16224-30		55
1240	Iron- and ruthenium-Lewis acid catalyzed asymmetric 1,3-dipolar cycloaddition reactions between enals and diaryl nitrones. <b>2008</b> , 3, 1298-311		39

1239	Formation of CO2on a carbonaceous surface: a quantum chemical study. 2008, 384, 1158-1164		54
1238	Packing of Planar Organic Molecules: Interplay of van der Waals and Electrostatic Interaction. <b>2008</b> , 8, 3053-3057		51
1237	Highly accurate first-principles benchmark data sets for the parametrization and validation of density functional and other approximate methods. Derivation of a robust, generally applicable, double-hybrid functional for thermochemistry and thermochemical kinetics. <i>Journal of Physical</i>	2.8	578
1236	Chemistry A, 2008, 112, 12868-86  Ab initio study of acrylate polymerization reactions: methyl methacrylate and methyl acrylate propagation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6772-82	2.8	68
1235	Double-hybrid functionals for thermochemical kinetics. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 3-8	2.8	194
1234	DFT calculation of 1J(119Sn,13C) and 2J(119Sn,1H) coupling constants in di- and trimethyltin(IV) compounds. <b>2008</b> , 47, 4796-807		43
1233	Experimental and computational study of the conrotatory ring opening of various 3-chloro-2-azetines. <i>Journal of Organic Chemistry</i> , <b>2008</b> , 73, 5481-8	4.2	32
1232	Consequences of spin contamination in unrestricted calculations on open-shell species: effect of Hartree-Fock and Mller-Plesset contributions in hybrid and double-hybrid density functional theory approaches. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13225-30	2.8	112
1231	Evidence for nonstatistical dynamics in the Wolff rearrangement of a carbene. <b>2008</b> , 130, 12085-94		50
1230	OH formation from O and H atoms physisorbed on a graphitic surface through the Langmuir-Hinshelwood mechanism: a quasi-classical approach. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 11921-30	2.8	35
1229	Origin of enantioselection in Hetero-Diels-Alder reactions catalyzed by naphthyl-TADDOL. <b>2008</b> , 10, 2749-52		74
1228	Interactions in large, polyaromatic hydrocarbon dimers: application of density functional theory with dispersion corrections. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 10968-76	2.8	131
1227	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> , <b>2008</b> , 4, 1849-68	6.4	784
1226	Probing the molecular and electronic structure of capsaicin: a spectroscopic and quantum mechanical study. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 5700-11	2.8	11
1225	Mechanical and electronic properties of endofullerene Ne@C60 studied via structure distortions. <b>2008</b> , 106, 703-716		11
1224	Hybrid QM/MM Investigations into the Structure and Properties of Oxygen-Donating Species in TS-1. <b>2008</b> , 112, 7173-7185		30
1223	The structure and binding energies of the van der Waals complexes of Ar and N2 with phenol and its cation, studied by high level ab initio and density functional theory calculations. <b>2008</b> , 128, 044313		22
1222	The onset of calcium carbonate nucleation: a density functional theory molecular dynamics and hybrid microsolvation/continuum study. <b>2008</b> , 112, 6965-75		46

#### (2008-2008)

1221	An Coordination Chemistry: Development of Benchmark Suites for Geometries, Dipole Moments, and Bond Dissociation Energies and Their Use To Test and Validate Density Functionals and Molecular Orbital Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 75-85	6.4	147
1220	Assessment of the accuracy of density functionals for prediction of relative energies and geometries of low-lying isomers of water hexamers. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 3976-84	2.8	135
1219	Stereochemistry of eudesmane cation formation during catalysis by aristolochene synthase from Penicillium roqueforti. <b>2008</b> , 6, 2346-54		34
1218	Thermochemistry and kinetics of acetonylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 7139-49	3.6	17
1217	Theoretical study on NO3-initiated oxidation of acenaphthene in the atmosphere. <b>2008</b> , 86, 129-137		10
1216	A computational analysis of the interaction between flavin and thiol(ate) groups. Implications for flavoenzyme catalysis. <b>2008</b> , 29, 415-424		6
1215	Computational organic chemistry. <b>2008</b> , 104, 394		13
1214	Theoretical exploration of the cooperative effect in NMF-NMF-amino acid residue hydrogen bonding system. <i>Physical Chemistry Chemical Physics</i> , <b>2008</b> , 10, 5607-15	3.6	5
1213	Computational study of the factors controlling enantioselectivity in ruthenium(II) hydrogenation catalysts. <b>2008</b> , 47, 2674-87		39
1212	Isostructural potassium and thallium salts of sterically crowded triazenes: a structural and computational study. <b>2008</b> , 47, 4401-12		43
1211	Catalysis of Addition Reactions by a Negatively Charged Silica Surface Site on a Dust Grain. <b>2008</b> , 112, 15419-15422		16
<b>121</b> 0	Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Drug-Like Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 1718-1732	6.4	12
1209	Theoretical study of the nitroalkane thermolysis. 1. Computation of the formation enthalpy of the nitroalkanes, their isomers and radical products. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 4458-64	2.8	32
1208	Carbene-alkene complexes between a nucleophilic carbene and electron-poor alkenes. <b>2008</b> , 130, 1463	4-9	11
1207	Jacobsen Catalyst Interaction with Polydimethylsiloxane/Tetraethoxysilane Network and Solvent Molecules: Theoretical Design of a New Polymeric Membrane. <b>2008</b> , 112, 14830-14834		8
1206	Understanding the participation of quadricyclane as nucleophile in polar [2sigma + 2sigma + 2pi] cycloadditions toward electrophilic pi molecules. <i>Journal of Organic Chemistry</i> , <b>2008</b> , 73, 8791-9	4.2	183
1205	Multicoefficient density functional theory (MC-DFT). Journal of Physical Chemistry A, 2008, 112, 1064-70	2.8	7
1204	Hybrid Meta-Generalized Gradient Functional Modeling of Boron-Nitrogen Coordinate Covalent Bonds. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 1249-53	6.4	22

1203	Strength of Calpha-HO=C hydrogen bonds in transmembrane proteins. 2008, 112, 1041-8		35
1202	Benchmark Data for Interactions in Zeolite Model Complexes and Their Use for Assessment and Validation of Electronic Structure Methods. <b>2008</b> , 112, 6860-6868		137
1201	Assessment of new meta and hybrid meta density functionals for predicting the geometry and binding energy of a challenging system: the dimer of H2S and benzene. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 6009-16	2.8	33
1200	One-electron reduction of 8-bromo-2-aminoadenosine in the aqueous phase: radiation chemical and DFT studies of the mechanism. <b>2008</b> , 112, 5209-17		8
1199	A quantum mechanical study on the formation of PCDD/Fs from 2-chlorophenol as precursor. <b>2008</b> , 42, 7301-8		77
1198	Spin-orbit and electron correlation effects on the structure of EF3 ( $E = I$ , At, and element 117). <b>2008</b> , 112, 16021-9		13
1197	Theoretical study of the mechanism and rate constant of the B + CO2 reaction. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 8148-53	2.8	2
1196	Theoretical investigation on the stability of ionic formic acid clusters. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13382-92	2.8	13
1195	Claisen rearrangement of aliphatic allyl vinyl ethers in the presence of copper(II) bisoxazoline. Journal of Organic Chemistry, <b>2008</b> , 73, 4800-9	4.2	12
1194	Spectral heterogeneity of PRODAN fluorescence in isotropic solvents revealed by multivariate photokinetic analysis. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13402-12	2.8	24
1193	Canonical variational transition-state theory study of the CF3CH2CH3 + OH reaction. <b>2008</b> , 112, 328-35		16
1192	Carbene proton attachment energies: theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 5269	92787	6
1191	Mechanism of thiolate-disulfide interchange reactions in biochemistry. <i>Journal of Organic Chemistry</i> , <b>2008</b> , 73, 12-21	4.2	106
1190	Tubular aggregates of cyclic oligothiophenes. A theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 3996-4003	2.8	18
1189	Halogen Bonding with Dihalogens and Interhalogens. <b>2007</b> , 65-104		55
1188	1,2,3-Triazines and their Benzo Derivatives. <b>2008</b> , 1-93		
1187	An ab initio investigation on (CO2)n and CO2(Ar)m clusters: geometries and IR spectra. <b>2008</b> , 128, 1243	10	32
1186	Mechanism and Kinetics of Cyanide Decomposition by Ferrate. 2008, 81, 1212-1218		23

1185	EPR and IR spectra of the FSO3 radical revisited: Strong vibronic interactions in the 2A2 electronic ground state. <b>2008</b> , 128, 084501		9
1184	Structure and properties of the Zn(+)-D(2) complex. <b>2009</b> , 131, 224304		15
1183	Post-CCSD(T) ab initio thermochemistry of halogen oxides and related hydrides XOX, XOOX, HOX, XOn, and HXOn (X = F, Cl), and evaluation of DFT methods for these systems. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 4802-16	2.8	71
1182	An efficient algorithm for the density-functional theory treatment of dispersion interactions. <b>2009</b> , 130, 124105		96
1181	Efficient global representations of potential energy functions: trajectory calculations of bimolecular gas-phase reactions by multiconfiguration molecular mechanics. <b>2009</b> , 130, 024105		12
1180	DFT Study of Molecules Confined Inside Fullerene and Fullerene-like Cages. <b>2009</b> , 58, 69-114		17
1179	Uncertainties in scaling factors for ab initio vibrational zero-point energies. 2009, 130, 114102		62
1178	Mechanism of OH-initiated atmospheric photooxidation of the organophosphorus insecticide (C2H5O)3PS. <b>2009</b> , 43, 4163-4170		14
1177	Determination of the catalytic pathway of a manganese arginase enzyme through density functional investigation. <b>2009</b> , 15, 8026-36		23
1176	Density functional studies on isomerization of prostaglandin H2 to prostacyclin catalyzed by cytochrome P450. <b>2009</b> , 15, 4464-73		14
1175	On the reaction of glycerol dehydratase with but-3-ene-1,2-diol. <b>2009</b> , 15, 4865-73		7
1174	The (3)[ndsigma*(n+1)psigma] emissions of linear silver(I) and gold(I) chains with bridging phosphine ligands. <b>2009</b> , 15, 10777-89		65
1173	A combined theoretical and experimental investigation on the enantioselective oxidation of aryl benzyl sulfides in the presence of a chiral titanium catalyst. <b>2009</b> , 15, 13417-26		35
1172	The Variable Strength of the SulfurBulfur Bond: 78 to 41 kcal ©3, CBS-Q, and DFT Bond Energies of Sulfur (S8) and Disulfanes XSSX (X = H, F, Cl, CH3, CN, NH2, OH, SH). <b>2009</b> , 2009, 1358-1368		21
1171	Theoretical Study of the RNA Hydrolysis Mechanism of the Dinuclear Zinc Enzyme RNase Z. <b>2009</b> , 2009, 2967-2972		14
1170	Noncovalent interactions in supramolecular complexes: a study on corannulene and the double concave buckycatcher. <b>2009</b> , 30, 51-6		69
1169	Comparison of some representative density functional theory and wave function theory methods for the studies of amino acids. <b>2009</b> , 30, 589-600		53
1168	Can the hybrid meta GGA and DFT-D methods describe the stacking interactions in conjugated polymers?. <b>2009</b> , 30, 1179-84		15

1167	Typical aromatic noncovalent interactions in proteins: A theoretical study using phenylalanine. <b>2009</b> , 30, 1392-404		42	
1166	Formation pathways of DMSO(2) in the addition channel of the OH-initiated DMS oxidation: A theoretical study. <b>2009</b> , 30, 1477-89		5	
1165	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of N-formyl-glycine amide and N-formyl-alanine amide radical cations. <b>2009</b> , 30, 1771-84		6	
1164	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for zinc complexes. <b>2009</b> , 30, 2752-63		45	
1163	Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H2O> H2O, CH3OH> H2O, and H2O> CH3OH dimers. <b>2010</b> , 31, 963-72		11	
1162	Evaluation of exchange-correlation functionals for time-dependent density functional theory calculations on metal complexes. <b>2010</b> , 31, 1008-14		24	
1161	Barrier heights for H-atom abstraction by H*O2 from n-butanola simple yet exacting test for model chemistries?. <b>2010</b> , 31, 1236-48		75	
1160	Quinoline alkaloids as intercalative topoisomerase inhibitors. <i>Journal of Molecular Modeling</i> , <b>2009</b> , 15, 1417-26	2	25	
1159	Gas-phase acidity, bond dissociation energy and enthalpy of formation of fluorine-substituted benzenes: A theoretical study. <b>2009</b> , 130, 621-628		19	
1158	Testing the performance of density functionals for the calculation of energetic properties of complex-forming radical-molecule reactions. <b>2009</b> , 96, 233-244		4	
1157	Theoretical study on the hydrolytic deamination mechanism of adenosine. <i>Structural Chemistry</i> , <b>2009</b> , 20, 685-691	1.8	11	
1156	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. <b>2009</b> , 52, 444-455		10	
1155	Excess charge delocalization in organic and biological molecules: some theoretical notions. <b>2009</b> , 123, 29-40		8	
1154	Density functional methods in the study of oxygen transfer reactions. <b>2009</b> , 123, 59-66		3	
1153	Formation pathways of CH3SOH from CH3S(OH)CH3 in the presence of O2: a theoretical study. <b>2009</b> , 123, 93-103		5	
1152	Interaction between uracil nucleobase and phenylalanine amino acid: the role of sodium cation in stacking. <b>2009</b> , 124, 115-122		33	
1151	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. <b>2009</b> , 124, 197-215		4	
1150	Chlorination of ammonia and aliphatic amines by Cl2: DFT study of medium and substituent effects. <b>2009</b> , 22, 59-68		10	

1149	Substituent effects in the BaeyerVilliger reaction of acetophenones: a theoretical study. <b>2009</b> , 22, 643-649	23
1148	Modeling excitation properties of iridium complexes. <b>2009</b> , 22, 845-856	24
1147	Addition of sulfenic acids to monosubstituted acetylenes: a theoretical and experimental study. <b>2009</b> , 22, 1048-1057	21
1146	Implementation and benchmark tests of the DFTB method and its application in the ONIOM method. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 1841-1854	50
1145	The reaction of N2O5 with H3O+: A first-principles direct molecular dynamics study of acid-catalyzed reactive uptake of N2O5. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 2143-2148	4
1144	Formation of H2on an olivine surface: a computational study. <b>2009</b> , 393, 1403-1407	36
1143	A potential energy surface bifurcation in terpene biosynthesis. <b>2009</b> , 1, 384-9	91
1142	Enantioselective recognition of 1,2-aminoalcohols by the binol receptor dangled with pyrrole-2-carboxamide and its analogues. <b>2009</b> , 65, 666-671	15
1141	Reaction of Moore's ketene (tert-butylcyanoketene) with 1,3-cyclopentadiene and 1,3-cyclohexadiene. Is periselectivity controlled by the dynamic of trajectories at the bifurcation point?. <b>2009</b> , 65, 7504-7509	7
1140	Assessment of mixed basis set and ONIOM methods on the activation energy of ring opening reactions of substituted cyclobutenes. <b>2009</b> , 893, 98-105	2
1139	Study on the Z/E thermal isomerization of acetaldehyde N,N-dimethylhydrazone in cyclohexane by density functional theory computations. <b>2009</b> , 893, 84-87	1
1138	Theoretical studies on bond dissociation energies for some pyridine N-oxide biological compounds by density functional theory and CBS-4M method. <b>2009</b> , 907, 126-130	11
1137	Computational study of the interaction of proflavine with d(ATATATAT)2 and d(GCGCGCGCGC)2. <b>2009</b> , 915, 86-92	22
1136	A partial exploration of the potential energy surfaces of SCN and HSCN: implications for the enzyme-mediated detoxification of cyanide. <b>2009</b> , 28, 183-6	4
1135	Kinetic studies of the reaction of atomic chlorine with chlorobenzene. <i>Chemical Physics Letters</i> , <b>2009</b> , 469, 266-269	4
1134	Reexamination of the reaction of 4-chlorophenol with hydroxyl radical. <i>Chemical Physics Letters</i> , 2009, 474, 62-66	22
1133	Molecular hydrogen encapsulation in spherophanes. <i>Chemical Physics Letters</i> , <b>2009</b> , 480, 225-230 2.5	5
1132	Theoretical studies on the kinetics and thermochemistry of the gas-phase addition and H-abstraction reactions of 4-picoline with OH radical. <i>Chemical Physics Letters</i> , <b>2009</b> , 480, 161-167	13

1131	What is the energy barrier for H2 dissociation on Group 13 sub-nanosized metal cluster to form dihydride? Density functional dependence study. <i>Chemical Physics Letters</i> , <b>2009</b> , 482, 15-19	2.5	8
1130	Charge carrier mobility in sulphonated and non-sulphonated Ni phthalocyanines: experiment and quantum chemical calculations. <b>2009</b> , 72, 385-395		20
1129	"Mindless" DFT Benchmarking. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 993-1003	6.4	191
1128	Ab initio kinetic simulation of gas-phase experiments: tautomerization of cytosine and guanine. <b>2009</b> , 113, 6140-50		50
1127	On the relative preference of enamine/iminium pathways in an organocatalytic Michael addition reaction. <b>2009</b> , 4, 714-24		24
1126	Comparative DFT study on the $\Box$ -glycosidic bond in reactive species of galactosyl diphosphates. <b>2009</b> , 63,		24
1125	Influence of alkoxyl substituent on 4,6-diphenyl-2,2'-bipyridine ligand on photophysics of cyclometalated platinum(II) complexes: admixing intraligand charge transfer character in low-lying excited states. <b>2009</b> , 48, 2407-19		63
1124	Stepwise hydration of protonated carbonic acid: a theoretical study. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 12260-75	2.8	24
1123	Unexpected Trimerization of Pyrazine in the Coordination Sphere of Low-Valent Titanocene Fragments. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2044-9	6.4	12
1122	Hydrogen abstraction from deoxyribose by a neighboring 3'-uracil peroxyl radical. <b>2009</b> , 113, 6574-8		7
1121	The remarkable cis effect in the ene reactions of nitrosocarbonyl intermediates. <i>Journal of Organic Chemistry</i> , <b>2009</b> , 74, 2301-10	4.2	18
1120	Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 324-33	6.4	283
1119	Mechanistic and kinetic studies on the homogeneous gas-phase formation of PCDD/Fs from 2,4,5-trichlorophenol. <b>2009</b> , 43, 4068-75		80
1118	DFT Study on the Propagation Kinetics of Free-Radical Polymerization of ∃-Substituted Acrylates. <b>2009</b> , 42, 3033-3041		66
1117	An analysis of the different behavior of DNA and RNA through the study of the mutual relationship between stacking and hydrogen bonding. <b>2009</b> , 113, 4907-14		42
1116	Benzene-water (BZWn (n = 1-10)) clusters. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 13845-52	2.8	86
1115	Comparison of isoelectronic 8-HO-G and 8-NH2-G derivatives in redox processes. <b>2009</b> , 131, 15895-902		10
1114	Non-Hermitian Multiconfiguration Molecular Mechanics. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 1454-61	6.4	15

## (2009-2009)

1113	Mechanism and thermal rate constants for the complete series reactions of chlorophenols with H. <b>2009</b> , 43, 4105-12		61
1112	Benchmark Data for Noncovalent Interactions in HCOOH Benzene Complexes and Their Use for Validation of Density Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2726-33	6.4	29
1111	Raman spectroscopy study and first-principles calculations of the interaction between nucleic acid bases and carbon nanotubes. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 3621-9	2.8	46
1110	Thermochemical kinetics for multireference systems: addition reactions of ozone. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 5786-99	2.8	106
1109	Dispersion Corrected Atom-Centered Potentials for Phosphorus. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2930-4	6.4	15
1108	H/Br exchange in BBr3 by HSiR3 (R = H, CH3, C2H5): origin of DFT failures to describe a seemingly innocuous reaction barrier. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 12035-43	2.8	12
1107	An embedded cluster study of the formation of water on interstellar dust grains. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 5431-6	3.6	65
1106	Critical role of substrate conformational change in the proton transfer process catalyzed by 4-oxalocrotonate tautomerase. <b>2009</b> , 131, 2687-98		13
1105	Theoretical study of the dimerization of calcium carbonate in aqueous solution under natural water conditions. <b>2009</b> , 73, 5394-5405		16
1104	Density functional theory for transition metals and transition metal chemistry. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 10757-816	3.6	1248
1104		3.6	1248 410
	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical		
1103	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a		410
1103	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a ferrocene-azaquinoxaline dyad. 2009, 48, 11566-75  Electronic structure, binding energy, and solvation structure of the streptavidin-biotin		410
1103 1102 1101	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a ferrocene-azaquinoxaline dyad. 2009, 48, 11566-75  Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. 2009, 113, 9958-67  Correction for dispersion and Coulombic interactions in molecular clusters with density functional		410 50 25
1103 1102 1101 1100	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a ferrocene-azaquinoxaline dyad. 2009, 48, 11566-75  Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. 2009, 113, 9958-67  Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: application to polycyclic aromatic hydrocarbon clusters. 2009, 130, 244304  Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH	6.4	410 50 25 81
1103 1102 1101 1100	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a ferrocene-azaquinoxaline dyad. 2009, 48, 11566-75  Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. 2009, 113, 9958-67  Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: application to polycyclic aromatic hydrocarbon clusters. 2009, 130, 244304  Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH with unsaturated aldehydes. Physical Chemistry Chemical Physics, 2009, 11, 7649-58  Mononuclear ferrocenophane structural motifs with two thiourea arms acting as a dual binding site	6.4	410 50 25 81 78
1103 1102 1101 1100 1099 1098	Chemical Physics, 2009, 11, 10757-816  The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-21  A selective redox and chromogenic probe for Hg(II) in aqueous environment based on a ferrocene-azaquinoxaline dyad. 2009, 48, 11566-75  Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. 2009, 113, 9958-67  Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: application to polycyclic aromatic hydrocarbon clusters. 2009, 130, 244304  Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH with unsaturated aldehydes. Physical Chemistry Chemical Physics, 2009, 11, 7649-58  Mononuclear ferrocenophane structural motifs with two thiourea arms acting as a dual binding site for anions and cations. 2009, 48, 1566-76  A new open benzodipyrrole-based chemosensor for hydrogenpyrophosphate anion in aqueous	6.4	410 50 25 81 78 48

1095	Large two-photon absorption cross section: molecular tweezer as a new promising class of compounds for nonlinear optics. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 2592-6	3.6	42
1094	OH radical gas phase reactions with aliphatic ethers: a variational transition state theory study. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 13913-20	2.8	91
1093	A multiresponsive two-arm ferrocene-based chemosensor molecule for selective detection of mercury. <b>2009</b> , 2121-9		37
1092	Biogenesis of sesquiterpene lactones pseudoguaianolides from germacranolides: theoretical study on the reaction mechanism of terminal biogenesis of 8-epiconfertin. <i>Journal of Organic Chemistry</i> , <b>2009</b> , 74, 874-83	4.2	28
1091	Comparison of Global Reactivity Descriptors Calculated Using Various Density Functionals: A QSAR Perspective. <i>Journal of Chemical Theory and Computation</i> , <b>2009</b> , 5, 2744-53	6.4	101
1090	Anchoring the potential energy surface of the diacetylene dimer. <b>2009</b> , 107, 923-928		7
1089	Intermolecular interaction-controlled tuning of the two-photon absorption of fullerene bound in a buckycatcher. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 5485-8	2.8	38
1088	Assessment of the accuracy of theoretical methods for calculating (27)Al nuclear magnetic resonance shielding tensors of aquated aluminum species. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 5138-43	2.8	20
1087	Reaction of hydrated electrons with guanine derivatives: tautomerism of intermediate species. <b>2009</b> , 113, 2170-6		11
1086	Multichannel RRKM-TST and direct-dynamics VTST study of the reaction of hydroxyl radical with furan. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 2838-46	2.8	36
1085	Fluorine substituent effects on dihydrogen bonding of transition metal hydrides. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 7231-40	3.6	10
1084	Localized orbital corrections for the calculation of barrier heights in density functional theory. Journal of Chemical Theory and Computation, <b>2009</b> , 5, 2996-3009	6.4	19
1083	Modelling doped (Ni, Pd, Pt) sulfur-nitrolic systems as new motifs for storage of hydrogen. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 11054-9	3.6	12
1082	A DFT study of carbon monoxide adsorption on a Si4 nano-cluster. <b>2009</b> , 107, 1805-1810		4
1081	Atomization energies of the carbon clusters C n (n = $210$ ) revisited by means of W4 theory as well as density functional, Gn, and CBS methods. <b>2009</b> , 107, 977-990		37
1080	Metal-histidine-glutamate as a regulator of enzymatic cycles: a case study of carbonic anhydrase. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 374-83	3.6	11
1079	Theoretical study of the gas-phase ozonolysis of beta-pinene (C10H16). <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 5643-56	3.6	76
1078	Nucleophile-dependent regioselective ring opening of 2-substituted N,N-dibenzylaziridinium ions: bromide versus hydride. <b>2009</b> , 2508-10		33

## (2010-2009)

1077	Dispersion-corrected DFT calculations on C(60)-porphyrin complexes. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 4365-74	3.6	23
1076	Orthogonal non-covalent binding forces in solid state supramolecular herringbone-shaped "interlocked dimers". Pseudopolymorphism in [(ppy)Pd(mu-pz)](2) (ppy = 2-(2-pyridyl)phenyl, pz = pyrazol-1-yl) complex. <b>2009</b> , 9625-36		28
1075	The gas-phase ozonolysis of beta-caryophyllene (C(15)H(24)). Part II: A theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2009</b> , 11, 4173-83	3.6	58
1074	Gas-phase reaction between calcium monocation and fluoromethane: Analysis of the potential energy hypersurface and kinetics calculations. <b>2009</b> , 131, 144309		8
1073	Reliable Electronic Structure Computations for Weak Noncovalent Interactions in Clusters. <b>2009</b> , 39-90		24
1072	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> , <b>2009</b> , 74, 96-101	4.2	14
1071	Hydroxyl radical initiated oxidation of s-triazine: hydrogen abstraction is faster than hydroxyl addition. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 8596-606	2.8	25
1070	Ammonia-water cation and ammonia dimer cation. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 6859-64	2.8	19
1069	pi Complexes in benzidine rearrangement. <b>2009</b> , 7, 4631-40		17
1068	What is the mechanism of amine conjugate additions to pyrazole crotonate catalyzed by thiourea catalysts?. <b>2009</b> , 7, 483-7		20
1067	The Baeyer-Villiger reaction: solvent effects on reaction mechanisms. <b>2009</b> , 7, 3682-90		66
1066	Imidazole-annelated ferrocene derivatives as highly selective and sensitive multichannel chemical probes for Pb(II) cations. <i>Journal of Organic Chemistry</i> , <b>2009</b> , 74, 4787-96	4.2	89
1065	Infrared spectra of SF6(-) $\times$ HCOOH $\times$ Ar(n) (n = 0-2): infrared triggered reaction and Ar-induced reactive inhibition. <b>2009</b> , 130, 174302		6
1064	Theoretical study of CH4-CH4, CHF3-CH4, CH4-H2O, and CHF3-H2O dimers. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 14818-23	2.8	29
1063	Modeling and spectral simulation of matrix-isolated molecules by density functional calculations: a case study on formic acid dimer. <b>2010</b> , 133, 214502		12
1062	Hydrogen Bonding and Proton Transfer in ionized DNA Base Pairs, Amino Acids and Peptides. <b>2010</b> , 219	9-243	5
1061	Computational Simulation of the Terminal Biogenesis of Sesquiterpenes: The Case of 8-Epiconfertin. <b>2010</b> , 623-642		1
1060	Computational explorations of mechanisms and ligand-directed selectivities of copper-catalyzed Ullmann-type reactions. <b>2010</b> , 132, 6205-13		294

1059	Mutual relationship between stacking and hydrogen bonding in DNA. Theoretical study of guanine-cytosine, guanine-5-methylcytosine, and their dimers. <b>2010</b> , 114, 10217-27	68
1058	A Theoretical Study of the Mechanism of the Desymmetrization of Cyclic meso-Anhydrides by Chiral Amino Alcohols. <b>2010</b> , 2, 1122-1129	17
1057	Mechanism of chain termination in lipid peroxidation by carotenes: a theoretical study. <b>2010</b> , 114, 16948-58	13
1056	Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate. <b>2010</b> , 43, 5602-5610	33
1055	Quantum chemical prediction of redox reactivity and degradation pathways for aqueous phase contaminants: an example with HMPA. <b>2010</b> , 44, 5868-74	17
1054	Theoretical study of the competitive decomposition and isomerization of 1-hexyl radical. <b>2010</b> , 126, 87-98	16
1053	A theoretical investigation on the spectroscopic properties and photosensitizing capability of 5, 10, 15, 20-tetraphenyl-26,28-diheterosapphyrins with two O, S, or Se Atoms. <b>2010</b> , 127, 475-484	15
1052	DFT studies on the Eglycosidase catalytic mechanism: The deglycosylation step. <b>2010</b> , 946, 125-133	21
1051	Theoretical studies on the gas-phase pyrolysis of 2-trimethylsilylethanol. <b>2010</b> , 941, 127-132	1
1050	Theoretical study on mechanism for O3-initiated atmospheric oxidation reaction of Etaryophyllene. <b>2010</b> , 947, 68-75	16
1049	Hydrogen-mediated Stone-Wales isomerization of dicyclopenta[de,mn]anthracene. <i>Journal of Molecular Modeling</i> , <b>2010</b> , 16, 1519-27	4
1048	Hydrogen bonding nature between calix[6]arene and piperidine/triethylamine. 2010, 66, 67-73	4
1047	Electron delocalization and aromaticity variations in the stacked nucleic acid base pairs. <i>Structural Chemistry</i> , <b>2010</b> , 21, 1069-1078	9
1046	Exploration of density functional methods for one-electron reduction potential of nitrobenzenes. <b>2010</b> , 31, 144-50	25
1045	A theoretical study on the catalytic mechanism of Mus musculus adenosine deaminase. <b>2010</b> , 31, 2238-47	3
1044	Comparison of aromatic NH	95
1043	A Selective Chromogenic and Fluorescent Molecular Probe for YbIII Based on a Bichromophoric Azadiene. <b>2010</b> , 2010, 697-703	10
1042	Systematic Study of Halide-Induced Ring Opening of 2-Substituted Aziridinium Salts and Theoretical Rationalization of the Reaction Pathways. <i>European Journal of Organic Chemistry</i> , <b>2010</b> , 3.2 2010, 4920-4931	58

1041	Selective metal-cation recognition by [2.2]ferrocenophanes: the cases of zinc- and lithium-sensing. <b>2010</b> , 16, 1532-42		37	
1040	Hydroxylation and ring-opening mechanism of an unusual flavoprotein monooxygenase, 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase: a theoretical study. <b>2010</b> , 16, 2557-66		8	
1039	First-principles prediction of nucleophilicity parameters for pi nucleophiles: implications for mechanistic origin of Mayr's equation. <b>2010</b> , 16, 2586-98		32	
1038	Origin of stability in branched alkanes. <b>2010</b> , 16, 6942-9		38	
1037	Asymmetric phase-transfer-catalyzed intramolecular N-alkylation of indoles and pyrroles: a combined experimental and theoretical investigation. <b>2010</b> , 16, 12462-73		54	
1036	Tunneln von Wasserstoffatomen kann zur Bildung von H2 im Weltraum beitragen. <b>2010</b> , 122, 7508-7511		9	
1035	Hydrogen-atom tunneling could contribute to H2 formation in space. <b>2010</b> , 49, 7350-2		64	
1034	Vibrational spectroscopy: can density functional theory cope with highly electronegative atoms?. <b>2010</b> , 77, 942-7		1	
1033	Solid state conformational preferences of the {M(EXPX)}2 core (X = O, S) in transition metal complexes. <i>Journal of Molecular Structure</i> , <b>2010</b> , 968, 52-58	4	3	
1032	Structural characterization of triorganotin(IV) complexes with sodium fusidate and DFT calculations. <b>2010</b> , 695, 1405-1413		6	
1031	Mechanistic elucidation of ketenimine <b>B</b> utynoate cycloaddition reaction: role of biradical intermediates in isotopomeric purity of benzyl (1,1a,6,6a-13C4)-6-methyl anthranilic ester. <b>2010</b> , 66, 3855-3860		11	
1030	A new bis(pyrenyl)azadiene-based probe for the colorimetric and fluorescent sensing of Cu(II) and Hg(II). <b>2010</b> , 66, 3662-3667		74	
1029	Evaluation of Density Functionals, SCC-DFTB, Neglect of Diatomic Differential Overlap (NDDO) Models and Molecular Mechanics Methods for Prolyl-Leucyl-Glycinamide (PLG) and Structural Derivatives. <b>2010</b> , 944, 76-82		1	
1028	Mechanism study on OH-initiated atmospheric degradation of the organophosphorus pesticide chlorpyrifos. <b>2010</b> , 952, 8-15		15	
1027	CN bond dissociation energies: An assessment of contemporary DFT methodologies. <b>2010</b> , 961, 97-100		20	
1026	Assessment of density functional methods for the study of olefin metathesis catalysed by ruthenium alkylidene complexes. <i>Chemical Physics Letters</i> , <b>2010</b> , 493, 273-278	.5	58	
1025	A practical implementation of semi-classical transition state theory for polyatomics. <i>Chemical Physics Letters</i> , <b>2010</b> , 499, 9-15	.5	81	
1024	Selectivity in radical alkylation of substituted pyrroles. <i>International Journal of Quantum Chemistry</i> , <b>2010</b> , 110, 697-705	.1	8	

1023	Theoretical calculations of structures, energetics, and kinetics of O (3P) + CH3OH reactions. <i>International Journal of Quantum Chemistry</i> , <b>2010</b> , 110, NA-NA	2.1	2
1022	2. The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. <b>2010</b> , 19-38		4
1021	QUANTUM-CHEMICAL PREDICTION OF FORMATION ENTHALPY OF CYCLOALKANE. <b>2010</b> , 09, 155-166		
1020	Adsorption of carbon monoxide on Si x Ge4 $\mathbb{R}$ (x = 0 $\mathbb{R}$ ) nano-clusters: a hybrid meta density functional study. <b>2010</b> , 108, 1317-1327		6
1019	The assessment of density functionals for DNAprotein stacked and T-shaped complexes. <b>2010</b> , 88, 815-8	330	36
1018	Gradient-based multiconfiguration Shepard interpolation for generating potential energy surfaces for polyatomic reactions. <b>2010</b> , 132, 084109		18
1017	Theoretical Study of the HOCH2OOD HO2D HO2D HO2D HO2D HO2D HO2D HO2D		7
1016	Communications: Is quantum chemical treatment of biopolymers accurate? Intramolecular basis set superposition error (BSSE). <b>2010</b> , 132, 231101		34
1015	Density-functional based determination of intermolecular charge transfer properties for large-scale morphologies. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 11103-13	3.6	178
1014	Opposite regiospecific ring opening of 2-(cyanomethyl)aziridines by hydrogen bromide and benzyl bromide: experimental study and theoretical rationalization. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 453	<del>6</del> -41	53
1013	Thermochemical properties of exo-tricyclo[5.2.1.0(2,6)]decane (JP-10 jet fuel) and derived tricyclodecyl radicals. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 9545-53	2.8	37
1012	Mechanistic insight into the alcohol oxidation mediated by an efficient green [CuBr(2)(2,2'-bipy)]-TEMPO catalyst by density functional method. <b>2010</b> , 49, 9392-9		42
1011	Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrum-the role of pyrophosphate in manipulating pathways to monoterpenes. <b>2010</b> , 8, 4589-600		65
1010	Absorption spectra of riboflavina difficult case for computational chemistry. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 10234-42	2.8	20
1009	The inactivation of lipid peroxide radical by quercetin. A theoretical insight. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 7662-70	3.6	83
1008	THEORETICAL STUDY OF THE HYDROGEN BOND CHARACTER BETWEEN THE FNO AND HO2 RADICAL. <b>2010</b> , 09, 925-934		1
1007	Quantification of mutual trans influence of ligands in Pd(II) complexes: a combined approach using isodesmic reactions and AIM analysis. <b>2010</b> , 39, 815-22		43
1006	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 2872-87	6.4	892

## (2010-2010)

1005	The effects of perfluorination on carbohydrate-pi interactions: computational studies of the interaction of benzene and hexafluorobenzene with fucose and cyclodextrin. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 7959-67	3.6	23
1004	Computational Modeling of the Nitrile Stretching Vibration of 5-Cyanoindole in Water. <b>2010</b> , 1, 781-786		34
1003	Kinetic properties for the complete series reactions of chlorophenols with OH radicals-relevance for dioxin formation. <b>2010</b> , 44, 1399-404		70
1002	Substitution effects of diborane on the interaction with borazine (inorganic benzene). <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 5565-72	2.8	21
1001	Mechanism of the hydride transfer between Anabaena Tyr303Ser FNR(rd)/FNR(ox) and NADP+/H. A combined pre-steady-state kinetic/ensemble-averaged transition-state theory with multidimensional tunneling study. <b>2010</b> , 114, 3368-79		25
1000	On the assessment of some new meta-hybrid and generalized gradient approximation functionals for calculations of anharmonic vibrational frequency shifts in hydrogen-bonded dimers. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 4354-63	2.8	5
999	Computational simulation of the lifetime of the methoxymethyl cation in water. A simple model for a glycosyl cation: when is an intermediate an intermediate?. <b>2010</b> , 114, 5769-74		11
998	Hydrogen abstraction from n-butanol by the hydroxyl radical: high level ab initio study of the relative significance of various abstraction channels and the role of weakly bound intermediates. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 5558-64	2.8	35
997	Atomistic details of the Catalytic Mechanism of Fe(III)-Zn(II) Purple Acid Phosphatase. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 2424-33	6.4	32
996	Reaction-path dynamics calculations of the Cl + NH(3) hydrogen abstraction reaction: the role of the intermediate complexes. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 4418-26	2.8	13
995	Theoretical investigation on the stability of negatively charged formic acid clusters. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 6917-26	2.8	8
994	Phosphate mono- and diesterase activities of the trinuclear zinc enzyme nuclease P1insights from quantum chemical calculations. <b>2010</b> , 49, 6883-8		30
993	Conformational properties of the germacradienolide 6-epidesacetyllaurenobiolide by theory and NMR analyses. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 2139-46	4.2	7
992	Theoretical study of the structures and hydrogen-bond properties of new alternated heterocyclic compounds. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 6413-22	2.8	10
991	Computational Study of Carbonyl Sulphide Formation on Model Interstellar Dust Grains. <b>2010</b> , 114, 1892	2-1900	) 23
990	Quantum chemical and kinetic study on dioxin formation from the 2,4,6-TCP and 2,4-DCP precursors. <b>2010</b> , 44, 3395-403		74
989	Dioxin formations from the radical/radical cross-condensation of phenoxy radicals with 2-chlorophenoxy radicals and 2,4,6-trichlorophenoxy radicals. <b>2010</b> , 44, 6745-51		45
988	Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 7782-93	3.6	135

987	Intramolecular pi-pi stacking interactions in 2-substituted N,N-dibenzylaziridinium ions and their regioselectivity in nucleophilic ring-opening reactions. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 885-96	4.2	64
986	The Minnesota Density Functionals and their Applications to Problems in Mineralogy and Geochemistry. <b>2010</b> , 71, 19-37		29
985	The role of exact exchange in the description of $Cu(2+)-(H(2)O)(n)$ (n = 1-6) complexes by means of DFT methods. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 10857-63	2.8	40
984	Improved density functional description of the electrochemistry and structure-property descriptors of substituted flavins. <b>2010</b> , 114, 14907-15		30
983	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 3647-3663	6.4	8
982	Challenges posed to bornyl diphosphate synthase: diverging reaction mechanisms in monoterpenes. <b>2010</b> , 132, 6349-60		81
981	Benchmarking of DFT Functionals for the Hydrolysis of Phosphodiester Bonds. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 2281-92	6.4	62
980	Enzyme catalysis by hydrogen bonds: the balance between transition state binding and substrate binding in oxyanion holes. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 1831-40	4.2	86
979	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. <b>2010</b> , 29, 2040-2045		27
978	A highly diastereoselective synthesis of $\Box$ -hydroxy- $\Box$ mino acid derivatives via a Lewis acid catalyzed three-component condensation reaction. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 7099-106	4.2	23
977	What is the preferred structure of the Meisenheimer-Wheland complex between sym-triaminobenzene and 4,6-dinitrobenzofuroxan?. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 3761-5	4.2	13
976	Reinvestigation of the reaction of ethylene and singlet oxygen by the approximate spin projection method. Comparison with multireference coupled-cluster calculations. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 7967-74	2.8	37
975	Direct Dynamics Implementation of the Least-Action Tunneling Transmission Coefficient. Application to the CH4/CD3H/CD4 + CF3 Abstraction Reactions. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 3015-25	6.4	11
974	A System-Dependent Density-Based Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 1990-2001	6.4	118
973	Bond dissociation energies of organophosphorus compounds: an assessment of contemporary ab initio procedures. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 2864-73	2.8	27
972	Favored reaction mechanism of calcium-dependent phospholipase A(2). Insights from density functional exploration. <b>2010</b> , 114, 11584-93		5
971	Stabilization and structure calculations for noncovalent interactions in extended molecular systems based on wave function and density functional theories. <b>2010</b> , 110, 5023-63		666
970	Thermochemical benchmarking of hydrocarbon bond separation reaction energies: Jacob's ladder is not reversed!. <b>2010</b> , 108, 2655-2666		45

## (2010-2010)

969	[2 + 2] Photocycloaddition of 2(5H)-furanone to unsaturated compounds. insights from first principles calculations and transient-absorption measurements. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 4392-401	4.2	16	
968	Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones. <b>2010</b> , 8, 4884-91		56	
967	Kinetic and Mechanistic Study onp-Quinodimethane Formation in the Sulfinyl Precursor Route for the Polymerization of Poly(p-phenylenevinylene) (PPV). <b>2010</b> , 43, 7424-7433		25	
966	The mechanism of the Stevens and Sommelet-Hauser rearrangements. A theoretical study. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 3608-17	4.2	55	
965	A theoretical approach for accurate predictions of the enthalpies of formation of carotenes. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 12334-44	2.8	4	
964	Reaction free energies in organic solvents: comparing different quantum mechanical methods. <b>2010</b> , 36, 1197-1207		4	
963	Solvent Effects on Free Radical Polymerization Reactions: The Influence of Water on the Propagation Rate of Acrylamide and Methacrylamide. <b>2010</b> , 43, 827-836		42	
962	Importance of the nature of ∃-substituents in pyrrolidine organocatalysts in asymmetric Michael additions. <i>Journal of Organic Chemistry</i> , <b>2010</b> , 75, 7310-21	4.2	30	
961	Role of Chain Transfer Agents in Free Radical Polymerization Kinetics. 2010, 43, 1823-1835		144	
960	An enthalpic scale of hydrogen-bond basicity. 4. Carbon pi bases, oxygen bases, and miscellaneous second-row, third-row, and fourth-row bases and a survey of the 4-fluorophenol affinity scale.  Journal of Organic Chemistry, <b>2010</b> , 75, 4105-23	4.2	71	
959	Validation of density functional methods for the calculation of small gold clusters. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 10297-308	2.8	42	
958	Investigating behaviours of hydrogen in a tungsten grain boundary by first principles: from dissolution and diffusion to a trapping mechanism. <b>2010</b> , 50, 025016		158	
957	Rhodamines in the gas phase: cations, neutrals, anions, and adducts with metal cations. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 11710-4	3.6	22	
956	Quantum mechanical study of secondary structure formation in protected dipeptides. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 4678-85	3.6	6	
955	New 7-azaindole palladium and platinum complexes: crystal structures and theoretical calculations. In vitro anticancer activity of the platinum compounds. <b>2010</b> , 39, 3290-301		62	
954	Optical properties of protonated Rhodamine 19 isomers in solution and in the gas phase. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 14121-7	3.6	25	
953	A multifaceted ferrocene-benzobisimidazole derivative: fluorogenic probe for Pb(2+) and Zn(2+) cations and unconventional fluorescence behaviour towards Cu(2+) metal cations. <b>2010</b> , 39, 5429-31		27	
952	Folding oligomers of difluorinated thienylfurans: a DFT study. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 523-32	3.6	5	

951	A computational study of the threshold energies of the 1,2-FCl interchange reaction of chlorofluoroethanes. <b>2010</b> , 88, 1112-1117		9
950	Modelling the binding of HIV-reverse transcriptase and nevirapine: an assessment of quantum mechanical and force field approaches and predictions of the effect of mutations on binding. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 7117-25	3.6	26
949	A significant role of alkaline cations on the Reimer-Tiemann reaction. <b>2011</b> , 9, 5109-14		7
948	DFT study on the mechanism for the substitution of F(-) into Al(III) complexes in aqueous solution. <b>2011</b> , 40, 567-72		10
947	The taxadiene-forming carbocation cascade. <b>2011</b> , 133, 18249-56		43
946	A neutral Pt3 stack unsupported by any bridging ligand. <b>2011</b> , 40, 5159-61		20
945	Modeling proton transfer in imidazole-like dimers: a density functional theory study. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 2627-34	2.8	23
944	Deuterium enrichment of interstellar methanol explained by atom tunneling. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10767-74	2.8	48
943	The origin of regio- and enantioselectivity in the Rh/chiral 1,4-diene-catalyzed addition of phenylboronic acid to enones: insights from DFT. <b>2011</b> , 47, 10969-71		38
942	Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with (CH3)(x)NH+(4-x), $x = 0-4$ . Physical Chemistry Chemical Physics, <b>2011</b> , 13, 954-65	3.6	10
941	Mechanism of OH-initiated atmospheric oxidation of diethyl phthalate. <b>2011</b> , 89, 1419-1427		6
940	On the performance of density functional schemes for computing the static dipole polarizability of 4d transition-metal monohalides. <b>2011</b> , 109, 1439-1452		5
939	Polarized Molecular Orbital Model Chemistry. II. The PMO Method. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 857-867	6.4	24
938	Electronic structures and charge transport of stacked annelated Erithiophenes. <b>2011</b> , 115, 5113-20		28
937	Mechanism and direct kinetic study of the polychlorinated dibenzo-p-dioxin and dibenzofuran formations from the radical/radical cross-condensation of 2,4-dichlorophenoxy with 2-chlorophenoxy and 2,4,6-trichlorophenoxy. <b>2011</b> , 45, 643-50		40
936	Theoretical study on the electronic excitations of a porphyrin-polypyridyl ruthenium(II) photosensitizer. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 11988-97	2.8	14
935	Quantum chemical and theoretical kinetics study of the O(3P) + CS2 reaction. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 4263-9	2.8	6
934	A proposal for mitochondrial processing peptidase catalytic mechanism. <b>2011</b> , 133, 17824-31		33

933	Mechanism for OH-initiated degradation of 2,3,7,8-tetrachlorinated dibenzo-p-dioxins in the presence of O2 and NO/H2O. <b>2011</b> , 45, 4756-62		36
932	Quantifying water-mediated protein-ligand interactions in a glutamate receptor: a DFT study. <b>2011</b> , 115, 7085-96		16
931	Mechanical and kinetic studies of the formation of polyhalogenated dibenzo-p-dioxins from hydroxylated polybrominated diphenyl ethers and chlorinated derivatives. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 13489-97	2.8	15
930	The Accuracy of Density Functional Theory in the Description of Cation-Land E-Hydrogen Bond Interactions. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2059-67	6.4	35
929	Thermal decomposition of 2-butanol as a potential nonfossil fuel: a computational study. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 2837-46	2.8	31
928	RI-MP2 and MPWB1K Study of EAnion-EComplexes: MPWB1K Performance and Some Additivity Aspects. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 3012-8	6.4	24
927	A theoretical rationale for why azetidine has a faster rate of formation than oxetane in TC(6-4) photoproducts. <b>2011</b> , 115, 9681-6		9
926	Ab initio study of the F + CH3NHNH2 reaction mechanism. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 805-14	2.8	5
925	Modeling Charge Resonance in Cationic Molecular Clusters: Combining DFT-Tight Binding with Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 44-55	6.4	42
924	Role of carbocation's flexibility in sesquiterpene biosynthesis: computational study of the formation mechanism of terrecyclene. <i>Journal of Organic Chemistry</i> , <b>2011</b> , 76, 1572-7	4.2	16
923	Charge transport properties of stacking bisindenoanthrazolines: DFT studies. <b>2011</b> , 115, 8409-16		10
922	Developing a computational model that accurately reproduces the structural features of a dinucleoside monophosphate unit within B-DNA. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 16373-8	3 <sup>3.6</sup>	41
921	Diffusion and aggregation of sodium fluorescein in aqueous solutions. <b>2011</b> , 115, 12896-904		63
920	Stability and aromaticity of charged MBius[4n]annulenes. <i>Journal of Organic Chemistry</i> , <b>2011</b> , 76, 35-41	4.2	18
919	The calculation of intermolecular interaction energies. <b>2011</b> , 107, 148		24
918	Accuracy of Density Functionals in the Prediction of Electronic Proton Affinities of Amino Acid Side Chains. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 3898-908	6.4	35
917	2-Chloroethylisocyanate. Thermal decomposition and spectroscopic properties. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 8608-15	2.8	4
916	Fluorescence and visual sensing of nitroaromatic explosives using electron rich discrete fluorophores. <b>2011</b> , 21, 9130		192

915	Multichannel RRKM-TST and CVT rate constant calculations for reactions of CH2OH or CH3O with HO2. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 3291-300	2.8	15
914	A QM/QM investigation of the hUNG2 reaction surface: the untold tale of a catalytic residue. <b>2011</b> , 50, 4218-27		25
913	Revisiting the effects of sequence and structure on the hydrogen bonding and Estacking interactions in nucleic acids. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 12800-8	2.8	15
912	Synthesis of 3-methoxyazetidines via an aziridine to azetidine rearrangement and theoretical rationalization of the reaction mechanism. <i>Journal of Organic Chemistry</i> , <b>2011</b> , 76, 2157-67	4.2	36
911	Performance of Density Functional Theory and Mller-Plesset Second-Order Perturbation Theory for Structural Parameters in Complexes of Ru. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 232	25: <del>3</del> 2	116
910	Computational calculations of pKa values of imidazole in Cu(II) complexes of biological relevance. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 7852-61	3.6	51
909	Kinetics and thermodynamics of limonene ozonolysis. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10911-	<b>-9</b> .8	29
908	Prediction of contaminant persistence in aqueous phase: a quantum chemical approach. <b>2011</b> , 45, 2236	-42	20
907	Infrared Spectroscopy of the Ag+⊞2 Complex: Exploring the Connection Between Vibrational Band-Shifts and Binding Energies. <b>2011</b> , 2, 719-724		21
906	Peripheral and Structural Effects on the Band Gap of AcceptorDonor Type Conducting Polymers Containing Pendant Bisfulleroid Groups. <b>2011</b> , 115, 25007-25018		3
905	The Mathematics and Topology of Fullerenes. 2011,		24
904	A theoretical study on structural, spectroscopic and energetic properties of acetamide clusters [CH3CONH2] (n=1-15). <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 15211-20	3.6	34
903	Mechanisms of reductive eliminations in square planar Pd(II) complexes: nature of eliminated bonds and role of trans influence. <b>2011</b> , 50, 8085-93		45
902	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. <b>2011</b> , 9, 6616-22		41
901	Calculations on the structure and spectral properties of cytochrome c551 using DFT and ONIOM methods. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 2866-76	2.8	7
900	PO bond dissociation enthalpies: High-level ab initio and DFT study. <b>2011</b> , 968, 1-7		8
899	Influence of the structure of the diphosphine ligand on the copper fluoride and copper hydride complexes. <b>2011</b> , 970, 23-29		6
898	Accurate prediction of experimental free energy of activation barriers for the aliphatic-Claisen rearrangement through DFT calculations. <b>2011</b> , 976, 167-182		13

897	DFT characterization of the first step of methyl acrylate polymerization: Performance of modern functionals in the complete basis limit. <b>2011</b> , 978, 88-97		10
896	Validation of electronic structure methods for isomerization reactions of large organic molecules. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13683-9	3.6	67
895	How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. <b>2011</b> , 9, 689-700		186
894	Reactivity of activated versus nonactivated 2-(bromomethyl)aziridines with respect to sodium methoxide: a combined computational and experimental study. <i>Journal of Organic Chemistry</i> , <b>2011</b> , 76, 8698-709	4.2	15
893	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 3567-77	6.4	322
892	Interaction of metal ions with biomolecular ligands: how accurate are calculated free energies associated with metal ion complexation?. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 11394-402	2.8	36
891	Theoretical determination of one-electron redox potentials for DNA bases, base pairs, and stacks. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 4804-10	2.8	63
890	Gas phase enthalpies of formation, isomerization, and disproportionation of mono-through tetra-substituted tetrahedranes: A G4MP2/G4 theoretical study. <b>2011</b> ,		
889	A New Series of Organocatalysts for Diels-Alder Cycloaddition Reactions and Theoretical Analysis. <b>2011</b> , 15, 3514-3522		3
888	An introduction to quantum chemical methods applied to drug design. <b>2011</b> , 3, 1061-78		
888	An introduction to quantum chemical methods applied to drug design. <b>2011</b> , 3, 1061-78  5,5-Diaryldipyrromethanes: syntheses and anion binding properties. <b>2011</b> , 52, 5995-5999		8
			8
887	5,5-Diaryldipyrromethanes: syntheses and anion binding properties. <b>2011</b> , 52, 5995-5999  A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction:	-135.8	
887 886	5,5-Diaryldipyrromethanes: syntheses and anion binding properties. <b>2011</b> , 52, 5995-5999  A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction: Evidence from DFT calculations. <b>2011</b> , 345, 37-43	-135.8	20
887 886 885	5,5-Diaryldipyrromethanes: syntheses and anion binding properties. <b>2011</b> , 52, 5995-5999  A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction: Evidence from DFT calculations. <b>2011</b> , 345, 37-43  Conformational and NMR analysis on cis 1,3-indanediol. <i>Journal of Molecular Structure</i> , <b>2011</b> , 1002, 151-Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study.	-13 <b>5.</b> ₿	20
887 886 885	5,5-Diaryldipyrromethanes: syntheses and anion binding properties. 2011, 52, 5995-5999  A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction: Evidence from DFT calculations. 2011, 345, 37-43  Conformational and NMR analysis on cis 1,3-indanediol. <i>Journal of Molecular Structure</i> , 2011, 1002, 151-Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. 2011, 52, 5503-5512  Conventional and density-fitting local Miler Plesset theory calculations of C60 and its endohedral		20 2 20
887 886 885 884 883	5,5-Diaryldipyrromethanes: syntheses and anion binding properties. 2011, 52, 5995-5999  A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction: Evidence from DFT calculations. 2011, 345, 37-43  Conformational and NMR analysis on cis 1,3-indanediol. <i>Journal of Molecular Structure</i> , 2011, 1002, 151-Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. 2011, 52, 5503-5512  Conventional and density-fitting local MllerPlesset theory calculations of C60 and its endohedral H2@C60 and 2H2@C60 complexes. <i>Chemical Physics Letters</i> , 2011, 513, 236-240  Structure and bonding in polybromide anions Br(Br2)n (n=18). <i>Chemical Physics Letters</i> , 2011,	2.5	20 2 20 8

879	Chemical mechanism and kinetics study on the ocimene ozonolysis reaction in atmosphere. <b>2011</b> , 45, 6197-6203		11
878	New insights on the molecular features and electrophysiological properties of dinotefuran, imidacloprid and acetamiprid neonicotinoid insecticides. <b>2011</b> , 19, 7623-34		27
877	A quantum theoretical study of reactions of methyldiazonium ion with DNA base pairs. <b>2011</b> , 388, 31-3	7	6
876	A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 6670-88	3.6	1347
875	Can the Gibbs free energy of adsorption be predicted efficiently and accurately: an M05-2X DFT study. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 2423-30	2.8	36
874	Coordination of methanol clusters to benzene: a computational study. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 10556-64	2.8	24
873	Quantum mechanical investigations of organocatalysis: mechanisms, reactivities, and selectivities. <b>2011</b> , 111, 5042-137		429
872	How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 1667-76	6.4	140
871	Density functional theory with London dispersion corrections. <b>2011</b> , 1, 211-228		1645
870	A new photoproduct of 5-methylcytosine and adenine: a theoretical study. <i>Structural Chemistry</i> , <b>2011</b> , 22, 951-955	1.8	3
869	On the mechanism of the N-glycosydic bond hydrolysis of 2?-deoxyguanosine: insights from first principles calculations. <b>2011</b> , 128, 619-626		14
868	How accurate are electronic structure methods for actinoid chemistry?. <b>2011</b> , 129, 657-666		58
867	A computational study on the relationship between formation and electrolytic dissociation of carbonic acid. <b>2011</b> , 130, 909-918		9
866	Theoretical study on photophysical properties of 2,1,3-benzothiadiazole-based star-shaped molecules. <b>2011</b> , 129, 833-845		5
865	Applications and validations of the Minnesota density functionals. <i>Chemical Physics Letters</i> , <b>2011</b> , 502, 1-13	2.5	568
864	Computational study of the one- and two-photon absorption properties of macrocyclic thiophene derivatives. <b>2011</b> , 91, 248-257		7
863	Infrared matrix-isolation spectroscopy of trifluoroacetic acid hydrates. <b>2011</b> , 382, 52-57		22
862	Cyclization tendencies in the free radical polymerization of allyl acrylate derivatives: A computational study. <b>2011</b> , 49, 2474-2483		8

## (2011-2011)

861	A computational study of C?X (X = H, C, F, Cl) bond dissociation enthalpies (BDEs) in polyhalogenated methanes and ethanes. <b>2011</b> , 24, 65-73		15
860	Is the neutral Knoevenagel reaction initiated by the carbanion formation?. <b>2011</b> , 24, 663-671		6
859	Electron correlation and the stability of substituted alkenes. <b>2011</b> , 24, 1222-1228		4
858	Is fullerene C60 large enough to host an aromatic molecule?. <i>International Journal of Quantum Chemistry</i> , <b>2011</b> , 111, 2398-2405	2.1	9
857	Interaction of the Mn2+, Co2+, Ni2+, and Zn2+ with prion protein HGGGW pentapeptide model. <i>International Journal of Quantum Chemistry</i> , <b>2011</b> , 111, 1152-1162	2.1	8
856	Organocatalytic Enantioselective Michael-Addition of Malonic Acid Half-Thioesters to ENitroolefins: From Mimicry of Polyketide Synthases to Scalable Synthesis of EAmino Acids. <b>2011</b> , 353, 3196-3202		119
855	Hydrogen motion in proton sponge cations: a theoretical study. <b>2011</b> , 12, 1118-29		18
854	Benchmarking density functional methods against the S66 and S66x8 datasets for non-covalent interactions. <b>2011</b> , 12, 3421-33		252
853	A method to calculate the one-electron reduction potentials for nitroaromatic compounds based on gas-phase quantum mechanics. <b>2011</b> , 32, 226-39		31
852	A comparison of the behavior of functional/basis set combinations for hydrogen-bonding in the water dimer with emphasis on basis set superposition error. <b>2011</b> , 32, 1519-27		109
851	Toward robust computational electrochemical predicting the environmental fate of organic pollutants. <b>2011</b> , 32, 2195-203		37
850	Intramolecular hydrogen bond energy and cooperative interactions in $\Box$ -, $\Box$ and $\Box$ - conformers. <b>2011</b> , 32, 2996-3004		34
849	Accurate prediction of the enthalpies of formation for xanthophylls. 2011, 32, 3175-87		2
848	Structural features and hydrogen-bond properties of galanthamine and codeine: an experimental and theoretical study. <b>2011</b> , 17, 11637-49		12
847	Competitive reactions of organophosphorus radicals on coke surfaces. <b>2011</b> , 17, 12027-36		21
846	Cooperative supramolecular polymerization and amplification of chirality in C3-symmetrical OPE-based trisamides. <b>2011</b> , 17, 7755-9		67
845	The diiodine basicity scale: toward a general halogen-bond basicity scale. <b>2011</b> , 17, 10431-44		109
844	Ruthenium(IV)-catalyzed isomerization of the C=C bond of o-allylic substrates: a theoretical and experimental study. <b>2011</b> , 17, 10583-99		42

843	A through-space charge transfer mechanism for explaining the oxidation of 2-chlorophenol on a tetrasulphonated nickel(III) phthalocyanine. <b>2011</b> , 963, 161-167		6
842	Kinetics and thermochemistry of the gas-phase reactions of 4-ethylpyridine with OH radical: A DFT study. <b>2011</b> , 965, 268-274		12
841	Theoretical study on the electronic structure and the absorption spectra of complexes of C60 and C59N with Extended derivatives of tetrathiafulvalene. <b>2011</b> , 965, 168-175		10
840	Theoretical Investigation of the gas-phase reactions of (CF3)2CHOCH3 with OH Radical. <i>Chemical Physics Letters</i> , <b>2011</b> , 502, 23-28	2.5	31
839	Density functional investigation of metal encapsulated X@C12Si8 heterofullerene (X=Li+, Na+, K+, Be2+, Mg2+, Ca2+, Al3+, Ga3+). <b>2011</b> , 406, 1471-1476		6
838	Influence of diosgenin structure on the polymerization kinetics of acrylamide: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , <b>2011</b> , 985, 34-47	3.4	2
837	Stress effects on stability and diffusion of H in W: A first-principles study. <b>2011</b> , 269, 1731-1734		30
836	Bond dissociation energies of ligands in square planar Pd(II) and Pt(II) complexes: An assessment using trans influence. <b>2011</b> , 696, 2086-2092		19
835	Highly energetic nitrogen species: reliable energetics via the correlation consistent Composite Approach (ccCA). <b>2011</b> , 186, 583-9		52
834	Trajectory calculations of OH radical- and Cl atom-initiated reaction of glyoxal: atmospheric chemistry of the HC(O)CO radical. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 6296-304	3.6	10
833	Adaptive integration grids in instanton theory improve the numerical accuracy at low temperature. <b>2011</b> , 134, 184107		62
832	Theoretical study of nitrogen monoxide adsorption on small Si x (x = $3B$ ) clusters. <b>2011</b> , 109, 229-237		5
831	Density functional study of multiplicity-changing valence and Rydberg excitations of p-block elements: delta self-consistent field, collinear spin-flip time-dependent density functional theory (DFT), and conventional time-dependent DFT. <b>2011</b> , 135, 044118		55
830	van der Waals density functional study of energetic, structural, and vibrational properties of small water clusters and ice Ih. <b>2011</b> , 84,		42
829	COMPARATIVE QUANTUM STUDY ON TERT-BUTYL RADICAL AND CATION. <b>2011</b> , 10, 325-348		4
828	Benchmark of density functional theory methods on the prediction of bond energies and bond distances of noble-gas containing molecules. <b>2011</b> , 134, 244110		46
827	Infrared absorption of trans-1-chloromethylallyl and trans-1-methylallyl radicals produced in photochemical reactions of trans-1,3-butadiene and Cl2 in solid para-hydrogen. <b>2012</b> , 137, 084310		20
826	Analysis of the Heyd-Scuseria-Ernzerhof density functional parameter space. <b>2012</b> , 136, 204117		112

S?O homolytic bond dissociation enthalpies in sulfones: high-level ab initio and DFT study. 2012, 33, 541-559 1 825 824 Designing Fullerene Separation Materials: A Theoretical Study. 2012, 20, 72-84 Constructing Potential Energy Surfaces for Polyatomic Systems: Recent Progress and New 823 16 Problems. **2012**, 2012, 1-19 Matrix-isolation infrared studies of 1:1 molecular complexes containing chloroform (CHCl3) and 822 26 Lewis bases: seamless transition from blue-shifted to red-shifted hydrogen bonds. 2012, 137, 014505 Mechanisms and kinetics for the thermal decomposition of 2-azido-N,N-dimethylethanamine 821 2.8 12 (DMAZ). Journal of Physical Chemistry A, 2012, 116, 3561-76 Theoretical assessment of the viability of thermal [2+2] processes for formation of plumisclerin A. 820 11 2012, 53, 6919-6922 Performance of recent and high-performance approximate density functionals for time-dependent 819 density functional theory calculations of valence and Rydberg electronic transition energies. 2012, 145 137, 244104 Elucidation of Strong Cooperative Effects Caused by Dispersion Interactions in a 818 Recognition-Mediated Diels-Alder Reaction. Journal of Chemical Theory and Computation, 2012, 8, 5064-714 9 Electron density distribution in endohedral complexes of fullerene CDcalculated based on the 817 4 Gauss law. 2012, 52, 1193-8 Theoretical studies on the kinetics and mechanism of the gas-phase reactions of CHF(2)OCHF (2) 816 34 with OH radicals. Journal of Molecular Modeling, 2012, 18, 4239-47 Mapping of the interaction sites of galanthamine: a quantitative analysis through pairwise 815 1 potentials and quantum chemistry. 2012, 26, 1111-26 S=O homolytic bond dissociation enthalpies in sulfoxides. 2012, 38, 1791-1806 814 813 An accurate theoretical study of energy barriers of alkaline hydrolysis of carboxylic esters. 2012, 38, 2175-219010 On the Performance of Local Density Approximation in Describing the Adsorption of Electron 812 32 Donating/Accepting Molecules on Graphene. 2012, 406, 78-85 Quantitative estimation of the strength of specific interactions in polyurethane elastomers, and 811 21 their effect on structure and properties. 2012, 48, 1854-1865 Quasi-classical trajectory and direct-dynamics CVT study on the initiation steps of methanol 810 combustion. 2012, 9, 957-969 Density functional theory for NIMO2 bond dissociation energies of N-nitroacylamide compounds in 809 acetonitrile Theoretical method assessment and prediction. 2012, 90, 526-533 Theoretical calculations on carbocations involved in the biosynthesis of bergamotenes and related 808 12 terpenes--the same and not the same. 2012, 48, 1571-3

807	Quantitative integral cross sections for the H + CO2 -> OH + CO reaction from a density functional theory-based potential energy surface. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 16699-702	3.6	7
806	Theoretical study on the chemical formation mechanism of a Emyrcene ozonolysis reaction under atmospheric conditions. <b>2012</b> , 90, 708-715		5
805	A theoretical study of the ring size effect on one- and two-photon absorption properties of macrocyclic thiophene derivatives. <b>2012</b> , 36, 947		5
804	Electrophilic reactivity of tetrabromorhodamine 123 is bromine induced: convergent interpretation through complementary molecular descriptors. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 11938-45	2.8	2
803	Click-chemistry approach to azacycloalkene monosulfonyl diamines: synthesis and computational analysis of the reaction mechanism. <b>2012</b> , 2, 10652		22
802	Tunneling and conformational flexibility play critical roles in the isomerization mechanism of vitamin D. <b>2012</b> , 134, 346-54		28
801	Theoretical investigations of spin-orbit coupling and kinetics in reaction W + NH3 -> N?WH3. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 2583-90	2.8	9
800	Combined effects of Estacking and hydrogen bonding on the (N1) acidity of uracil and hydrolysis of 2'-deoxyuridine. <b>2012</b> , 116, 2622-32		14
799	Effects of alkyl groups in the rate determining step of the Baeyer-Villiger reaction of phenyl alkyl ketones: a quantum chemistry study. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 7712-7	2.8	4
798	Computational study of Xe(OH)4, XeO(OH)3(-), and XeO2(OH)2(2-). <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 10397-402	2.8	2
797	Anharmonic vibrational frequency shifts upon interaction of phenol+ with the open shell ligand O2. The performance of DFT methods versus MP2. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 1939-49	2.8	5
796	Benchmark Database for Ylidic Bond Dissociation Energies and Its Use for Assessments of Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2824-34	6.4	58
795	Mechanism and kinetic study on the OH-initiated degradation of 2,3,7,8-tetrachlorinated dibenzofuran in atmosphere. <b>2012</b> , 435-436, 53-60		11
794	A critical theoretical study on linear and nonlinear optical properties of macrocyclic thiophene derivatives with different connecting Econjugated bridge and ring size. <b>2012</b> , 53, 2991-3000		9
793	Gauging the flexibility of the active site in soybean lipoxygenase-1 (SLO-1) through an atom-centered density matrix propagation (ADMP) treatment that facilitates the sampling of rare events. <b>2012</b> , 116, 10145-64		21
792	The role of acid catalysis in the Baeyer-Villiger reaction. A theoretical study. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 6801-15	4.2	25
791	How Evenly Can Approximate Density Functionals Treat the Different Multiplicities and Ionization States of 4d Transition Metal Atoms?. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 4112-26	6.4	34
790	Unraveling the mechanisms of carboxyl ester bond hydrolysis catalyzed by a vanadate anion. <b>2012</b> , 51, 9619-28		7

## (2012-2012)

Accurate prediction of rate constants of Diels-Alder reactions and application to design of Diels-Alder ligation. <b>2012</b> , 10, 2673-82	41
Kinetic study on the linalool ozonolysis reaction in the atmosphere. <b>2012</b> , 90, 353-361	4
Mechanism and kinetic study on the gas-phase reactions of OH radical with carbamate insecticide isoprocarb. <b>2012</b> , 60, 460-466	8
Addition of carbon centered radicals to methyl 3-(methylamino)acrylate: The regioselectivity of radical addition to enamino esters. <b>2012</b> , 979, 17-21	3
Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. <b>2012</b> , 979, 1-9	8
SingletEriplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. <b>2012</b> , 983, 69-75	7
Libxc: A library of exchange and correlation functionals for density functional theory. <b>2012</b> , 183, 2272-2281	323
Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes.  Chemical Physics Letters, <b>2012</b> , 541, 7-11	17
Kinetic modeling for hydrogen-abstraction reaction of methylcyclohexane with the CH3 radical. <b>2012</b> , 79, 200-209	5
Solvent-catalyzed ring-chain-ring tautomerization in axially chiral compounds. <b>2012</b> , 18, 12725-32	11
Benchmark Ab Initio Calculations of the Barrier Height and Transition-State Geometry for Hydrogen Abstraction from a Phenolic Antioxidant by a Peroxy Radical and Its Use to Assess the Performance of Density Functionals. <b>2012</b> , 3, 2834-2839	30
The performance of density functional based methods in the description of selected biological systems and processes. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 14943-53	27
Nucleation and growth of nanoparticles in the atmosphere. <b>2012</b> , 112, 1957-2011	75 <sup>8</sup>
Atmospheric chemical reactions of 2,3,7,8-tetrachlorinated dibenzofuran initiated by an OH radical: mechanism and kinetics study. <b>2012</b> , 46, 8148-55	51
MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. <b>2012</b> , 02, 1230006	7
The catalytic mechanism of HIV-1 integrase for DNA 3'-end processing established by QM/MM calculations. <b>2012</b> , 134, 13436-47	47
Nonlinear optical properties for a class of hexa-peri-hexabenzocoronene chromophores: a computational investigation. <b>2012</b> , 41, 12416-27	4
Origins of the stability of imidazole-imidazole, benzene-imidazole, and benzene-indole dimers: CCSD(T)/CBS and SAPT calculations. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 1694-700	22
	Diels-Alder ligation. 2012, 10, 2673-82  Kinetic study on the linalool ozonolysis reaction in the atmosphere. 2012, 90, 353-361  Mechanism and kinetic study on the gas-phase reactions of OH radical with carbamate insecticide isoprocarb. 2012, 60, 460-466  Addition of carbon centered radicals to methyl. 3-(methylamino)acrylate: The regioselectivity of radical addition to enamino esters. 2012, 979, 17-21  Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. 2012, 979, 1-9  Singlettriplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. 2012, 983, 69-75  Libxc: A library of exchange and correlation functionals for density functional theory. 2012, 183, 2272-2281  Assessment of density functionals on intramolecular dispersion interaction in large normal alkanes. Chemical Physics Letters, 2012, 541, 7-11  Kinetic modeling for hydrogen-abstraction reaction of methylcyclohexane with the CH3 radical. 2012, 79, 200-209  Solvent-catalyzed ring-chain-ring tautomerization in axially chiral compounds. 2012, 18, 12725-32  Benchmark Ab Initio Calculations of the Barrier Height and Transition-State Geometry for Hydrogen Abstraction from a Phenolic Antioxidant by a Peroxy Radical and its Use to Assess the Performance of Density Functionals. 2012, 3, 2834-2839  The performance of density functional based methods in the description of selected biological systems and processes. Physical Chemistry Chemical Physics, 2012, 14, 14943-53  Nucleation and growth of nanoparticles in the atmosphere. 2012, 112, 1957-2011  Atmospheric chemical reactions of 2.3.7, 8-tetrachlorinated dibenzofuran initiated by an OH radical: mechanism and kinetics study. 2012, 46, 8148-55  MOLECULAR BIOLOGY AT THE QUANTUM LEVEL: CAN MODERN DENSITY FUNCTIONAL THEORY FORGE THE PATH?. 2012, 02, 1230006  The catalytic mechanism of HIV-1 integrase for DNA 3'-end processing established by QM/MM calculations. 2012, 134, 13436-47  Nonlinear optical properties

771	Why calcium inhibits magnesium-dependent enzyme phosphoserine phosphatase? A theoretical study. <b>2012</b> , 131, 1		7
77°	An experimental and theoretical approach to the molecular structure of 3-{[4-(3-Methyl-3-phenyl-cyclobutyl)-thiazol-2-yl]-hydrazono}-1,3-dihydro- indol-2-one. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 1566-1578	2.1	3
769	Analytical potential energy surface for the reaction with intermediate complexes NH3 + Cl -> NH2 + HCl: Application to the kinetics study. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 1887-190	3 <sup>2.1</sup>	16
768	Recognition of aromatic amino acids and proteins with p-sulfonatocalix[4]arene [A luminescence and theoretical approach. <b>2012</b> , 25, 1217-1227		22
767	Possible DNA damage by oxidation products of guanine: A density functional and electron propagator theoretical study. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 2840-2847	2.1	7
766	Reaction mechanism of hydrogenation and direct desulfurization routes of dibenzothiophene-like compounds: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 3599-3605	2.1	15
765	Correlations between computation and experimental thermodynamics of halogen bonding. <i>Journal of Organic Chemistry</i> , <b>2012</b> , 77, 3483-91	4.2	84
764	Density functional theory study of 1,2-dioxetanone decomposition in condensed phase. <b>2012</b> , 33, 2118	-23	11
763	Response to Domment on density functional theory study of 1,2-dioxetanone decomposition in condensed phase D2012, 33, 2127-2130		6
762	Kinetic Study of 1,5-Hydrogen Transfer Reactions of Methyl Acrylate and Butyl Acrylate Using Quantum Chemistry. <b>2012</b> , 21, 461-469		29
761	Quantum Chemical Investigation of Secondary Reactions in Poly(vinyl chloride) Free-Radical Polymerization. <b>2012</b> , 6, 330-345		11
760	Prereactive complexes in chlorination of benzene, triazine, and tetrazine: a quantum chemical study. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 1298-306	2.8	16
759	Synthesis, structural characterization, photophysics, and broadband nonlinear absorption of a platinum(II) complex with the 6-(7-benzothiazol-2'-yl-9,9-diethyl-9 H-fluoren-2-yl)-2,2'-bipyridinyl ligand. <b>2012</b> , 18, 4593-606		27
75 <sup>8</sup>	Substituent effect on the linkers in triphenylamine dyes for sensitized solar cells: a DFT/TDDFT study. <b>2012</b> , 13, 3320-9		33
757	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists. <b>2012</b> , 95-133		2
756	Polarized continuum model study of bond dissociation energies of the ONO2 bond A density functional theory study and natural bond order analysis. <b>2012</b> , 90, 433-440		
755	The entrance complex, transition state, and exit complex for the F + H2O -> HF + OH reaction. Definitive predictions. Comparison with popular density functional methods. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 10891-5	3.6	60
754	Time-dependent density functional theory benchmarking for the calculations of atomic spectra: efficiency of exc-ETDZ basis set. <b>2012</b> , 131, 1		7

753	A systematical comparison of DFT methods in reproducing the interaction energies of halide series with protein moieties. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 2079-98	2	6
75 <sup>2</sup>	The OH-induced degradation mechanism of 4-chloro-2-methylphenoxyacetic acid (MCPA) with two forms in the water: a DFT comparison. <b>2012</b> , 88, 39-48		7
751	Proton exchange in acidBase complexes induced by reaction coordinates with heavy atom motions. <b>2012</b> , 402, 105-112		1
750	Binding of molecular hydrogen to halide anions: A computational exploration of eco-friendly materials for hydrogen storage. <i>Chemical Physics Letters</i> , <b>2012</b> , 519-520, 83-88	2.5	7
749	Fine tuning of the one- and two-photon absorption properties of macrocyclic thiophene-based derivatives. <b>2012</b> , 93, 1519-1531		6
748	Theoretical study of the reaction mechanism and kinetics of low-molecular-weight atmospheric aldehydes (C1tt4) with NO2. <b>2012</b> , 54, 288-295		23
747	Mechanism and kinetics study on the OH-initiated oxidation of organophosphorus pesticide trichlorfon in atmosphere. <b>2012</b> , 419, 144-50		16
746	Metal ion shuttling mechanism through thiacalix[4]crown: a computational study. <b>2012</b> , 53, 2009-2012		7
745	Mechanism for the reaction of 2-naphthol with N-methyl-N-phenyl-hydrazine suggested by the density functional theory investigations. <b>2012</b> , 33, 220-30		6
744	An improved theoretical approach to the empirical corrections of density functional theory. <b>2012</b> , 26, 199-213		2
743	Computational study of the electronic structures, UV-Vis spectra and static second-order nonlinear optical susceptibilities of macrocyclic thiophene derivatives. <i>Journal of Molecular Modeling</i> , <b>2012</b> , 18, 393-404	2	4
742	Theoretical study of the pH-dependent antioxidant properties of vitamin C. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 1945-52	2	8
741	Theoretical study of gas phase reactions of important SOA intermediates: (cis- and trans-) BEPOX and EEPOX with OH radical. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 1162-1170	2.1	
740	Mechanistic aspects regarding the elimination of H2O2 from C(4a)-hydroperoxyflavin. The role of a proton shuttle required for H2O2 elimination. <i>Journal of Organic Chemistry</i> , <b>2013</b> , 78, 8585-93	4.2	13
739	A density functional theory study for the role of end groups on the antioxidative potency of carotenoids. <b>2013</b> , 132, 1		5
738	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3872-7	6.4	248
737	Tests of Exchange-Correlation Functional Approximations Against Reliable Experimental Data for Average Bond Energies of 3d Transition Metal Compounds. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3965-77	6.4	82
736	Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. <b>2013</b> , 34, 2079-90		27

735	Experimental and theoretical studies on polar DielsAlder reactions of 1-nitronaphathalene developed in ionic liquids. <b>2013</b> , 3, 13825		8
734	Polymerization of Methyl Methacrylate with Lithium Triflate. A Kinetic and Structural Study. <b>2013</b> , 46, 5445-5454		14
733	A computational methodology for accurate predictions of rate constants in solution: application to the assessment of primary antioxidant activity. <b>2013</b> , 34, 2430-45		203
732	The influence of (5?R) and (5?S)-5?,8-cyclo-2?-deoxyadenosine for the electronic properties of nucleosides pairs. The theoretical quantum mechanics studies. <b>2013</b> , 11, 1079-1090		O
731	Electrosteric Activation by using Ion-Tagged Prolines: A Combined Experimental and Computational Investigation. <b>2013</b> , 5, 2913-2924		7
730	Theoretical investigation of the gas-phase reactions of CF2ClC(O)OCH3 with the hydroxyl radical and the chlorine atom at 298 K. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 3263-70	2	20
729	DFT comparison of the OH-initiated degradation mechanisms for five chlorophenoxy herbicides. Journal of Molecular Modeling, <b>2013</b> , 19, 2249-63	2	28
728	Acylglucuronide in alkaline conditions: migration vs. hydrolysis. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 2423-32	2	4
727	The OH-initiated atmospheric reaction mechanism and kinetics for levoglucosan emitted in biomass burning. <b>2013</b> , 93, 2004-10		34
726	Dynamics in Carbene Reactions. <b>2013</b> , 131-165		1
725	Formation of bromophenoxy radicals from complete series reactions of bromophenols with H and OH radicals. <b>2013</b> , 92, 382-90		21
724	Selective and Practical Oxidation of Sulfides to Diastereopure Sulfoxides: A Combined Experimental and Computational Investigation. <b>2013</b> , 355, 191-202		15
723	The atmospheric degradation reaction of dehydroabietic acid (DHAA) initiated by OH radicals and O3. <b>2013</b> , 92, 933-40		5
722	A DFT study of the Altaletalyzed Friedel-Crafts acylation of phenyl aromatic compounds. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 4947-58	2	11
721	Understanding CI bond formation in polar reactions. An ELF analysis of the Friedel Trafts reaction between indoles and nitroolefins. <b>2013</b> , 3, 7520		21
720	Synthesis, Molecular Characterization and Preliminary Antioxidant Activity Evaluation of Quercetin Fatty Esters. <b>2013</b> , 90, 1751-1759		23
719	Hydrogen-bond acidity of OH groups in various molecular environments (phenols, alcohols, steroid derivatives, and amino acids structures): experimental measurements and density functional theory calculations. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 13184-93	2.8	36
718	Antioxidant properties of phenolic Schiff bases: structure-activity relationship and mechanism of action. <b>2013</b> , 27, 951-64		63

717	Economical and accurate protocol for calculating hydrogen-bond-acceptor strengths. 2013, 53, 3262-7	2	14
716	TD-DFT accuracy in determining excited-state structures and fluorescence spectra of firefly emitter. <b>2013</b> , 29, 982-985		4
715	Accurate treatment of two-dimensional non-separable hindered internal rotors. 2013, 138, 134112		36
714	A DFT study of the applicability of the charge balance model in two-metal enzymes: The case of cAMP-dependent protein kinase. <i>Chemical Physics Letters</i> , <b>2013</b> , 571, 66-70	2.5	7
713	Theoretical study of the Omcl interaction in fluorinated dimethyl ethers complexed with a Cl atom: is it through a two-center-three-electron bond?. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 8010-6	2.8	15
712	Theoretical and experimental analysis of the reaction mechanism of MrTPS2, a triquinane-forming sesquiterpene synthase from chamomile. <b>2013</b> , 19, 13590-600		28
711	The atmospheric chemical reaction of 4-tert-butylphenol initiated by OH radicals. 2013, 10, 111		2
710	Theoretical study on the OH-initiated atmospheric reaction of N-methyl perfluorobutane sulfonamidoethanol (C4F9SO2N(CH3)CH2CH2OH). <b>2013</b> , 91, 1161-1167		O
709	Theoretical study on the reaction mechanism of vinyl acetate with OH radicals in the atmosphere. <b>2013</b> , 91, 241-247		6
708	Consistent descriptions of metalligand bonds and spin-crossover in inorganic chemistry. <b>2013</b> , 257, 196-209		153
707	Electronic structure of [Ni(II)S4] complexes from S K-edge X-ray absorption spectroscopy. <b>2013</b> , 257, 564-578		30
706	Theoretical study on the regioselectivity of Baeyer-Villiger Reaction of ⊞-Me-, -F-, -CF3-cyclohexanones. <i>Journal of Organic Chemistry</i> , <b>2013</b> , 78, 146-53	4.2	18
7°5	What occurs by replacing Mn2+ with Co2+ in human arginase I: first-principles computational analysis. <b>2013</b> , 52, 655-9		18
704	ONIOM (DFT:MM) study of the catalytic mechanism of myo-inositol monophosphatase: essential role of water in enzyme catalysis in the two-metal mechanism. <b>2013</b> , 117, 833-42		8
703	Halogen-bond interactions: a crystallographic basicity scale towards iodoorganic compounds. <b>2013</b> , 15, 3212		50
702	Chemiluminescence of 1,2-dioxetanone studied by a closed-shell DFT approach. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 1709-1716	2.1	5
701	Intricacies of Describing Weak Interactions Involving Halogen Atoms within Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 955-64	6.4	21

699	A computational study on the reactivity enhancement in the free radical polymerization of alkyl ∃-hydroxymethacrylate and acrylate derivatives. <b>2013</b> , 51, 880-889		6
698	Theoretical investigations on kinetics, mechanism and thermochemistry of the gas phase reactions of CHF2OCF2CHF2 with OH radicals. <b>2013</b> , 1022, 50-58		25
697	N-NO2 bond dissociation energies in acetonitrile: an assessment of contemporary computational methods. <b>2013</b> , 43, 66-71		2
696	Origins of the solvent effect on the propagation kinetics of acrylic acid and methacrylic acid. <b>2013</b> , 51, 2024-2034		23
695	Theoretical investigation of two-photon absorption and fluorescence properties of cypridina luciferin-based derivatives: 2,3,5-trisubstituted pyrazine compounds. <b>2013</b> , 26, 822-833		8
694	Theoretical study on the kinetics and branching ratios of the gas phase reactions of 4,4,4-trifluorobutanal (TFB) with OH radical in the temperature range of 250월00K and atmospheric pressure. <b>2013</b> , 154, 60-66		14
693	Quantum chemical and direct dynamic study on homogeneous gas-phase formation of PBDD/Fs from 2,4,5-tribromophenol and 3,4-dibromophenol. <b>2013</b> , 93, 512-20		12
692	New interpretation of proton and deuteron tunneling in 2?-methylacetophenone. <i>Chemical Physics Letters</i> , <b>2013</b> , 586, 61-66	2.5	
691	Application of two-layer ONIOM for studying the interaction of N-substituted piperazinylfluoroquinolones with ds-DNA. <b>2013</b> , 1006, 9-18		5
690	Density functional theory calculations of stable isomers for trifluoroacetic acid (TFA)[H2O)4 complexes. <b>2013</b> , 1016, 48-53		7
689	Introducing copper as catalyst for oxidative alkane dehydrogenation. 2013, 135, 3887-96		66
688	Why do five-membered heterocyclic compounds sometimes not participate in polar Diels-Alder reactions?. <i>Journal of Organic Chemistry</i> , <b>2013</b> , 78, 2462-71	4.2	38
687	Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 1803-1811	2.1	7
686	Efficient and accurate theoretical methods to investigate anion-linteractions in protein model structures. <b>2013</b> , 117, 3315-22		23
685	Assessing the Accuracy of Density Functional and Semiempirical Wave Function Methods for Water Nanoparticles: Comparing Binding and Relative Energies of (H2O)16 and (H2O)17 to CCSD(T) Results. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 995-1006	6.4	43
684	Free radical scavenging by natural polyphenols: atom versus electron transfer. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 2082-92	2.8	172
683	Acid-catalyzed nucleophilic additions to carbonyl groups: is the accepted mechanism the rule or an exception?. <i>Journal of Organic Chemistry</i> , <b>2013</b> , 78, 2327-35	4.2	14
682	Assessment of density functional methods for thermochemistry of chromium oxo compounds and their application in a study of chromiaBilica system. <i>Chemical Physics Letters</i> , <b>2013</b> , 561-562, 87-91	2.5	13

681	Computational study on the attack of EOH radicals on aromatic amino acids. 2013, 19, 6862-73		29
680	EH3 (E = N, P, As) and H2 activation with N-heterocyclic silylene and germylene homologues. <b>2013</b> , 19, 7835-46		25
679	Theoretical investigation of the coupling between hydrogen-atom transfer and stacking interaction in adenine-thymine dimers. <b>2013</b> , 14, 1256-63		15
678	Cycloaddition of ozone to allyl alcohol, acrylic acid and allyl aldehyde: A comparative DFT study. <b>2013</b> , 415, 161-167		2
677	Rh2(OAc)4-catalyzed reaction of ⊞-diazocarbonyl compounds with 2-carbonyl-substituted 2H-azirines. <b>2013</b> , 69, 4546-4551		22
676	Benchmark quantum-chemical calculations on a complete set of rotameric families of the DNA sugar-phosphate backbone and their comparison with modern density functional theory. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 7295-310	3.6	25
675	Theoretical study on rate constants for the reactions of CF3CH 2NH 2 (TFEA) with the hydroxyl radical at 298 K and atmospheric pressure. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 2189-95	2	15
674	Structures, stabilization energies, and binding energies of quinoxaline(H2O)(n), quinoxaline dimer, and quinoxaline(H2O)(n), quinoxaline(H2O)	2.8	18
673	Theoretical study on the mechanism of the reaction of alkylmethylimidazolium cation with benzaldehyde involved in the base-catalyzed Baylis Hillman reaction. <b>2013</b> , 1014, 24-28		6
672	Quantum chemistry investigation of secondary reaction kinetics in acrylate-based copolymers. Journal of Physical Chemistry A, <b>2013</b> , 117, 4358-66	2.8	23
671	Theoretical investigations on the kinetics of H-abstraction reactions from CF3CH(OH)CF3 by OH radicals. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 4534-44	2.8	30
670	Performance of density functional methods. Some difficult cases for small systems containing Cu, Ag, or Au. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 2619-28	2.8	6
669	Atmospheric degradation of 2,3,7,8-tetrachlorinated dibenzo-p-dioxins in the presence of NO3 at night. <b>2013</b> , 91, 398-405		2
668	Selecting DFT methods for use in optimizations of enzyme active sites: applications to ONIOM treatments of DNA glycosylases. <b>2013</b> , 91, 559-572		14
667	Mechanistic and kinetics study of the gas phase reactions of methyltrifluoroacetate with OH radical and Cl atom. <b>2013</b> , 111, 860-867		23
666	Computational design of two-photon fluorescent probes for a zinc ion based on a Salen ligand. <b>2013</b> , 52, 5702-13		24
665	Binding interactions in dimers of phenalenyl and closed-shell analogues. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 3642-9	2.8	33
664	New insights on the molecular recognition of imidacloprid with Aplysia californica AChBP: a computational study. <b>2013</b> , 117, 3944-53		18

663	Quantum chemical and kinetics study of the thermal gas phase decomposition of 2-chloropropene. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 10218-27	8
662	Methane Dehydrogenation by Niobium Ions: A First-Principles Study of the Gas-Phase Catalytic Reactions. <b>2013</b> , 32, 989-999	23
661	DFT STUDY OF THE PROTONATION AND DEPROTONATION ENTHALPIES OF BENZOXAZOLE, 1,2-BENZISOXAZOLE AND 2,1-BENZISOXAZOLE AND IMPLICATIONS FOR THE STRUCTURES AND ENERGIES OF THEIR ADDUCTS WITH EXPLICIT WATER MOLECULES. <b>2013</b> , 12, 1350070	11
660	Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 3848-54	2
659	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> , <b>2013</b> , 117, 12821-30 <sup>2.8</sup>	14
658	Theoretical study on the OH-initiated atmospheric reaction of 1,1,1-trichloro-2,2-bis(4-chlorophenyl) ethane (DDT). <b>2013</b> , 67, 177-183	10
657	OH-initiated oxidation mechanisms and kinetics of 2,4,4'-Tribrominated diphenyl ether. <b>2013</b> , 47, 8238-47	16
656	Theoretical and experimental insights into the electrochemical mineralization mechanism of perfluorooctanoic acid. <b>2013</b> , 47, 14341-9	129
655	Theoretical studies on OH and Cl initiated hydrogen atom abstraction of HFE-227pc (CF3OCF2CHF2). <b>2013</b> , 70, 257-268	2
654	A Density Functional Theory Study of Secondary Reactions in n-Butyl Acrylate Free Radical Polymerization. <b>2013</b> , 22, 127-135	38
653	DFT Study on Homolytic Dissociation Enthalpies of CliBonds. <b>2013</b> , 26, 541-548	9
652	Direct-dynamics VTST study of hydrogen or deuterium abstraction and C-C bond formation or dissociation in the reactions of CH3 + CH4, CH3 + CD4, CH3D + CD3, CH3CH3 + H, and CH3CD3 + D. <b>2013</b> , 138, 194305	9
651	DUAL-LEVEL DIRECT DYNAMICS STUDIES ON THE HYDROGEN ABSTRACTION REACTION OF CF3CHFCF3 (HFC-227ea) WITH Cl ATOM. <b>2013</b> , 12, 1250119	
650	Assessment of theoretical methods for the study of hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation (IUPAC Technical Report). <b>2013</b> , 85, 1901-1918	6
649	Theoretical study of a reaction mechanism of tropospheric interest: CH3CH2F + OH. <b>2013</b> , 38, 342-358	
648	Accurate Prediction of Au?P Bond Strengths by Density Functional Theory Methods. <b>2013</b> , 31, 200-208	7
647	Competing mechanisms of catalytic H2 formation and dissociation on ultrasmall silicate nanocluster dust grains. <b>2013</b> , 435, 1486-1492	14
646	A theoretical rationale why furan-side monoadduct is more favorable toward diadduct formation in 8-methoxypsoralen and thymine complexes. <b>2013</b> , 89, 891-9	3

645	Linking molecular level chemistry to macroscopic combustion behavior for nano-energetic materials with halogen containing oxides. <b>2013</b> , 139, 074701		15
644	On the interactions between poly(ethylene oxide) and graphite oxide: a comparative study by different computational methods. <b>2013</b> , 138, 094308		3
643	Atmospheric oxidation mechanism of polyfluorinated sulfonamides IA quantum chemical and kinetic study. <b>2013</b> , 91, 472-478		1
642	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. <b>2013</b> , 19, 14081-9		42
641	Computational Study of Cage Like (ZnO)12 Cluster Using Hybrid and Hybrid Meta Functionals. Journal of the Chinese Chemical Society, <b>2013</b> , 60, 1082-1091	1.5	4
640	Interaction of selected gases with zinc phthalocyanine thin films: theoretical and experimental studies. <b>2013</b> , 64, 10202		7
639	Applications of density functional theory to iron-containing molecules of bioinorganic interest. <b>2014</b> , 2, 14		16
638	. 2014,		55
637	Electronic and optical properties at organic/organic interfaces in organic solar cells. <b>2014</b> , 352, 103-50		5
636	Computational study on the kinetics of OH initiated oxidation of methyl difluoroacetate (CF2HCOOCH3). <b>2014</b> , 112, 1892-1898		12
635	Assessment of density-functionals for describing the X(-) + CH3ONO2 gas-phase reactions with X = F, OH, CH2CN. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 26769-78	3.6	11
634	Density Functional Theory Calculations on Nilligand Bond Dissociation Enthalpies. <b>2014</b> , 27, 640-646		1
633	Chemosensors for detection of nitroaromatic compounds (explosives). <b>2014</b> , 83, 783-819		56
632	Theoretical investigation on mechanism and kinetics of the Cl-initiated hydrogen abstraction reactions of ethyl trifluoroacetate at 298 K. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2475	2	7
631	Kinetics of radical-molecule reactions in aqueous solution: a benchmark study of the performance of density functional methods. <b>2014</b> , 35, 2019-26		151
630	Accurate Prediction of Ir?H Bond Dissociation Enthalpies by Density Functional Theory Methods. <b>2014</b> , 32, 269-275		11
629	Assessment of a Cost-Effective Approach to the Calculation of Kinetic and Thermodynamic Properties of Methyl Methacrylate Homopolymerization: A Comprehensive Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 5668-76	6.4	16
628	Anthraquinone-based intramolecular charge-transfer compounds: computational molecular design, thermally activated delayed fluorescence, and highly efficient red electroluminescence. <b>2014</b> , 136, 1807	70-81	628

627	Theoretical investigation on the atmospheric fate of CF3C(O)OCH 2O radical: alpha-ester rearrangement vs oxidation at 298 K. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2444	2	4
626	CHIand CFIInteractions Lead to Structural Changes of N-Heterocyclic Carbene Palladium Complexes. <b>2014</b> , 126, 1307-1311		6
625	A computational perspective on mechanism and kinetics of the reactions of CF3C(O)OCH2CF3 with OH radicals and Cl atoms at 298K. <b>2014</b> , 160, 64-71		21
624	A theoretical investigation on the kinetics, mechanism and thermochemistry of gas-phase reactions of methyl acetate with chlorine atoms at 298 K. <i>Chemical Physics Letters</i> , <b>2014</b> , 595-596, 43-47	2.5	20
623	Mechanism and rate constants for complete series reactions of 19 fluorophenols with atomic H. <b>2014</b> , 26, 154-9		2
622	Micro-mechanism and rate constants for OH-initiated degradation of methomyl in atmosphere. <b>2014</b> , 107, 331-335		6
621	Hydroxyl radical reactions with 2-chlorophenol as a model for oxidation in supercritical water. <b>2014</b> , 40, 973-990		8
620	Mechanism for OH-initiated atmospheric oxidation of the organophosphorus insecticide phorate. <i>Structural Chemistry</i> , <b>2014</b> , 25, 275-284	1.8	5
619	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. <b>2014</b> , 372, 20120476		514
618	Halogen bonds with benzene: an assessment of DFT functionals. <b>2014</b> , 35, 386-94		65
618 617	Halogen bonds with benzene: an assessment of DFT functionals. <b>2014</b> , 35, 386-94  Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <b>2014</b> , 133, 1		6 <sub>5</sub>
	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate	1.8	
617	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <b>2014</b> , 133, 1  A theoretical investigation on the kinetics and reactivity of the gas-phase reactions of ethyl	1.8	33
617 616	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <b>2014</b> , 133, 1  A theoretical investigation on the kinetics and reactivity of the gas-phase reactions of ethyl chlorodifluoroacetate with OH radical and Cl atom at 298 K. <i>Structural Chemistry</i> , <b>2014</b> , 25, 463-470  Quantum mechanical investigation on bimolecular hydrogen abstractions in butyl acrylate-based		33
<ul><li>617</li><li>616</li><li>615</li></ul>	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. 2014, 133, 1  A theoretical investigation on the kinetics and reactivity of the gas-phase reactions of ethyl chlorodifluoroacetate with OH radical and Cl atom at 298 K. Structural Chemistry, 2014, 25, 463-470  Quantum mechanical investigation on bimolecular hydrogen abstractions in butyl acrylate-based free radical polymerization processes. Journal of Physical Chemistry A, 2014, 118, 1799-806  Theoretical investigations on the kinetics of p-cymene+OH reaction. Chemical Physics Letters, 2014,	2.8	33 14 9
<ul><li>617</li><li>616</li><li>615</li><li>614</li></ul>	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. 2014, 133, 1  A theoretical investigation on the kinetics and reactivity of the gas-phase reactions of ethyl chlorodifluoroacetate with OH radical and Cl atom at 298 K. Structural Chemistry, 2014, 25, 463-470  Quantum mechanical investigation on bimolecular hydrogen abstractions in butyl acrylate-based free radical polymerization processes. Journal of Physical Chemistry A, 2014, 118, 1799-806  Theoretical investigations on the kinetics of p-cymene+OH reaction. Chemical Physics Letters, 2014, 597, 75-85  CH-land CF-linteractions lead to structural changes of N-heterocyclic carbene palladium	2.8	33 14 9
<ul><li>617</li><li>616</li><li>615</li><li>614</li><li>613</li></ul>	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. 2014, 133, 1  A theoretical investigation on the kinetics and reactivity of the gas-phase reactions of ethyl chlorodifluoroacetate with OH radical and Cl atom at 298 K. Structural Chemistry, 2014, 25, 463-470  Quantum mechanical investigation on bimolecular hydrogen abstractions in butyl acrylate-based free radical polymerization processes. Journal of Physical Chemistry A, 2014, 118, 1799-806  Theoretical investigations on the kinetics of p-cymene+OH reaction. Chemical Physics Letters, 2014, 597, 75-85  CH-Iand CF-IInteractions lead to structural changes of N-heterocyclic carbene palladium complexes. 2014, 53, 1283-7  Theoretical investigation on gas-phase reaction of CF3CH2OCH3 with OH radicals and fate of	2.8	33 14 9 10 26

609	Atmospheric chemistry of 2,3,7,8-TCDD/F: Mechanism and kinetics study. <b>2014</b> , 2, 1098-1103	3
608	A DFT study on kinetics of the gas phase reactions of CH3CH2OCF3 with OH radicals and Cl atoms. <b>2014</b> , 159, 57-64	15
607	Aromaticity from the viewpoint of molecular geometry: application to planar systems. <b>2014</b> , 114, 6383-422	340
606	Solution-Phase Organic Chemistry. <b>2014</b> , 445-503	
605	Quantum Mechanics for Organic Chemistry. <b>2014</b> , 1-60	1
604	The mechanism of ionic DielsAlder reactions. A DFT study of the oxa-Povarov reaction. <b>2014</b> , 4, 16567-16577	22
603	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 102-21	55
602	Water interaction with ion pairs from ionic liquids. Computational study and performance assessment of several common functionals. <i>Chemical Physics Letters</i> , <b>2014</b> , 593, 181-188	19
601	Biosynthetic consequences of multiple sequential post-transition-state bifurcations. <b>2014</b> , 6, 104-11	103
600	Theoretical prediction of hydrogen-bond basicity pKBHX using quantum chemical topology descriptors. <b>2014</b> , 54, 553-61	24
599	Quantum-chemical predictions of pKa's of thiols in DMSO. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 606-22	42
598	A DFT study on the NHC catalysed Michael addition of enols to ∃,⊞nsaturated acyl-azoliums. A base catalysed C-C bond-formation step. <b>2014</b> , 12, 895-904	28
597	New understanding of the formation of PCDD/Fs from chlorophenol precursors: a mechanistic and kinetic study. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 449-56	17
596	Understanding the selectivity in the formation of Elactams vs. Elactams in the Staudinger reactions of chloro-cyan-ketene with unsaturated imines. A DFT study. <b>2014</b> , 4, 58559-58566	13
595	Theoretical study on the degradation reaction of octachlorinated dibenzo-p-dioxin with atomic oxygen O((3)P) in dielectric barrier discharge reactor. <b>2014</b> , 26, 2283-9	1
594	DielsAlder reactions of pinacol alkenylboronates: an experimental and theoretical study. <b>2014</b> , 4, 36385-3640	012
593	Theoretical investigation on the atmospheric fate of the CF3C(O)OCH(O)CF3 radical: alpha-ester rearrangement vs. oxidation. <b>2014</b> , 4, 16759	16
592	Challenges in modelling the reaction chemistry of interstellar dust. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 18623-43	24

591	Charting the mechanism and reactivity of zirconium oxalate with hydroxamate ligands using density functional theory: implications in new chelate design. <b>2014</b> , 43, 9872-84		39
590	Accurate predictions of C-SO2R bond dissociation enthalpies using density functional theory methods. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 20964-70	3.6	19
589	Understanding the mechanism of the Povarov reaction. A DFT study. <b>2014</b> , 4, 25268		41
588	A new CII bond formation model based on the quantum chemical topology of electron density. <b>2014</b> , 4, 32415-32428		347
587	Theoretical investigation on unimolecular decomposition of malonic acid: a potential sink for ketene. <b>2014</b> , 4, 38034		4
586	Theoretical insights into the absorption and emission properties of blue luminescent copper(I) complexes based on the pyrazolyl-pyridine ligands. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 1685-1691	2.1	4
585	A new exchange-correlation functional free of delocalization and static correlation errors. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 16373-7	3.6	3
584	Insight into the promiscuous activity of human carbonic anhydrase against the cyanic acid substrate from a combined QM and QM/MM investigation. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 16671-6	3.6	17
583	Quantum chemistry investigation of fluorinated polymer systems of industrial interest. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 238-47	2.8	11
582	What Dominates the Error in the CaO Diatomic Bond Energy Predicted by Various Approximate Exchange-Correlation Functionals?. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2291-305	6.4	13
581	Explanation of the Source of Very Large Errors in Many Exchange-Correlation Functionals for Vanadium Dimer. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2399-409	6.4	23
580	Understanding the polar mechanism of the ene reaction. A DFT study. <b>2014</b> , 12, 7581-90		31
579	Lifetimes of carbocations encountered along reaction coordinates for terpene formation. <b>2014</b> , 5, 3301	l	25
578	Density differences in embedding theory with external orbital orthogonality. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 9182-200	2.8	30
577	Catalytic, regioselective, and green methods for rearrangement of 1,2-diaryl epoxides to carbonyl compounds employing metallic triflates, BrBsted-acidic ionic liquids (ILs), and IL/microwave; experimental and computational substituent effect study on aryl versus hydrogen migration. <b>2014</b> ,		16
576	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> , <b>2014</b> , 118, 3004-13	2.8	6
575	A theoretical investigation on kinetics, mechanism, and thermochemistry of the gas-phase reactions of methyl fluoroacetate with OH radicals and fate of alkoxy radical. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 8779-86	2.8	10
574	Interactions of the Watson Trick nucleic acid base pairs with carbon nanotubes and graphene: DFT and MP2 study. <i>Chemical Physics Letters</i> , <b>2014</b> , 610-611, 186-191	2.5	10

573	Reactions of benzene and 3-methylpyrrole with the DH and DOH radicals: an assessment of contemporary density functional theory methods. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 2667-82	2.8	5
572	A computational study of pyrazinamide: Tautomerism, acidBase properties, micro-solvation effects and acid hydrolysis mechanism. <b>2014</b> , 1046, 30-41		23
571	Energies and 2'-Hydroxyl Group Orientations of RNA Backbone Conformations. Benchmark CCSD(T)/CBS Database, Electronic Analysis, and Assessment of DFT Methods and MD Simulations. Journal of Chemical Theory and Computation, 2014, 10, 463-80	6.4	20
570	CIIN vs CIII Activation: Actual Mechanism of the Reaction between [(dippe)PtH]2 and Benzonitrile Evidenced by a DFT Computational Investigation. <b>2014</b> , 33, 4173-4182		9
569	Performance of Density Functional Theory Procedures for the Calculation of Proton-Exchange Barriers: Unusual Behavior of M06-Type Functionals. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 3777-83	6.4	37
568	MP2, DFT and DFT-D study of the dimers of diazanaphthalenes: a comparative study of their structures, stabilisation and binding energies. <b>2014</b> , 40, 1131-1146		8
567	Benchmarking of Density Functionals for the Accurate Description of Thiol-Disulfide Exchange. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 4842-56	6.4	26
566	Understanding the electron density reorganization upon stacking vs. H-bonding interaction in methyl gallatellaffeine complexes. <b>2014</b> , 4, 25018-25027		5
565	Promising density functional theory methods for predicting the structures of uranyl complexes. <b>2014</b> , 4, 50261-50270		4
564	Computational Tools for Structure, Spectroscopy and Thermochemistry. <b>2014</b> , 249-320		
563	Computational Tools for Structure, Spectroscopy and Thermochemistry. <b>2014</b> , 249-320  Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. <b>2014</b> , 133, 1		5
,	Performance of recent density functionals to discriminate between olefin and nitrogen binding to	9066	5
563	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. <b>2014</b> , 133, 1	9066	
563	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. <b>2014</b> , 133, 1  Theoretical Study of Chain Transfer to Agent Kinetics in Butyl Acrylate Polymerization. <b>2014</b> , 53, 9058-9  Calculation of the two-dimensional non-separable partition function for two molecular systems.		15
563 562 561	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. <b>2014</b> , 133, 1  Theoretical Study of Chain Transfer to Agent Kinetics in Butyl Acrylate Polymerization. <b>2014</b> , 53, 9058-5  Calculation of the two-dimensional non-separable partition function for two molecular systems. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2190  Theoretical mechanistic study of the formic acid decomposition assisted by a Ru(II)-phosphine	2	15 6
563 562 561 560	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. 2014, 133, 1  Theoretical Study of Chain Transfer to Agent Kinetics in Butyl Acrylate Polymerization. 2014, 53, 9058-9  Calculation of the two-dimensional non-separable partition function for two molecular systems.   Journal of Molecular Modeling, 2014, 20, 2190  Theoretical mechanistic study of the formic acid decomposition assisted by a Ru(II)-phosphine catalyst.   Journal of Molecular Modeling, 2014, 20, 2250  Reaction of chlorine radical with tetrahydrofuran: a theoretical investigation on mechanism and	2	15 6 9
563 562 561 560	Performance of recent density functionals to discriminate between olefin and nitrogen binding to palladium. 2014, 133, 1  Theoretical Study of Chain Transfer to Agent Kinetics in Butyl Acrylate Polymerization. 2014, 53, 9058-9058-9058-9058-9058-9058-9058-9058-	2 2 2	15 6 9 2

555	Stereoselective propagation in free radical polymerization of acrylamides: a DFT study. 2014, 49, 55-67		7
554	Asymmetric modular synthesis of a semirigid dipeptide mimetic by cascade cycloaddition/ring rearrangement and borohydride reduction. <i>Journal of Organic Chemistry</i> , <b>2014</b> , 79, 3094-102	4.2	22
553	Theoretical investigation of the atmospheric chemistry of methyl difluoroacetate: reaction with Cl atoms and fate of alkoxy radical at 298 K. <i>Structural Chemistry</i> , <b>2014</b> , 25, 1475-1482	1.8	9
552	Theoretical kinetic study of the unimolecular decomposition of 2-bromopropene. <i>Chemical Physics Letters</i> , <b>2014</b> , 608, 386-392	2.5	3
551	Computational Insight into the Explosive Detection Mechanisms in Silafluorene- and Silole-Containing Photoluminescent Polymers. <b>2014</b> , 118, 6385-6397		14
550	Supramolecular analyte recognition: experiment and theory interplay. <b>2014</b> , 4, 11980-11999		10
549	Computational study on the kinetics and mechanism of the carbaryl + OH reaction. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 7776-81	2.8	3
548	Novel [2 + 1] Concerted Reaction Path for Disilacyclobutenes with Acetylene. <b>2014</b> , 33, 763-770		5
547	Theoretical vibrational Raman and surface-enhanced Raman scattering spectra of water interacting with silver clusters. <b>2014</b> , 15, 4067-76		6
546	Gas-phase tropospheric chemistry of 2,3,7,8-tetrafuorinated dibenzo-p-dioxin. <b>2014</b> , 468-469, 104-10		8
545	Computational study on the mechanisms and rate constants of the OH-initiated oxidation of ethyl vinyl ether in atmosphere. <b>2014</b> , 111, 61-9		8
544	Stable isomers for trifluoroacetic acid (TFA) pentahydrates obtained from density functional calculations. <b>2014</b> , 71, 57-61		3
543	Mechanism and kinetic properties of NO3-initiated atmospheric degradation of DDT. 2014, 26, 601-7		8
542	Kinetics, mechanism and thermochemistry of the gas phase reactions of CF3CH2OCH2CF3 with OH radicals: A theoretical study. <b>2014</b> , 161, 51-59		27
541	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. <b>2014</b> , 70, 4519-4525		64
540	Direct dynamics investigation of the reaction S(3P) + CH4-> CH3+ SH(2l). <i>Chemical Physics Letters</i> , <b>2014</b> , 591, 103-108	2.5	7
539	TICT based fluorescence Burn-onlhydrazine probes. <b>2014</b> , 199, 93-100		67
538	Mechanism and kinetics study on the ozonolysis reaction of 2,3,7,8-TCDD in the atmosphere. <b>2014</b> , 26, 181-8		7

537	The theoretical assessment and prediction of CBr bond dissociation enthalpies. 2014, 1027, 116-124	11
536	Accurate binding energies of hydrogen, halogen, and dihydrogen bonded complexes and cation enhanced binding strengths. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 885-894	8
535	Investigation of the reactions of U, U+ and U2+ with ammonia: mechanisms and topological analysis. <b>2014</b> , 4, 29806	19
534	Unravelling the S -> O linkage photoisomerization mechanisms in cis- and trans-[Ru(bpy)2(DMSO)2](2+) using density functional theory. <b>2014</b> , 53, 6752-60	32
533	Generalized Energy-Based Fragmentation CCSD(T)-F12a Method and Application to the Relative Energies of Water Clusters (H2O)20. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 1546-53	51
532	Kinetics and quantitative structure-activity relationship study on the degradation reaction from perfluorooctanoic acid to trifluoroacetic acid. <i>International Journal of Molecular Sciences</i> , <b>2014</b> , 15, 14153-65	6
531	Antioxidant activity of hispidin oligomers from medicinal fungi: a DFT study. <b>2014</b> , 19, 3489-507	29
530	Influence of Fluorination on the Conformational Properties and Hydrogen-Bond Acidity of Benzyl Alcohol Derivatives. <b>2015</b> , 21, 11462-74	20
529	Spectroscopic characterization, X-ray structure and DFT studies on 4-[3-(2,5-dimethylphenyl)-3-methylcyclobutyl]-N-methylthiazol-2-amine. <b>2015</b> , 56, 1342-1352	2
528	SN2 Reaction of IOD+ CH3Cl: An Ab Initio and DFT Benchmark Study. <b>2015</b> , 88, 110-116	4
527	The mechanism and kinetic studies on oxidation reaction of acetofenate initiated by HOx, NO3, O3, and Cl radicals. <b>2015</b> , 5, 96518-96524	2
526	DFT Mechanistic Investigation of the Gold(I)-Catalyzed Synthesis of Azepino[1,2-a]indoles. <b>2015</b> , 7, 2480-2484	<b>1</b> 14
525	Triesterase and promiscuous diesterase activities of a di-Co(II)-containing organophosphate degrading enzyme reaction mechanisms. <b>2015</b> , 21, 3736-45	16
524	A Quantum Mechanical Study on the Propagation Kinetics of N-methylacrylamide: Comparison With N,N-Dimethylacrylamide in Free Radical Polymerization. <b>2015</b> , 24, 218-231	2
523	Quantum Chemical and Kinetic Study on Polychlorinated Naphthalene Formation from 3-Chlorophenol Precursor. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 20620-40	4
522	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. <b>2015</b> , 169-201	
521	Formation of Chlorotriophenoxy Radicals from Complete Series Reactions of Chlorotriophenols with H and OH Radicals. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 18714-31	8
520	Quantitative Structure-Activity Relationships Study on the Rate Constants of Polychlorinated Dibenzo-p-Dioxins with OH Radical. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 18812-24	2

519	Mechanistic and Kinetic Studies on the Homogeneous Gas-Phase Formation of PCTA/DTs from 2,4-Dichlorothiophenol and 2,4,6-Trichlorothiophenol. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 20449-67	6.3	8
518	Theoretical Mechanistic and Kinetic Studies on Homogeneous Gas-Phase Formation of Polychlorinated Naphthalene from 2-Chlorophenol as Forerunner. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 25641-56	6.3	8
517	Computational studies on hypervalent iodonium(III) compounds as activated precursors for 18F radiofluorination of electron-rich arenes. <b>2015</b> , 1066, 34-46		12
516	Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1\$\mathbb{U}\$5 oxygenates. <b>2015</b> , 113, 1630-1635		3
515	Components of the Bond Energy in Polar Diatomic Molecules, Radicals, and Ions Formed by Group-1 and Group-2 Metal Atoms. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2968-83	6.4	24
514	OH radical-initiated oxidation degradation and atmospheric lifetime of N-ethylperfluorobutyramide in the presence of OMNOx. <b>2015</b> , 134, 241-9		9
513	Theoretical investigations of the gas phase reaction of limonene (C10H16) with OH radical. <b>2015</b> , 113, 3202-3215		12
512	Generation of a substituted 1,2,4-thiadiazole ring via the [3+2] cycloaddition reaction of benzonitrile sulfide toward trichloroacetonitrile. A DFT study of the regioselectivity and of the molecular mechanism. <b>2015</b> , 18, 1277-1283		9
511	EDH Oxidation Toward S- and OH-Containing Amino Acids. 2015, 119, 15430-42		15
510	Can Silica Particles Reduce Air Pollution by Facilitating the Reactions of Aliphatic Aldehyde and NO2?. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 11376-83	2.8	10
509	Ionic DielsAlder reaction of 3-bromofuran toward the highly electron deficient cyclobuteniminium cation: a regio- and stereoselectivity, and molecular mechanism study using DFT. <b>2015</b> , 5, 98538-98548		4
508	Kinetics and mechanism for OH-initiated gas-phase chemistry of ⊞-terpineol. <b>2015</b> , 5, 95096-95103		4
507	Theoretical study for OH radical-initiated atmospheric oxidation of ethyl acrylate. <b>2015</b> , 119, 626-633		21
506	Theoretical investigation on the role of mineral dust aerosol in atmospheric reaction: A case of the heterogeneous reaction of formaldehyde with NO 2 onto SiO 2 dust surface. <b>2015</b> , 103, 207-214		16
505	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. <b>2015</b> , 13, 2034-43		14
504	Computational study on kinetics and mechanism of Cl-initiated hydrogen abstraction of methyl fluoroacetate. <b>2015</b> , 172, 74-79		4
503	HCN elimination from vinyl cyanide: product energy partitioning, the role of hydrogen-deuterium exchange reactions and a new pathway. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 6948-55	3.6	21
502	Dispersion correction derived from first principles for density functional theory and Hartree-Fock theory. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 2161-8	2.8	12

501	Bicyclobutonium ions in biosynthesisinterconversion of cyclopropyl-containing sterols from orchids. <b>2015</b> , 137, 2085-8	16
500	Computational prediction for emission energy of iridium (III) complexes based on TDDFT calculations using exchange-correlation functionals containing various HF exchange percentages. 2  Journal of Molecular Modeling, 2015, 21, 22	6
499	Ferrocenyl pyrazoline based multichannel receptors for a simple and highly selective recognition of Hg2+ and Cu2+ ions. <b>2015</b> , 780, 20-29	22
498	Kinetics and mechanism of the reactions of OH radicals with p-nitroaniline in gas-phase and aqueous solution. <b>2015</b> , 1055, 68-77	7
497	An automated method to find transition states using chemical dynamics simulations. <b>2015</b> , 36, 222-34	111
496	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. <b>2015</b> , 71, 2421-2427	20
495	Regio- and diastereoselectivity of the 1,3-dipolar cycloaddition of ∃-aryl nitrone with methacrolein. A theoretical investigation. <b>2015</b> , 5, 22126-22134	4
494	A theoretical study on CH bond dissociation enthalpies of oxygen-containing fused heterocyclic compounds. <b>2015</b> , 41, 7207-7225	1
493	A comparison of the C-H bond dissociation enthalpies of sulfur-containing fused heterocyclic compounds to the C-H bond dissociation enthalpies in other heterocycles. <b>2015</b> , 36, 155-169	6
492	Computational investigation on NO3-initiated degradation of p,p?-DDE in atmosphere: Mechanism and kinetics. <b>2015</b> , 1068, 21-29	1
491	Atmospheric Degradation of CH2?C(CH3)C(O)OCH3 Initiated by OH Radicals: Mechanistic Study and Quantification of CH3C(O)C(O)OCH3 in NOx Free Air. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 8775-83 <sup>2.8</sup>	5
490	Antioxidative Reaction of Carotenes against Peroxidation of Fatty Acids Initiated by Nitrogen Dioxide: A Theoretical Study. <b>2015</b> , 119, 9640-50	10
489	Trends in the adsorption and reactivity of hydrogen on magnesium silicate nanoclusters. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 8951-63	7
488	The mechanism and kinetic model on the OH-initiated degradation of acetofenate in the atmosphere. <b>2015</b> , 103, 357-364	3
487	Theoretical investigation on mechanism, kinetics and thermochemistry of gas-phase reactions of ethyl trifluoroacetate with OH radicals. <b>2015</b> , 178, 79-85	1
486	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. <b>2015</b> , 5, 58464-58477	43
485	Structure and optoelectronic properties of helical pyridine-furan, pyridine-pyrrole and pyridine-thiophene oligomers. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 20647-57	10
484	Theoretical Investigation on Mechanistic and Kinetic Transformation of 2,2',4,4',5-Pentabromodiphenyl Ether. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 6404-11	17

483	Modeling Cu2+-Altomplexes from computational approaches. <b>2015</b> , 5, 092402		16
482	Chemical conversion pathways and kinetic modeling for the OH-initiated reaction of triclosan in gas-phase. <i>International Journal of Molecular Sciences</i> , <b>2015</b> , 16, 8128-41	3 (	3
481	Atmospheric degradation of lindane and 1,3-dichloroacetone in the gas phase. Studies at the EUPHORE simulation chamber. <b>2015</b> , 138, 112-9		12
480	On the stability of noble gas bound 1-tris(pyrazolyl)borate beryllium and magnesium complexes. <b>2015</b> , 39, 6778-6786	:	23
479	Validation of Methods for Computational Catalyst Design: Geometries, Structures, and Energies of Neutral and Charged Silver Clusters. <b>2015</b> , 119, 9617-9626	;	26
478	PBCDD/F formation from radical/radical cross-condensation of 2-Chlorophenoxy with 2-Bromophenoxy, 2,4-Dichlorophenoxy with 2,4-Dibromophenoxy, and 2,4,6-Trichlorophenoxy with 2,4,6-Tribromophenoxy. <b>2015</b> , 295, 104-11	:	11
477	DFT-ONIOM study of the dopamineECD complex: NBO and AIM analysis. <b>2015</b> , 93, 1115-1121	:	11
476	Quantum chemical investigation on the mechanism and kinetics of OH radical-initiated atmospheric oxidation of PCB-47. <b>2015</b> , 133, 53-60	:	15
475	Homolytic C-O cleavage in phosphates and sulfonates. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 3488-9 <u>9</u> .8	3 ;	7
474	A DFT Study of Inter- and Intramolecular Aryne Ene Reactions. <i>European Journal of Organic Chemistry</i> , <b>2015</b> , 2015, 2826-2834	2 :	23
473	Encapsulation of fluoroethanols in pristine and Stone Wales defect boron nitride nanotube DA DFT study. <i>Applied Surface Science</i> , <b>2015</b> , 345, 369-378	7 ]	7
472	How the intercalation of phenanthroline affects the structure, energetics, and bond properties of DNA base pairs: theoretical study applied to adenine-thymine and guanine-cytosine tetramers. 6.2 Journal of Chemical Theory and Computation, <b>2015</b> , 11, 2714-28	<b>1</b> -	22
471	Do Practical Standard Coupled Cluster Calculations Agree Better than Kohn-Sham Calculations with Currently Available Functionals When Compared to the Best Available Experimental Data for  Dissociation Energies of Bonds to 3d Transition Metals?. Journal of Chemical Theory and	1 !	91
470	Computation, <b>2015</b> , 11, 2036-52  Feasibility of intramolecular proton transfers in terpene biosynthesisguiding principles. <b>2015</b> , 137, 4134-4	40 :	26
469	Distinct photoproducts of hydroxylated polybromodiphenyl ethers from different photodegradation pathways: a case study of 2'-HO-BDE-68. <b>2015</b> , 17, 351-7	(	6
468	Understanding the role of the trifluoromethyl group in reactivity and regioselectivity in [3+2] cycloaddition reactions of enol acetates with nitrones. A DFT study. <i>Journal of Molecular Modeling</i> , 2 <b>2015</b> , 21, 104		3
467	Tension between Internal and External Modes of Stabilization in Carbocations Relevant to Terpene Biosynthesis: Modulating Minima Depth via C-HIIInteractions. <b>2015</b> , 17, 5388-91		19
466	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained C∃-Tetrasubstituted ∃-Amino Acids in Aib-based Peptides. <b>2015</b> , 119, 14003-13	:	14

465	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. <b>2015</b> , 5, 37119-37129		22
464	Competing mechanisms for the reaction of dichloropropynylborane with 2-tert-butylbutadiene. DielsAlder reaction versus alkynylboration. <b>2015</b> , 5, 70147-70155		6
463	Understanding the participation of 3-nitropyridine in polar DielsAlder reactions. A DFT study. <b>2015</b> , 1072, 37-42		12
462	A DFT study of the mechanism of Brlisted acid catalysed Povarov reactions. <b>2015</b> , 71, 9339-9345		13
461	Polar DielsAlder reaction of isoprene toward 2-bromocyclobutenone followed by a subsequent sodium hydroxide-assisted ring contraction reaction. A regio- and stereoselectivity and molecular mechanism study using DFT. <b>2015</b> , 39, 9525-9534		10
460	Homogeneous gas-phase formation of polychlorinated naphthalene from dimerization of 4-chlorophenoxy radicals and cross-condensation of phenoxy radical with 4-chlorophenoxy radical: Mechanism and kinetics study. <i>Chemical Physics Letters</i> , <b>2015</b> , 638, 153-160	2.5	6
459	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. <b>2015</b> , 5, 84797-84809		17
458	Understanding the molecular mechanism in a regiospecific [3 + 2] cycloaddition reaction including CD and CB interactions: an ELF topological analysis. <b>2015</b> , 5, 72959-72970		18
457	Influence of water on the homogeneous gas-phase formation mechanism of polyhalogenated dioxins/furans from chlorinated/brominated phenols as precursors. <b>2015</b> , 137, 142-8		13
456	Theoretical study on homolytic C(sp2) <b>D</b> cleavage in ethers and phenols. <b>2015</b> , 39, 6935-6943		7
456 455	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. <b>2015</b> , 5, 81153-81161		5
	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated	3.4	
455	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. <b>2015</b> , 5, 81153-81161  Intramolecular hydrogen bonding in N-salicylideneaniline: FT-IR spectrum and quantum chemical		5
455 454	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. <b>2015</b> , 5, 81153-81161  Intramolecular hydrogen bonding in N-salicylideneaniline: FT-IR spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , <b>2015</b> , 1102, 314-322  Non-classical CH?O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl		5
455 454 453	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. 2015, 5, 81153-81161  Intramolecular hydrogen bonding in N-salicylideneaniline: FT-IR spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2015, 1102, 314-322  Non-classical CH?O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. 2015, 5, 99299-993  Mechanism of stabilization of helix secondary structure by constrained CH-tetrasubstituted		5 14 29
455 454 453 452	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. 2015, 5, 81153-81161  Intramolecular hydrogen bonding in N-salicylideneaniline: FT-IR spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2015, 1102, 314-322  Non-classical CH?O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. 2015, 5, 99299-993  Mechanism of stabilization of helix secondary structure by constrained CH-tetrasubstituted H-amino acids. 2015, 119, 1350-61  Influence of the density functional and basis set on the relative stabilities of oxygenated isomers of diiron models for the active site of [FeFe]-hydrogenase. <i>Journal of Chemical Theory and</i>	11	5 14 29 21
455 454 453 452 451	Mechanism and kinetic study on the ring-opening degradation of 2,3,7,8-tetrachlorinated dibenzofuran initiated by OH radicals in waste incineration. 2015, 5, 81153-81161  Intramolecular hydrogen bonding in N-salicylideneaniline: FT-IR spectrum and quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2015, 1102, 314-322  Non-classical CH?O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. 2015, 5, 99299-993  Mechanism of stabilization of helix secondary structure by constrained CH-tetrasubstituted H-amino acids. 2015, 119, 1350-61  Influence of the density functional and basis set on the relative stabilities of oxygenated isomers of diiron models for the active site of [FeFe]-hydrogenase. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 205-14  Accurate, precise, and efficient theoretical methods to calculate anion-linteraction energies in	6.4	5 14 29 21 13

447	Polar DielsAlder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study. <i>Journal of Molecular Structure</i> , <b>2015</b> , 1079, 47-53	4	21
446	Localized Polycentric Orbital Basis Set for Quantum Monte Carlo Calculations Derived from the Decomposition of Kohn-Sham Optimized Orbitals. <b>2016</b> , 4, 10		2
445	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. <b>2016</b> , 21,		475
444	Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry. <b>2016</b> , 21,		218
443	A mechanistic insight into the effect of piperidine as an organocatalyst on the [3 + 2] cycloaddition reaction of benzalacetone with phenyl azide from a computational study. <b>2016</b> , 14, 7324-33		3
442	Scrutinizing "Invisible" astatine: A challenge for modern density functionals. <b>2016</b> , 37, 1345-54		29
441	Copper(II) and Zinc(II) Complexes of Conformationally Constrained Polyazamacrocycles as Efficient Catalysts for RNA Model Substrate Cleavage in Aqueous Solution at Physiological pH. <b>2016</b> , 22, 10426-37		16
440	Ionic S(N)i-Si Nucleophilic Substitution in N-Methylaniline-Induced Si-Si Bond Cleavages of Si2Cl6. <b>2016</b> , 22, 5010-6		10
439	The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. <b>2016</b> , 138, 16620-16631		15
438	Hartree potential dependent exchange functional. <b>2016</b> , 145, 084110		10
438	Hartree potential dependent exchange functional. <b>2016</b> , 145, 084110  The Physical Chemistry of Polyphenols. <b>2016</b> , 1-35		10
		6	
437	The Physical Chemistry of Polyphenols. <b>2016</b> , 1-35  Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO ->	Ó	4
437	The Physical Chemistry of Polyphenols. <b>2016</b> , 1-35  Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO -> HO + OH. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 33021-33030	6	4 26
437 436 435	The Physical Chemistry of Polyphenols. <b>2016</b> , 1-35  Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO -> HO + OH. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 33021-33030  Mechanism and kinetic properties for the gas-phase ozonolysis of Elonone. <b>2016</b> , 6, 114256-114263		4 26 1
437 436 435 434	The Physical Chemistry of Polyphenols. 2016, 1-35  Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO -> HO + OH. Physical Chemistry Chemical Physics, 2016, 18, 33021-33030  Mechanism and kinetic properties for the gas-phase ozonolysis of Elonone. 2016, 6, 114256-114263  Perspective: Kohn-Sham density functional theory descending a staircase. 2016, 145, 130901  Benchmark Calculations for Bond Dissociation Enthalpies of Unsaturated Methyl Esters and the	8	4 26 1
437 436 435 434 433	The Physical Chemistry of Polyphenols. 2016, 1-35  Quantum tunneling during interstellar surface-catalyzed formation of water: the reaction H + HO -> HO + OH. Physical Chemistry Chemical Physics, 2016, 18, 33021-33030  Mechanism and kinetic properties for the gas-phase ozonolysis of Bonone. 2016, 6, 114256-114263  Perspective: Kohn-Sham density functional theory descending a staircase. 2016, 145, 130901  Benchmark Calculations for Bond Dissociation Enthalpies of Unsaturated Methyl Esters and the Bond Dissociation Enthalpies of Methyl Linolenate. Journal of Physical Chemistry A, 2016, 120, 4025-36  Mechanism and kinetic properties of OH-initiated atmospheric oxidation degradation of	8	4 26 1 186 36

429	Kinetic Isotope Effects in Multipath VTST: Application to a Hydrogen Abstraction Reaction. <b>2016</b> , 120, 1911-8		7
428	Tautomerization mechanism and spectral properties of porphyringlucose complexes as models of antibacterial material. <b>2016</b> , 135, 1		9
427	A donor-acceptor triptycene-coumarin hybrid dye featuring a charge separated excited state and AIE properties. <b>2016</b> , 14, 5007-11		7
426	Theoretical studies on the mechanism and kinetics of the hydrogen abstraction reactions from C4F9OC2H5 (HFE-7200) by OH and Cl radicals. <b>2016</b> , 187, 9-14		5
425	Distributions, profiles and formation mechanisms of polychlorinated naphthalenes in cement kilns co-processing municipal waste incinerator fly ash. <b>2016</b> , 155, 348-357		41
424	A mechanistic insights into manganese-catalyzed oxidative homocoupling reactions of Grignard reagents: A computational DFT investigation. <b>2016</b> , 814, 25-34		9
423	MN15: A Kohn-Sham global-hybrid exchange-correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. <b>2016</b> , 7, 5032-5051		491
422	The polythiophene molecular segment as a sensor model for H2O, HCN, NH3, SO3, and H2S: a density functional theory study. <i>Journal of Molecular Modeling</i> , <b>2016</b> , 22, 127		18
421	Structure and mode of action of organophosphate pesticides: A computational study. <b>2016</b> , 1088, 9-23		17
420	Theoretical investigation of the singlet-triplet splittings for carbazole-based thermally activated delayed fluorescence emitters. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 26623-26629	5	36
419	Weakly bounded intermediates as a previous step towards highly-enantioselective iminium type additions of Eketo-sulfoxides and -sulfones. <b>2016</b> , 423, 308-318		9
418	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. <b>2016</b> , 14, 10427-10436		13
417	Thermodynamics of Metal Nanoparticles: Energies and Enthalpies of Formation of Magnesium Clusters and Nanoparticles as Large as 1.3 nm. <b>2016</b> , 120, 26110-26118		14
416	Theoretical kinetics study of thymine tautomerism and interaction of Na+ with its tautomers. <b>2016</b> , 114, 3356-3374		4
415	Correlated-Participating-Orbitals Pair-Density Functional Method and Application to Multiplet Energy Splittings of Main-Group Divalent Radicals. <i>Journal of Chemical Theory and Computation</i> , 6.2016, 12, 4274-83	4	41
414	A DFT study of the mechanism of NHC catalysed annulation reactions involving ∃,£unsaturated acyl azoliums and £haphthol. <b>2016</b> , 14, 8338-45		7
413	The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. <b>2016</b> , 94, 1133-1143		28
412	Destabilization of the metal site as a hub for the pathogenic mechanism of five ALS-linked mutants of copper, zinc superoxide dismutase. <b>2016</b> , 8, 1141-1150		4

411	A theoretical study on the antioxidant properties of methoxy-substituted chalcone derivatives: A case study of kanakugiol and pedicellin through their Fe (II and III) coordination ability. <b>2016</b> , 15, 1650048	15
410	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4778-4792	159
409	Mechanism for the growth of polycyclic aromatic hydrocarbons from the reactions of naphthalene with cyclopentadienyl and indenyl. <b>2016</b> , 162, 345-54	22
408	Computational study of H-abstraction reactions from CHOCHCHCl/CHCHOCHCHCl by Cl atom and OH radical and fate of alkoxy radicals. <i>Environmental Science and Pollution Research</i> , <b>2016</b> , 23, 23467-23484	16
407	Noble gas bound beryllium chromate and beryllium hydrogen phosphate: a comparison with noble gas bound beryllium oxide. <b>2016</b> , 6, 92786-92794	15
406	Multiscale Treatment for the Molecular Mechanism of a Diels-Alder Reaction in Solution: A QM/MM-MD Study. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 4735-4742	12
405	Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 22712-8	21
404	How the mechanism of a [3 + 2] cycloaddition reaction involving a stabilized N-lithiated azomethine ylide toward a Edeficient alkene is changed to stepwise by solvent polarity? What is the origin of its regio- and endo stereospecificity? A DFT study using NBO, QTAIM, and NCI analyses. <b>2016</b> , 6, 75299-75314	19
403	Cover Picture: Hierarchical Hybrids of Mesoporous NiCo2O4 Needles/Graphene/Carbon Nanotubes with High Performance for Lithium Ion Batteries and Oxygen Reduction Reactions (ChemNanoMat 12/2016). <b>2016</b> , 2, 1064-1064	
402	Restricted-Open-Shell G4(MP2)-Type Procedures. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 9299-9304 2.8	11
401	Size-Dependent Ligand Quenching of Ferromagnetism in Co(benzene) Clusters Studied with X-ray Magnetic Circular Dichroism Spectroscopy. <b>2016</b> , 7, 4568-4575	19
400	A DFT study of [3+2] cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole. <b>2016</b> , 70, 296-304	16
399	Ionisation energy, electron affinity, and mass spectral decomposition mechanisms of RDX isomers upon electron attachment and electron ionisation. <b>2016</b> , 114, 3556-3566	4
398	A computational study of radical initiated protein backbone homolytic dissociation on all natural amino acids. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 30972-30981	6
397	Mass spectral decomposition mechanisms of RDX isomers upon electron attachment and electron ionisation: a DFT study of normal mode activation incorporating Duschinsky rotations. <b>2016</b> , 114, 3277-3293	2
396	Variational transition state theory with multidimensional tunnelling and kinetic isotope effects in the reactions of C2H6, C2H5D and C2D6 with .CCl3 to produce CHCl3 and CDCl3. <b>2016</b> , 114, 2195-2203	5
395	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mgn0, $\exists$ 1, n = 1 $\blacksquare$ . <b>2016</b> , 120, 13275-13286	27
394	Thermolysis biradical mechanisms in endoperoxides: A challenge for density functional theory?. <b>2016</b> , 135, 1	2

393	Theoretical kinetic study of the reaction of SF5 radical with F2, Cl2 and SF5. <b>2016</b> , 1090, 41-46	5
392	Understanding the carbenoid-type reactivity of nitrile ylides in [3+2] cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study. <b>2016</b> , 135, 1	20
391	Rate coefficients for hydrogen abstraction reaction of pinonaldehyde (C10H16O2) with Cl atoms between 200 and 400 K: A DFT study. <b>2016</b> , 128, 977-989	1
390	The choice of appropriate density functional for the calculation of static first hyperpolarizability of azochromophores and stacking dimers. <i>International Journal of Quantum Chemistry</i> , <b>2016</b> , 116, 103-112 <sup>2.1</sup>	16
389	Products, mechanism, and kinetics of OH radical-initiated oxidation degradation of 2,4,4?-trichlorobiphenyl in the atmosphere. <b>2016</b> , 6, 61794-61802	6
388	Theoretical study of the regio- and stereoselectivity of the intramolecular Povarov reactions yielding 5H-chromeno[2,3-c] acridine derivatives. <b>2016</b> , 6, 15759-15769	6
387	Gas phase enthalpies of formation, isomerization, and disproportionation of mono-through tetra-substituted tetrahedranes: A G4(MP2)/G4 theoretical study. <b>2016</b> , 1075, 30-37	4
386	Hydrogen-Bond Accepting Properties of New Heteroaromatic Ring Chemical Motifs: A Theoretical Study. <b>2016</b> , 56, 322-34	19
385	Design of new disulfide-based organic compounds for the improvement of self-healing materials. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 1758-70	98
384	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. <b>2016</b> , 120, 1894-910	19
383	Methane CH bond activation by niobium oxides: Theoretical analyses of the bonding and reactivity properties of Nbomn+ (m = 1, 2; n = 0, 1, 2). <b>2016</b> , 802, 49-59	8
382	MllerPlesset 2 and density functional theory studies of the interaction between aromatic compounds and Zn-porphyrins. <b>2016</b> , 1084, 133-139	3
381	Photodissociation of acryloyl chloride at 193 nm: interpretation of the product energy distributions, and new elimination pathways. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 5019-26	8
380	Antioxidant activity of mildbone and mildbenone secondary metabolites of Erythrina mildbraedii Harms: A theoretical approach. <b>2016</b> , 1077, 106-112	8
379	A new model for Cl bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of [3+2] cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes. <b>2016</b> , 72, 1524-1532	52
378	Terthiophene as a model sensor for some atmospheric gases: theoretical study. <b>2016</b> , 114, 584-591	15
377	Theoretical investigation on ratiometric two-photon fluorescent probe for Zn2+ detection based on ICT mechanism. <i>Journal of Molecular Structure</i> , <b>2016</b> , 1114, 65-77	6
376	QSAR study of the acute toxicity to fathead minnow based on a large dataset. SAR and QSAR in Environmental Research, <b>2016</b> , 27, 147-64	18

375	Computational study on alkenyl/aryl C(sp2) <b>D</b> homolytic cleavage of carboxylates and carbamates. <b>2016</b> , 6, 26514-26525		3
374	Looking for the interactions between omeprazole and amoxicillin in a disordered phase. An experimental and theoretical study. <b>2016</b> , 156, 70-7		16
373	Theoretical characterization of first and second generation Grubbs catalysts in styrene cross-metathesis reactions: insights from conceptual DFT. <b>2016</b> , 6, 755-766		12
372	Investigation of the effect of Btacking interaction on the properties of IONH2 functional group of benzamide. <i>Structural Chemistry</i> , <b>2016</b> , 27, 731-737	1.8	5
371	Structure and stability of clusters of Elanine in the gas phase: importance of the nature of intermolecular interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 5465-5476	3.6	4
370	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with ketenes. <b>2017</b> , 15, 1618-1627		27
369	Predicting bond dissociation energy and bond length for bimetallic diatomic molecules: a challenge for electronic structure theory. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 5839-5854	3.6	16
368	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists. <b>2017</b> , 225-267	,	1
367	Chromium(III) complexes bearing bis(benzotriazolyl)pyridine ligands: synthesis, characterization and ethylene polymerization behavior. <b>2017</b> , 70, 803-818		5
366	Rhodium Complexes Promoting C-O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. <b>2017</b> , 23, 5232-5243		6
365	A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds. <i>SAR and QSAR in Environmental Research</i> , <b>2017</b> , 28, 133-150	3.5	8
364	Synthesis of three crystalline forms of Al2O3 featuring rod-like fibers and their effect on the gaseous degradation of 1-chloronaphthalene. <b>2017</b> , 4, 994-1004		9
363	Efficient protocol for quantum Monte Carlo calculations of hydrogen abstraction barriers: Application to methanol. <i>International Journal of Quantum Chemistry</i> , <b>2017</b> , 117, e25361	2.1	11
362	A theoretical study of phosphorescent Cu(I) complexes with 2-(2'quinolyl)imidazole and POP mixed ligands. <b>2017</b> , 45, 9-19		12
361	A Benchmark Study of Kinetic Isotope Effects and Barrier Heights for the Finkelstein Reaction. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 2311-2321	2.8	9
360	In silico environmental chemical science: properties and processes from statistical and computational modelling. <b>2017</b> , 19, 188-202		16
359	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. <b>2017</b> , 73, 1718-1724		52
358	How hydroxylation affects hydrogen adsorption and formation on nanosilicates. <b>2017</b> , 7, 1-8		7

357	Can Kohn-Sham density functional theory predict accurate charge distributions for both single-reference and multi-reference molecules?. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 12898-12912	40
356	Toward understanding regioselectivity and molecular mechanism in the synthesis of CF2H-containing 2-pyrazolines: A molecular electron-density theory study. <b>2017</b> , 199, 77-91	11
355	A turn-on type stimuli-responsive fluorescent dye with specific solvent effect: Implication for a new prototype of paper using water as the ink. <b>2017</b> , 184, 7-12	11
354	Assessment of electronic structure methods for the determination of the ground spin states of Fe(ii), Fe(iii) and Fe(iv) complexes. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 13049-13069	72
353	Non-pericyclic cycloaddition of gem-difluorosubstituted azomethine ylides to the C[double bond, length as m-dash]O bond: computational study and synthesis of fluorinated oxazole derivatives. <b>2017</b> , 15, 4579-4586	3
352	Accurate Relative Energies and Binding Energies of Large Ice-Liquid Water Clusters and Periodic Structures. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 4030-4038	15
351	Benchmarking Quantum Chemical Methods: Are We Heading in the Right Direction?. <b>2017</b> , 56, 11011-11018	90
350	Influence of Alcohol Fluorination on Hydrogen-Bond Acidity of Conformationally Flexible Substrates. <b>2017</b> , 23, 2811-2819	24
349	Desulfination by 2'-hydroxybiphenyl-2-sulfinate desulfinase proceeds electrophilic aromatic substitution by the cysteine-27 proton. <b>2017</b> , 8, 5078-5086	7
348	A DFT computational study on the molecular mechanism of reaction between pyridinium salts and Eleficient ethylenes: Why furan derivatives are formed instead of feasible cyclopropane derivatives and [3 + 2] cycloadducts?. <b>2017</b> , 1114, 87-100	5
347	A molecular electron density theory study of the $[3 + 2]$ cycloaddition reaction of nitrones with strained allenes. <b>2017</b> , 7, 26879-26887	19
346	Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. <b>2017</b> , 115, 2315-2372	891
345	Theoretical Study of the BF-Promoted Rearrangement of Oxiranyl N-Methyliminodiacetic Acid Boronates. <i>Journal of Organic Chemistry</i> , <b>2017</b> , 82, 5917-5925	12
344	Mechanistic insights on the reduction of glutathione disulfide by protein disulfide isomerase. <b>2017</b> , 114, E4724-E4733	31
343	Theoretical and experimental insights into the EDH-mediated mineralization mechanism of flutriafol. <b>2017</b> , 235, 223-232	14
342	Transportation of hydrogen atom and molecule through X 12 Y 12 nano-cages. <b>2017</b> , 42, 11439-11451	40
341	Convergence of Computed Aqueous Absorption Spectra with Explicit Quantum Mechanical Solvent. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 2159-2171  6.4	46
340	Molecular Mechanism of Dioxin Formation from Chlorophenol based on Electron Paramagnetic Resonance Spectroscopy. <b>2017</b> , 51, 4999-5007	31

339	Hydrogenation and Deuteration of C2H2and C2H4on Cold Grains: A Clue to the Formation Mechanism of C2H6with Astronomical Interest. <b>2017</b> , 837, 155	19
338	Ab Initio Studies on the Clathrate Hydrates of Some Nitrogen- and Sulfur-Containing Gases. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 2620-2626	12
337	Computational study on <b>CB</b> homolytic bond dissociation enthalpies of organoboron compounds. <b>2017</b> , 41, 1346-1362	9
336	Synthesis, X-ray, 1H-NMR and DFT analysis of the phthalimidellydrazone probes as selective anion sensor. <b>2017</b> , 29, 417-429	10
335	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 3.6 <b>2017</b> , 19, 32184-32215	738
334	Theoretical study on homolytic B <b>B</b> cleavages of diboron(4) compounds. <b>2017</b> , 7, 49251-49272	6
333	Experimental and theoretical studies of the [3,3]-sigmatropic rearrangement of prenyl azides. <b>2017</b> , 7, 47527-47538	9
332	Reactivity of 3-Oxo-Elactams with Respect to Primary Amines-An Experimental and Computational Approach. <b>2017</b> , 23, 18002-18009	5
331	Theoretical studies on the mechanism and kinetics of the hydrogen abstraction reactions of threo-CF3CHFCHFC2F5 and erythro-CF3CHFCHFC2F5 (HFC-43-10mee) by OH radicals. <b>2017</b> , 1119, 59-64	5
330	Impact of Donor Substitution Pattern on the TADF Properties in the Carbazolyl-Substituted Triazine Derivatives. <b>2017</b> , 121, 23618-23625	42
329	Following the Molecular Mechanism of Decarbonylation of Unsaturated Cyclic Ketones Using Bonding Evolution Theory Coupled with NCI Analysis. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 8504-8517	32
328	Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction. 2017, 846, 43	22
327	The growth mechanism of polycyclic aromatic hydrocarbons from the reactions of anthracene and phenanthrene with cyclopentadienyl and indenyl. <b>2017</b> , 189, 265-276	23
326	Experimental and Theoretical Investigation of the Reaction of Amines with Methyl Propiolate.  ChemistrySelect, 2017, 2, 8465-8470	
325	A molecular electron density theory study of [3 + 2] cycloaddition reactions of chiral azomethine ylides with Ehitrostyrene. <b>2017</b> , 136, 1	16
324	Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study. <i>Journal of Molecular Structure</i> , <b>2017</b> , 1150, 447-458	13
323	Theoretical tuning of the singlet-triplet energy gap to achieve efficient long-wavelength thermally activated delayed fluorescence emitters: the impact of substituents. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 21639-21647	11
322	Understanding the Reactivity of CO and NO Radicals toward S-Containing and Aromatic Amino Acids. <b>2017</b> , 121, 7621-7632	7

321	Density functional evaluation and a feasibility study of intramolecular thionethiol tautomerization. <i>International Journal of Quantum Chemistry</i> , <b>2017</b> , 117, e25427	2.1	4	
320	Adsorption properties of the phosgene molecule on pristine graphyne, BN- and Si-doped graphynes: DFT study. <b>2017</b> , 7, 2626-2631		24	
319	MNgCCH (M = Cu, Ag, Au; Ng = Xe, Rn): The First Set of Compounds with M-Ng-C Bonding Motif.  Journal of Physical Chemistry A, <b>2017</b> , 121, 6491-6499	2.8	22	
318	Quantenchemische Methoden im Leistungsvergleich: Stimmt die Richtung noch?. <b>2017</b> , 129, 11155-1116	53	11	
317	Why are GGAs so accurate for reaction kinetics on surfaces? Systematic comparison of hybrid vs. nonhybrid DFT for representative reactions. <b>2017</b> , 146, 234103		10	
316	A Theoretical Study on the Dynamics of O(3P) + H2S(1A1) Reaction on an Interpolated Potential Energy Surface. <b>2017</b> , 90, 1141-1151		3	
315	Atmospheric chemistry of CH3O: its unimolecular reaction and reactions with H2O, NH3, and HF. <b>2017</b> , 7, 56211-56219		11	
314	Tunneling Reaction Kinetics for the Hydrogen Abstraction Reaction H + HS -> H + HS in the Interstellar Medium. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 9736-9741	2.8	18	
313	Performance of tertiary amines as the absorbents for CO 2 capture: Quantum mechanics and molecular dynamics studies. <b>2017</b> , 47, 154-166		13	
312	How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne, and Ne?. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 6068-6077	6.4	19	
311	The Hydrogen Abstraction Reaction HS + OH -> HO + SH: Convergent Quantum Mechanical Predictions. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 9136-9145	2.8	8	
310	Kinetic investigations of Cl atom initiated photo-oxidation reactions of cyclic unsaturated hydrocarbons in the gas phase: an experimental and theoretical study. <b>2017</b> , 41, 7491-7505		13	
309	Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products. <i>Environmental Science and Pollution Research</i> , <b>2017</b> , 24, 18458-18469	5.1	17	
308	OH-initiated atmospheric oxidation mechanism of 1-chloropyrene: A theoretical study. <b>2017</b> , 1115, 144-	150	3	
307	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd , Mn , and Zn -Fe Promiscuous Organophosphate-Degrading Enzyme: Reaction Mechanisms. <b>2017</b> , 23, 13742-13753		6	
306	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> , <b>2017</b> , 13, 3478-3492	6.4	22	
305	Applications of metal-organic frameworks in adsorption/separation processes via hydrogen bonding interactions. <b>2017</b> , 310, 197-215		277	
304	Electrophilic activation of CO2 in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. <b>2017</b> , 136, 1		6	

303	Application of quantum mechanics/molecular mechanics methods in the study of enzymatic reaction mechanisms. <b>2017</b> , 7, e1281		104
302	A DFT study of the mechanism and selectivities of the $[3]$ cycloaddition reaction between 3-(benzylideneamino)oxindole and trans-Ehitrostyrene. <b>2017</b> , 30, e3637		17
301	Unveiling the Reaction Machinery of the [AuI]-Catalyzed Synthesis of Substituted Acenes by a [1,5]-H Shift Cascade Reaction. <b>2017</b> , 9, 316-321		2
300	Are boat transition states likely to occur in Cope rearrangements? A DFT study of the biogenesis of germacranes. <b>2017</b> , 13, 1969-1976		2
299	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. <b>2017</b> , 22,		48
298	A theoretical investigation on the neutral Cu(I) phosphorescent complexes with azole-based and phosphine mixed ligand. <b>2018</b> , 116, 898-909		2
297	Theoretical study of radiative and nonradiative decay rates for Cu(i) complexes with double heteroleptic ligands. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 9419-9428	3.6	11
296	Kinetic and mechanistic insight into the formation of amphetamine using the Leuckart Wallach reaction and interaction of the drug with GpCECpG base-pair step of DNA: a DFT study. <b>2018</b> , 149, 1045-	1057	5
295	A dichotomy in the enantioselective oxidation of aryl benzyl sulfides: A combined experimental and computational work. <b>2018</b> , 74, 2041-2047		6
294	Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF, FeF Ethane, and FeF Ethylene. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 2563-2579	2.8	8
293	A molecular electron density theory study of the $[3]$ cycloaddition reaction between an azomethine imine and electron deficient ethylenes. <b>2018</b> , 31, e3830		18
292	Computational Study on N-N Homolytic Bond Dissociation Enthalpies of Hydrazine Derivatives. Journal of Physical Chemistry A, <b>2018</b> , 122, 2764-2780	2.8	5
291	Reactivity of cycloparaphenylenes: Studying the possible growth of single-walled carbon nanotubes with DFT methods. <i>Chemical Physics Letters</i> , <b>2018</b> , 697, 17-22	2.5	2
290	Magnetic behavior of Si-Ge bond in SixGe4-x nano-clusters. <b>2018</b> , 549, 58-60		
289	Oxidation of Acid, Base, and Amide Side-Chain Amino Acid Derivatives via Hydroxyl Radical. <b>2018</b> , 122, 4956-4971		3
288	Solvent effects and potential of mean force study of the S N 2 reaction of CH 3 +CN In water. <b>2018</b> , 27, 033401		1
287	Theoretical study on the reactions of a series of polybromobenzenes with OH radicals: mechanism, kinetics, and QSAR. <b>2018</b> , 96, 436-446		
286	Covalent or Non-Covalent? A Mechanistic Insight into the Enantioselective Brfisted Acid Catalyzed Dearomatization of Indoles with Allenamides. <b>2018</b> , 10, 2442-2449		14

285	Effect of electron-withdrawing terminal group on BDT-based donor materials for organic solar cells: a theoretical investigation. <b>2018</b> , 137, 1		10
284	Mechanism and thermal rate constants for complete series reactions of bromochlorophenols with H. <b>2018</b> , 8, 4259-4272		3
283	An infrared measurement of chemical desorption from interstellar ice analogues. <b>2018</b> , 2, 228-232		40
282	Understanding the molecular mechanism of thio-Claisen rearrangement of allyl phenyl sulfide and allyl vinyl sulfide using bonding evolution theory coupled with NCI analysis. <b>2018</b> , 39, 350-366		7
281	Atmospheric chemistry of CHCHO: the hydrolysis of CHCHO catalyzed by HSO. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 7701-7709	3.6	24
280	Supramolecular polymer chemistry meets computational chemistry: theoretical simulations on advanced self-assembling chiral materials. <b>2018</b> , 30, 876-890		2
279	Hydrogen's isotopic exchange reaction in the C-methyl sides in the medicinal agent xymedon: NMR spectroscopy and ab initio calculations. <b>2018</b> , 31, e3804		1
278	The experimental observation, mechanism and kinetic studies on the reaction of hexachloro-1,3-butadiene initiated by typical atmospheric oxidants. <b>2018</b> , 627, 256-263		7
277	The Role of Planarity versus Nonplanarity in the Electronic Communication of TCAQ-Based Push-Pull Chromophores. <b>2018</b> , 83, 300-307		12
276	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives. <i>Journal of Organic Chemistry</i> , <b>2018</b> , 83, 2182-2197	4.2	72
275	An intramolecular oxa-Michael reaction on $\Box$ , $\Box$ insaturated $\Box$ -amino- $\Box$ hydroxycarboxylic acid esters. Synthesis of functionalized 1,3-dioxanes. <b>2018</b> , 16, 1277-1286		5
274	A combined experimental and theoretical study of the thermal [3+2] cycloaddition of carbonyl ylides with activated alkenes. <i>Journal of Molecular Structure</i> , <b>2018</b> , 1157, 276-287	3.4	7
273	Rational Density Functional Selection Using Game Theory. <b>2018</b> , 58, 61-67		15
272	A new mechanism for internal nucleophilic substitution reactions. <b>2018</b> , 16, 1101-1112		1
271	Formation of Fluorinated Amido Esters through Unexpected C3-C4 Bond Fission in 4-Trifluoromethyl-3-oxo-Elactams. <b>2018</b> , 13, 421-431		3
270	Theoretical insight into the photodeactivation pathway of the tetradentate Pt(II) complex: The Etonjugation effect. <b>2018</b> , 32, e4220		4
269	A molecular electron density theory study of the chemo- and regioselective [3 + 2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. <b>2018</b> , 501, 128-137		9
268	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. <i>European Journal of Organic Chemistry</i> , <b>2018</b> , 2018, 1107-1120	3.2	47

267	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, <b>2018</b> , 14, 2596-2608	6.4	122
266	Role of 6-Mercaptopurine in the potential therapeutic targets DNA base pairs and G-quadruplex DNA: insights from quantum chemical and molecular dynamics simulations. <b>2018</b> , 36, 1369-1401		14
265	Theoretical studies on microstructures, stabilities and formation conditions of some sour gas in the type I, II, and H clathrate hydrates. <i>Journal of Molecular Structure</i> , <b>2018</b> , 1153, 292-298	3.4	О
264	Stable NCNgNSi (Ng=Kr, Xe, Rn) Compounds with Covalently Bound C-Ng-N Unit: Possible Isomerization of NCNSi through the Release of the Noble Gas Atom. <b>2018</b> , 24, 2879-2887		18
263	Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound M[] B Clusters (M=Nb, Ta). <b>2018</b> , 24, 3590-3598		14
262	Alternating phenylene and furan/pyrrole/thiophene units-based oligomers: A computational study of the structures and optoelectronic properties. <i>Chemical Physics Letters</i> , <b>2018</b> , 692, 152-159	2.5	3
261	Hydrogen bonding cooperation in glycine-(water)n clusters studied by density functional theory calculations. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25556	2.1	
260	A possible reason behind the initial formation of pentagonal dodecahedron cavities in sl-methane hydrate nucleation: A DFT study. <i>Chemical Physics Letters</i> , <b>2018</b> , 691, 415-420	2.5	1
259	Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenyl-based organic pollutants. <i>International Journal of Quantum Chemistry</i> , <b>2018</b> , 118, e25533	2.1	11
258	All-Thiophene-Based Double Helix: Synthesis, Crystal Structure, Chiroptical Property and Arylation. <b>2018</b> , 3, 16014-16020		6
257	Density functional benchmark studies on structure and energetics of 3d transition metal mononitrides. <b>2018</b> , 130, 1		3
256	Molecular Mechanism of ATP Hydrolysis in an ABC Transporter. <b>2018</b> , 4, 1334-1343		38
255	QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase. <b>2018</b> , 8, 10267-10278		19
254	Theoretical insight into structural and electronic properties of cationic Scn+ (n=2-13): A benchmark study. <b>2018</b> , 86, 60-68		2
253	Theoretical and Kinetic Properties of OH Radical-Initiated Oxidation of Galaxolide in the Atmosphere. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 9151-9159	2.8	4
252	Tunnelling dominates the reactions of hydrogen atoms with unsaturated alcohols and aldehydes in the dense medium. <i>Astronomy and Astrophysics</i> , <b>2018</b> , 617, A25	5.1	8
251	Multipath VTST rate constants for D + methyl formate reactions: Importance of torsional anharmonicity and conformational flexibility for combustion chemistry. <i>Chemical Physics Letters</i> , <b>2018</b> , 711, 132-137	2.5	5
250	Mechanistic Studies of a Flavin Monooxygenase: Sulfur Oxidation of Dibenzothiophenes by DszC. <b>2018</b> , 8, 9298-9311		10

## (2018-2018)

249	Effect of the Number and Substitution Pattern of Carbazole Donors on the Singlet and Triplet State Energies in a Series of Carbazole-Oxadiazole Derivatives Exhibiting Thermally Activated Delayed Fluorescence. <b>2018</b> , 30, 6389-6399		14
248	Cycloaddition reactions of pristine and endohedral fullerene molecules: possible anticancer activity. <i>Journal of Molecular Modeling</i> , <b>2018</b> , 24, 268	2	4
247	From interstellar carbon monosulfide to methyl mercaptan: paths of least resistance. <i>Astronomy and Astrophysics</i> , <b>2018</b> , 615, L2	5.1	16
246	### Estacking Interactions of 3a-Aryl-2,3,3a,4-tetrahydro-1H-benzo[d]pyrrolo[1,2-a]imidazol-1-ones, X-Ray and DFT Study. <b>2018</b> , 2, 1120		
245	Theoretical study on abnormal trans-effect of chloride, bromide and iodide ligands in iridium complexes. <b>2018</b> , 1138, 1-6		2
244	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> , <b>2018</b> , 122, 4790-4800	2.8	27
243	When Hartree-Fock exchange admixture lowers DFT-predicted barrier heights: Natural bond orbital analyses and implications for catalysis. <b>2018</b> , 148, 244106		20
242	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 23175-23194	3.6	68
241	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , <b>2018</b> , 83, 10959-10973	4.2	24
240	Guanidinium cationWater clusters. <b>2018</b> , 137, 1		7
239	Design of a Novel Series of Donor-Acceptor Frameworks via Superalkali-Superhalogen Assemblage to Improve the Nonlinear Optical Responses. <b>2018</b> , 57, 9335-9347		31
	the production of the contract of the production		
238	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. <b>2018</b> , 16, 5474-5482		5
238	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and	39 <b>1:3</b> 740	
	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. <b>2018</b> , 16, 5474-5482	89 <b>1</b> : <b>7</b> 40	
237	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. <b>2018</b> , 16, 5474-5482  Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 73  Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes.	89 <b>1</b> : <b>7</b> 40	0120
237	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. <b>2018</b> , 16, 5474-5482  Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 73  Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. <b>2018</b> , 23,  A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels? Alder and Polar	3.6	<b>01</b> 20
<ul><li>237</li><li>236</li><li>235</li></ul>	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. 2018, 16, 5474-5482  Noble Gas Inserted Metal Acetylides (Metal = Cu, Ag, Au). <i>Journal of Physical Chemistry A</i> , 2018, 122, 73  Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. 2018, 23,  A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels?Alder and Polar Alder-ene Reactions. 2018, 23,  Cyanide-isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal		7 9

231	Statistically representative databases for density functional theory via data science. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 19092-19103	3.6	13
230	Importance of Conformational Change in Excited States for Efficient Thermally Activated Delayed Fluorescence. <b>2019</b> , 123, 19322-19332		11
229	Multicomponent solid forms of the uric acid reabsorption inhibitor lesinurad and cocrystal polymorphs with urea: DFT simulation and solubility study. <b>2019</b> , 75, 1102-1117		8
228	Mechanism and kinetic study of the reaction of benzoic acid with OH, NO and SO radicals in the atmosphere <b>2019</b> , 9, 18971-18977		6
227	Formation of interstellar propanal and 1-propanol ice: a pathway involving solid-state CO hydrogenation. <i>Astronomy and Astrophysics</i> , <b>2019</b> , 627, A1	5.1	16
226	Theoretical Study of the Potential Energy Profile of the HBr + CO -> HOCO + BrEReaction. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 9791-9799	2.8	3
225	Hypercoordinated organotin(IV) compounds containing C,O- and C,N- chelating ligands: Synthesis, characterisation, DFT studies and polymerization behaviour. <b>2019</b> , 900, 120910		7
224	Evaluating Computational Chemistry Methods for Isotopic Fractionation between CO(g) and HO(g). <b>2019</b> , 59, 4663-4677		1
223	Understanding H Formation on Hydroxylated Pyroxene Nanoclusters: Ab Initio Study of the Reaction Energetics and Kinetics. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 9282-9291	2.8	5
222	A Mechanistic Insight into the Cu(II)-Catalyzed CN and CD Coupling Reaction of Arylglyoxylic Acids with Isatins; A DFT Investigation. <i>European Journal of Organic Chemistry</i> , <b>2019</b> , 2019, 6776-6782	3.2	O
221	Application of quantum chemical methods in polymer chemistry. <b>2019</b> , 38, 343-403		10
220	Stereoselective cyclopropanation of olefins through ammonium ylides: A molecular electron density theory study. <b>2019</b> , 32, e4008		1
219	Substitution induced tunable emission of an airplane-like pyrene-based fluorophore: First-principles study. <i>Chemical Physics Letters</i> , <b>2019</b> , 734, 136726	2.5	1
218	Computational investigation on the reaction of dimethyl ether with nitric dioxide. I. Underlying mechanism and accurate energetics. <b>2019</b> , 138, 1		2
217	The effect of heteroatoms in carbonaceous surfaces: computational analysis of H chemisorption on to a PANH and Si-doped PAH. <b>2019</b> , 490, 172-180		3
216	Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical: Hydrogen and Chlorine Atom Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 8954-8967	2.8	6
215	Quantum approach to the mechanism of monothiopyrophosphate isomerization. <i>Journal of Molecular Modeling</i> , <b>2019</b> , 25, 286	2	3
214	Understanding the mechanism of HS oxidation by flavin-dependent sulfide oxidases: a DFT/IEF-PCM study. <i>Journal of Molecular Modeling</i> , <b>2019</b> , 25, 308	2	2

213	Formation of amines: hydrogenation of nitrile and isonitrile as selective routes in the interstellar medium. <i>Astronomy and Astrophysics</i> , <b>2019</b> , 628, A15	5.1	8
212	Hierarchy of Commonly Used DFT Methods for Predicting the Thermochemistry of Rh-Mediated Chemical Transformations. <b>2019</b> , 4, 15435-15443		7
211	Strong cooperative interaction of lithium and hydrogen bonds between 4-aminobenzoic acid modified interlayer and polysulfides for lithium-sulfur batteries. <b>2019</b> , 155, 553-561		11
210	Mechanisms and kinetic studies of OH-initiated atmospheric oxidation of methoxyphenols in the presence of O and NO. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 21856-21866	3.6	14
209	Investigation on the Thermal Dissociation of Vinyl Nitrite with a Saddle Point Involved. <b>2019</b> , 4, 16052-1	16061	2
208	New Insight into an Old Problem: Analysis, Interpretation, and Theoretical Modeling of the Absorption and Magnetic Circular Dichroism Spectra of Monomeric and Dimeric Zinc Phthalocyanine Cation Radical. <b>2019</b> , 58, 14120-14135		9
207	Unveiling the high reactivity of cyclohexynes in $[3 + 2]$ cycloaddition reactions through the molecular electron density theory. <b>2019</b> , 17, 498-508		8
206	Benchmark DFT studies on C-CN homolytic cleavage and screening the substitution effect on bond dissociation energy. <i>Journal of Molecular Modeling</i> , <b>2019</b> , 25, 47	2	11
205	Theoretical Insights into the Role of Water Molecules in the Guanidinium-Based Protein Denaturation Process in Specific to Aromatic Amino Acids. <b>2019</b> , 123, 2191-2202		10
204	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 2966-2990	2.8	45
203	Benchmark of Density Functionals for the Calculation of the Redox Potential of Fe/Fe Within Protein Coordination Shells. <b>2019</b> , 7, 391		6
202	On the nature of organic electron density transfer complexes within molecular electron density theory. <b>2019</b> , 17, 6478-6488		6
201	How effectively bonding evolution theory retrieves and visualizes curly arrows: The cycloaddition reaction of cyclic nitrones. <i>International Journal of Quantum Chemistry</i> , <b>2019</b> , 119, e25985	2.1	9
200	Mechanistic and Kinetic Study on Self-/Cross- Condensation of PCTA/DT Formation Mechanisms from Three Types of Radicals of 2,4-Dichlorothiophenol. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	1
199	Design of a novel series of small molecule donors for application in organic solar cells. <b>2019</b> , 186, 72-83		10
198	Alcohols on the Rocks: Solid-State Formation in a H3CC?CH + OH Cocktail under Dark Cloud Conditions. <i>ACS Earth and Space Chemistry</i> , <b>2019</b> , 3, 986-999	3.2	10
197	The mechanism and kinetics of the gas-phase reactions of OH radicals with O,O-diethyl methylphosphonothioate, (C2H5O)2P(S)CH3: Theoretical investigations. <b>2019</b> , 1158, 36-40		
196	Kinetic and mechanistic insight into the OH-initiated atmospheric oxidation of 2,3,7,8-tetrachlorodibenzo-p-dioxin via OH-addition and hydrogen abstraction pathways: A theoretical investigation. <b>2019</b> , 679, 106-114		8

195	Quantum Chemical and Kinetic Study on Radical/Molecule Formation Mechanism of Pre-Intermediates for PCTA/PT/DT/DFs from 2-Chlorothiophenol and 2-Chlorophenol Precursors. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	2
194	Long-range screened hybrid-functional theory satisfying the local-density linear response. <b>2019</b> , 99,		10
193	Cu(II) and Zn(II) Complexes with Dinitrobenzoates and Pyrazolyl Ligands: Structural and Thermal Stability Influence of N⊞ Moiety. <b>2019</b> , 19, 3348-3357		5
192	DFT study on the regio- and stereoselectivity of the organocatalytic aza-Diels-Alder reaction of crotonaldehyde and cyclic 1-aza-1,3-butadiene. <i>Structural Chemistry</i> , <b>2019</b> , 30, 1831-1842	1.8	1
191	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. <b>2019</b> , 75, 2807-2816		3
190	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 3761-3781	2.8	53
189	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. <b>2019</b> , 75, 1961-1967		18
188	A molecular electron density theory study of Diels-Alder reaction between Danishefsky's diene and (2E)-3-phenyl-2-(trifluoromethyl) acrylonitrile. <b>2019</b> , 32, e3937		1
187	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from $\square$ -Santonin. <b>2019</b> , 24,		21
186	Reinvestigation of Acetophenones Oxidation by Performic Acid in Formic Acid. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 1968-1972	2.8	O
185	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> , <b>2019</b> , 21, 7412-7428	3.6	23
184	Computational Study on the Atmospheric Oxidation Mechanism of 6-Chlorobenzo[a]pyrene Initiated by OH Radicals. <b>2019</b> , 93, 2710-2717		
183	The Gas-Phase Formation Mechanism of Dibenzofuran (DBF), Dibenzothiophene (DBT), and Carbazole (CA) from Benzofuran (BF), Benzothiophene (BT), and Indole (IN) with Cyclopentadienyl Radical. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	1
182	A Molecular Electron Density Theory Study of the Synthesis of Spirobipyrazolines through the Domino Reaction of Nitrilimines with Allenoates. <b>2019</b> , 24,		5
181	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. <b>2019</b> , 24,		5
180	A Novel Design Strategy for Suppressing Efficiency Roll-Off of Blue Thermally Activated Delayed Fluorescence Molecules through Donor-Acceptor Interlocking by C-C Bonds. <b>2019</b> , 9,		6
179	Fine Structural Tuning of Thieno[3,2- b] Pyrrole Donor for Designing Banana-Shaped Semiconductors Relevant to Organic Field Effect Transistors. <b>2019</b> , 59, 1930-1945		9
178	Toward the comprehensive calculations on the relationship between H, C, P chemical shifts, J, and the bonding structure of different phosphoryl benzamides. <b>2019</b> , 57, S108-S116		1

177	Theoretical kinetic study of the reaction between dimethyl disulfide and OH radicals. 2019, 40, 185-194	2
176	[3 + 2] cycloaddition reaction of N,N? cyclic azomethine imines toward highly electron-deficient nitroalkenes: A molecular electron density theory study. <b>2019</b> , 32, e3925	2
175	Kinetics and Mechanisms of the Hydrogen Abstraction Reactions of CF3CF2CH2CH2F and CF3CH2CH2CF3 with Hydroxyl Radicals: Theoretical Studies. <b>2019</b> , 218, 116-121	
174	Density functional theories study of the interactions between host ECyclodextrin and guest 8-Anilinonaphthalene-1-sulfonate: Molecular structure, HOMO, LUMO, NBO, QTAIM and NMR analyses. <b>2019</b> , 280, 218-229	20
173	Brominated dioxins and furans in a cement kiln co-processing municipal solid waste. <b>2019</b> , 79, 339-345	12
172	Hydrogen Abstraction Reaction HSe + OH -> HO + SeH: Comparison with the Analogous Hydrogen Sulfide and Water Reactions. <b>2019</b> , 58, 2069-2079	1
171	Scaling Procedures in Vibrational Spectroscopy. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2019</b> , 49-95	2
170	Influence of fluorination on alcohol hydrogen-bond donating properties. 2019, 301-324	2
169	The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree-Fock and Its Use in the reHISSB-D Density Functional Theory Method. <b>2019</b> , 40, 29-38	5
168	Ibuprofen-based chemosensor for efficient binding and sensing of Cu2+ ion in aqueous medium. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1199, 127003	9
167	Finding chemical concepts in the Hilbert space: Coupled cluster analyses of noncovalent interactions. <b>2020</b> , 10, e1442	25
166	Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of C-Mg bond of Grignard reagent. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26106	1
165	Elucidation of the Mechanism of Silver-Catalyzed Inverse Electron-Demand Diels-Alder (IEDDA) Reaction of 1,2-Diazines and Siloxy Alkynes. <b>2020</b> , 12, 366-372	2
164	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Diels-Alder reactions. <b>2020</b> , 18, 292-304	19
163	An excited state managing molecular design platform of blue thermally activated delayed fluorescence emitters by Elinker engineering. <b>2020</b> , 8, 1736-1745	10
162	Theoretical insight into the degradation of p-nitrophenol by OH radicals synergized with other active oxidants in aqueous solution. <b>2020</b> , 389, 121901	34
161	Density functional theory thermal rate constant calculation of hydrogen abstraction reactions of trans-cyc-CF2CF2CHFCHF and cyc-CF2CF2CF2CHFCH2 with OH radicals. <b>2020</b> , 229, 109415	
160	The aromatic character of the transition state structures (TSs) involved in pseudocyclic reactions of fluorinated compounds. <b>2020</b> , 229, 109421	1

159	Role of Microsolvation and Quantum Effects in the Accurate Prediction of Kinetic Isotope Effects: The Case of Hydrogen Atom Abstraction in Ethanol by Atomic Hydrogen in Aqueous Solution. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 847-859	6.4	6
158	Effect of ultrasound pretreatment on bromination of double-walled carbon nanotubes. <b>2020</b> , 259, 116	233	6
157	Stereoselective aziridination of imines via ammonium ylides: A molecular electron density theory study. <b>2020</b> , 57, 419-427		3
156	Are the Absorption Spectra of Doxorubicin Properly Described by Considering Different Tautomers?. <b>2020</b> , 60, 513-521		2
155	Shedding light on the energetics, regioselectivity, stereoselectivity, and mechanistic aspects of [3 + 2] cycloaddition reaction between azomethine imines and 2-sulfolene through molecular electron density theory. <b>2020</b> , 33, e4042		1
154	Exploring effects of the trifluoromethyl substituent on the chemoselectivity and regioselectivity of [3+2] cycloadditions of thiocarbonyl S-methanides with $\oplus$ , Eunsaturated ketones. <i>Journal of the Chinese Chemical Society</i> , <b>2020</b> , 67, 703-710	1.5	2
153	A benzothiazolinic spiropyran for highly selective, sensitive and visible light controlled detection of copper ions in aqueous solution. <b>2020</b> , 390, 112265		8
152	Isomers in Interstellar Environments. I. The Case of Z- and E-cyanomethanimine. <b>2020</b> , 897, 158		9
151	Generalizing Double-Hybrid Density Functionals: Impact of Higher-Order Perturbation Terms. Journal of Chemical Theory and Computation, <b>2020</b> , 16, 7413-7430	6.4	7
150	Revealing the Origin of 🛮 facial and Regioselectivity in the Diels-Alder Reaction of Unsymmetrical, Cage-annulated 1,3-Cyclohexadiene with Ethyl Propiolate Dienophile: a DFT Study. <i>ChemistrySelect</i> , <b>2020</b> , 5, 13524-13529	1.8	1
149	A theoretical study on the role of stability of cytosine and its tautomers in DNA (deoxyribonucleic acid), and investigation of interactions of Na, K, Mg, Ca, Zn metal ions and OH radical with cytosine tautomers. <b>2020</b> , 1-18		О
148	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadium-Ligand Bonds. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 9757-9770	2.8	3
147	Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory. <b>2020</b> , 76, 131458		6
146	Unravelling the strain-promoted [3+2] cycloaddition reactions of phenyl azide with cycloalkynes from the molecular electron density theory perspective. <b>2020</b> , 44, 13633-13643		13
145	Revisiting immiscibility through DFT chemical descriptors. <b>2020</b> , 139, 1		О
144	The theoretical investigation of OH-induced degradation mechanisms of isoproturon. <i>Journal of Molecular Modeling</i> , <b>2020</b> , 26, 232	2	1
143	5-(-Trifluoromethylcarboxy)aminouracil as a Potential DNA Radiosensitizer and Its Radiochemical Conversion into -Uracil-5-yloxamic Acid. <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	0
142	Theoretical Prediction on the New Types of Noble Gas Containing Anions OBONgO and OCNNgO (Ng = He, Ar, Kr and Xe). <b>2020</b> , 25,		1

141	Understanding the Reactivity of Trimethylsilyldiazoalkanes Participating in [3+2] Cycloaddition Reactions towards Diethylfumarate with a Molecular Electron Density Theory Perspective. <b>2020</b> , 1, 3-	18	3
140	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> , <b>2020</b> , 22, 24951-24963	3.6	2
139	Theoretical analysis of the regio- and stereoselective synthesis of spiroisoxazolines. <i>Journal of Molecular Modeling</i> , <b>2020</b> , 26, 117	2	2
138	The inclusion behavior of 8-Anilino-1-naphthalene sulfonate into Cucurbit[7]uril: A DFT approach. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1217, 128390	3.4	3
137	Relationships between Orbital Energies, Optical and Fundamental Gaps, and Exciton Shifts in Approximate Density Functional Theory and Quasiparticle Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 4337-4350	6.4	10
136	Spin Splitting Energy of Transition Metals: A New, More Affordable Wave Function Benchmark Method and Its Use to Test Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 4416-4428	6.4	17
135	Rate coefficients and product branching ratios for (E)-2-butenal + H reactions. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 14246-14254	3.6	1
134	Theoretical studies on the kinetics of the hydrogen-abstraction reactions from 1,3,5-trioxane and 1,4-dioxane by OH radicals. <b>2020</b> , 45, 146867831989925		1
133	Curcumin based supramolecular ensemble for optical detection of Cu2+ and Hg2+ ions. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1211, 128091	3.4	5
132	Multi-coefficients correlation methods. <b>2020</b> , 10, e1474		3
131	Unveiling the Different Chemical Reactivity of Diphenyl Nitrilimine and Phenyl Nitrile Oxide in [3+2] Cycloaddition Reactions with (R)-Carvone through the Molecular Electron Density Theory. <b>2020</b> , 25,		19
130			
	Unravelling the regio- and stereoselective synthesis of bicyclic N,O-nucleoside analogues within the molecular electron density theory perspective. <i>Structural Chemistry</i> , <b>2020</b> , 31, 1-14	1.8	4
129		1.8	1
	molecular electron density theory perspective. <i>Structural Chemistry</i> , <b>2020</b> , 31, 1-14  The Impact of Macrocycle Conformation on the Taxadiene-Forming Carbocation Cascade: Insight Gained from Sobralene, a Recently Discovered Verticillene Isomer. <i>Journal of Organic Chemistry</i> ,		
129	molecular electron density theory perspective. <i>Structural Chemistry</i> , <b>2020</b> , 31, 1-14  The Impact of Macrocycle Conformation on the Taxadiene-Forming Carbocation Cascade: Insight Gained from Sobralene, a Recently Discovered Verticillene Isomer. <i>Journal of Organic Chemistry</i> , <b>2020</b> , 85, 4507-4514  Extension of Econjugation and enhancement of electron-withdrawing ability at terminal		1
129	molecular electron density theory perspective. <i>Structural Chemistry</i> , <b>2020</b> , 31, 1-14  The Impact of Macrocycle Conformation on the Taxadiene-Forming Carbocation Cascade: Insight Gained from Sobralene, a Recently Discovered Verticillene Isomer. <i>Journal of Organic Chemistry</i> , <b>2020</b> , 85, 4507-4514  Extension of Etonjugation and enhancement of electron-withdrawing ability at terminal indenedione for A-ED-EA small molecules for application in organic solar cells. <b>2020</b> , 81, 105679  Improvement of Antioxidative Activity of Apigenin by B12N12 Nanocluster: Antioxidative	4.2	5
129 128 127	molecular electron density theory perspective. Structural Chemistry, 2020, 31, 1-14  The Impact of Macrocycle Conformation on the Taxadiene-Forming Carbocation Cascade: Insight Gained from Sobralene, a Recently Discovered Verticillene Isomer. Journal of Organic Chemistry, 2020, 85, 4507-4514  Extension of Etonjugation and enhancement of electron-withdrawing ability at terminal indenedione for A-ED-EA small molecules for application in organic solar cells. 2020, 81, 105679  Improvement of Antioxidative Activity of Apigenin by B12N12 Nanocluster: Antioxidative Mechanism Analysis. ChemistrySelect, 2020, 5, 1829-1836  A DFT study on the reaction mechanism of enantioselective reduction of ketones with borane catalyzed by a B-methoxy-oxazaborolidine catalyst derived from (-)-Epinene. Journal of Molecular	1.8	1 5 4

123	Hexamethylphosphanetriamine-mediated aziridination of imines with alpha-ketoesters: A molecular electron density theory study. <b>2020</b> , 33, e4058		3
122	A new database and benchmark of the bond energies of noble-gas-containing molecules. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26238	2.1	2
121	Anharmonic Frequencies of (MO) and Related Hydrides for M = Mg, Al, Si, P, S, Ca, and Ti and Heuristics for Predicting Anharmonic Corrections of Inorganic Oxides. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 3191-3204	2.8	11
120	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions <b>2020</b> , 10, 15394-15405		57
119	Double hybrid DFT calculations with Slater type orbitals. <b>2020</b> , 41, 1660-1684		10
118	High-temperature rate constants for CH3OCOH + OH reactions: the effects of multiple structures and paths. <b>2020</b> , 139, 1		3
117	Spin-Controlled Binding of Carbon Dioxide by an Iron Center: Insights from Ultrafast Mid-Infrared Spectroscopy. <b>2021</b> , 60, 2519-2525		5
116	A molecular electron density theory study of polar Diels-Alder reaction between 2,4EimethylEEthoxyoxazole and ethyl 4,4,4Erifluorocrotonate. <i>Structural Chemistry</i> , <b>2021</b> , 32, 805-817	1.8	1
115	Ultrahigh Thermoresistant Lightweight Bioplastics Developed from Fermentation Products of Cellulosic Feedstock. <b>2021</b> , 5, 2000193		7
114	Novel complexes with ONNO tetradentate coumarin schiff-base donor ligands: x-ray structures, DFT calculations, molecular dynamics and potential anticarcinogenic activity. <b>2021</b> , 34, 119-140		2
113	Spin-Controlled Binding of Carbon Dioxide by an Iron Center: Insights from Ultrafast Mid-Infrared Spectroscopy. <b>2021</b> , 133, 2549-2555		1
112	Structures, energetics, and kinetics of H-atom abstraction from methyl propionate by molecular oxygen: Ab initio and DFT investigations. <b>2021</b> , 1196, 113119		7
111	HF and SiF4 adsorption on carbon graphite (1 1 1) surface in aqueous medium: A combined DFT and MD simulation approach. <b>2021</b> , 37, 3987-3993		3
110	Tricyclo[2.1.0.0]pent-3-ylidene: Stereoelectronic Control of Bridge-Flapping within a Nonclassical Nucleophilic Carbene. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 878-891	4.2	1
109	Understanding the uniqueness of the stepwise [4 + 1] cycloaddition reaction between conjugated nitroalkenes and electrophilic carbene systems with a molecular electron density theory perspective. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26440	2.1	5
108	Review: Simulation Models for Materials and Biomolecules. <b>2021</b> , 27-82		1
107	Failure of molecular dynamics to provide appropriate structures for quantum mechanical description of the aqueous chloride ion charge-transfer-to-solvent ultraviolet spectrum. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 9109-9120	3.6	
106	Mechanism and kinetic properties for the complete series reactions of chloro(thio)phenols with O(P) under high temperature conditions <b>2021</b> , 11, 17683-17693		

105	Perfluorobicyclo[2.2.0]hex-1(4)-ene as unique partner for DielsAlder reactions with benzene: a density functional theory study. <b>2021</b> , 140, 1		2
104	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. <b>2021</b> , 3, 74-93		5
103	The homogeneous gas-phase formation mechanisms of PCPTs/PCDTs/PCDFs from the radical/radical cross-condensation of 2-CPR and 2-CTPR: a theoretical, mechanistic and kinetics study <b>2021</b> , 11, 12626-12640		
102	Topological unraveling of the [3+2] cycloaddition (32CA) reaction between N-methylphenylnitrone and styrene catalyzed by the chromium tricarbonyl complex using electron localization function and catastrophe theory.		1
101	Revisiting the OH + H2 -> H2O + H reaction at the molecular level: the plausible catalytic role of ice in its own reconstruction. <i>Astronomy and Astrophysics</i> , <b>2021</b> , 646, A163	5.1	2
100	A high-performance Cu-doped vanadium pentoxide thin-film cathode for lithium-ion batteries. <b>2021</b> , 27, 2335-2344		4
99	Experimental and Theoretical Mechanistic Study on the Thermal Decomposition of 3,3-diphenyl-4-(trichloromethyl)-5-nitropyrazoline. <b>2021</b> , 26,		5
98	Copper(II)-Catalyzed Aminohalogenation of Alkynyl Carbamates. <i>European Journal of Organic Chemistry</i> , <b>2021</b> , 2021, 1750-1757	3.2	2
97	Predicting Excited-State and Luminescence Properties of a Cyclometalated Iridium(III) Complex: Quantum Mechanics/Molecular Mechanics Study. <b>2021</b> , 125, 5670-5677		5
96	An investigation of the regio-, chemo-, and stereoselectivity of cycloaddition reactions of 2-phenylsulfonyl-1,3-butadiene and its 3-phenylsulfanyl derivative: a DFT study. <i>Structural Chemistry</i> , <b>2021</b> , 32, 1819-1831	1.8	Ο
95	A computational investigation of the selectivity and mechanism of the Lewis acid catalyzed oxa-Diels-Alder cycloaddition of substituted diene with benzaldehyde. <b>2021</b> , 42, 1296-1311		3
94	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 2783-2806	6.4	18
93	Clues to the non-carcinogenicity of certain N-Nitroso compounds: Role of alkylated DNA bases. <b>2021</b> , 271, 106539		0
92	Hydrogenation of small aromatic heterocycles at low temperatures. <b>2021</b> , 505, 3157-3164		4
91	Unveiling $[3 + 2]$ cycloaddition reactions of benzonitrile oxide and diphenyl diazomethane to cyclopentene and norbornene: a molecular electron density theory perspective. <b>2021</b> , 140, 1		0
90	1,2-Phenylene-Incorporated Smallest Expanded Calix[4]pyrrole via One-Step Synthesis of Tetrapyrrane: A Fluorescent Host for Fluoride Ion. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 10536-10543	4.2	2
89	Benchmarking of Density Functionals for -Azoarene Half-Lives via Automated Transition State Search. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 6474-6485	2.8	1
88	Unveiling the Different Reactivity of Bent and Linear Three-Atom-Components Participating in [3 + 2] Cycloaddition Reactions. <b>2021</b> , 2, 274-286		3

87	A Statistically Supported Antioxidant Activity DFT Benchmark-The Effects of Hartree-Fock Exchange and Basis Set Selection on Accuracy and Resources Uptake. <b>2021</b> , 26,		3
86	Density Functional Theory for Electrocatalysis.		12
85	Photo-induced primary processes of trans-[Co(acac)2(N3)(py)] in liquid solution studied by femtosecond vibrational and electronic spectroscopies. e1964043		
84	The Molecular Mechanism of the Formation of Four-Membered Cyclic Nitronates and Their Retro (3 + 2) Cycloaddition: A DFT Mechanistic Study. <b>2021</b> , 26,		1
83	Understanding the Participation of Fluorinated Azomethine Ylides in Carbenoid-Type [3 + 2] Cycloaddition Reactions with Ynal Systems: A Molecular Electron Density Theory Study. <i>Journal of Organic Chemistry</i> , <b>2021</b> , 86, 12644-12653	4.2	5
82	Computational insight into networking H-bonds in open and cyclic forms of glucose. e4285		1
81	Theoretical design study on the origin of the improved phosphorescent efficiency of DPEphos quinoline-substituted derivatives for OLEDs. <b>2021</b> , 97, 106185		0
80	High-efficient esterification of rosin and glycerol catalyzed by novel rare earth Lewis acidic ionic liquid: Reaction development and mechanistic study. <b>2021</b> , 127, 1-6		O
79	Theoretical study on adiabatic electron affinity of fatty acids. <b>2021</b> , 45, 16892-16905		
78	Hohenberg-Kohn-Sham Density Functional Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2007</b> , 153-201	0.7	1
77	Potential Energy Surfaces for Reaction Catalyzed by Metalloenzymes from Quantum Chemical Computations. <b>2009</b> , 275-313		1
76	Endohedral Fullerene Complexes and In-Out Isomerism in Perhydrogenated Fullerenes. <b>2011</b> , 117-151		5
75	A theoretical study on 1H/13C/31P NMR chemical shifts, and the correlation between 2JPH and the electronic structure of different phosphoryl benzamide derivatives. <i>Journal of Molecular Structure</i> , <b>2019</b> , 1183, 230-240	3.4	3
74	Effects of oxygenation on the intercalation of 1,10-phenanthroline-5,6/4,7-dione between DNA base pairs: a computational study. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 16638-16649	3.6	13
73	Reconstruction of water ice: the neglected process OH + OH -> H2O + O. <i>Astronomy and Astrophysics</i> , <b>2020</b> , 638, A125	5.1	2
72	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. <b>2020</b> , 152, 044111		11
71	Insights from the density functional performance of water and water-solid interactions: SCAN in relation to other meta-GGAs. <b>2020</b> , 153, 214116		6
70	Crystal structures, packing features, Hirshfeld surface analyses and DFT calculations of hydrogen-bond energy of two homologous 8a-aryl-2,3,4,7,8,8a-hexahydropyrrolo[1,2-a]pyrimidin-6(1H)-ones. <b>2020</b> , 76, 483-489		1

## (2020-2017)

69	()-7-[(4-Nitro-phen-yl)diazen-yl]-3a-(-tol-yl)-2,3,3a,4-tetra-hydro-1-benzo[]pyrrolo-[1,2-]imidazol-1-one 0.58-dimethyl sulfoxide 0.42-aceto-nitrile solvate: crystal structure, Hirshfeld analysis and DFT estimation of the energy of inter-molecular inter-actions. <b>2017</b> , 73, 1590-1594	1
68	Cosmic and Atmospheric Nanosilicates. <b>2016</b> , 369-412	1
67	Thermal Isomerization of [Co(acac)2(N3)(py)] in Liquid Solution Studied by Time-Resolved Fourier-Transform Infrared Spectroscopy. <b>2020</b> , 234, 1549-1566	3
66	Chirality Conversion of Dipeptides in the Schiff Bases of Binol Aldehydes with Multiple Hydrogen Bond Donors. <b>2009</b> , 30, 409-414	4
65	Computational Study on the Conformational Characteristics of Calix[4]pyrrole Derivatives. <b>2009</b> , 30, 423-428	4
64	Molecular Dynamics Simulation and Density Functional Theory Investigation for Thiacalix[4]biscrown and its Complexes with Alkali-Metal Cations. <b>2010</b> , 31, 453-456	5
63	Density Functional Theory Study on D-EA-type Organic Dyes Containing Different Electron-Donors for Dye-Sensitized Solar Cells. <b>2013</b> , 34, 3211-3217	12
62	Spin-orbit Effects on the Structure of Haloiodomethane Cations CH2XI+(X=F, Cl, Br, and I). <b>2014</b> , 35, 775-782	4
61	Computational Study on OH and Cl Initiated Oxidation of 2,2,2-Trifluoroethyl Trifluoroacetate (CF3C(O)OCH2CF3). <b>2014</b> , 35, 1385-1390	5
60	mPW1PW91 Calculated Conformational Study of Calix[n]arene (n = 4,5,6): Hydrogen Bond. <b>2009</b> , 53, 640-652	1
59	The first-principles study on properties of B-doped at interstitial site of CuB grain boundary. <b>2013</b> , 62, 117102	3
58	Differences in the torsional anharmonicity between reactant and transition state: the case of 3-butenal + H abstraction reactions. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 25414-25423	2
57	Insights into the origin of selectivity for [2+2] cycloaddition step reaction involved in the mechanism of enantioselective reduction of ketones with borane catalyzed by a B-methoxy oxazaborolidine catalyst derived from (	O
56	A theoretical screening of the O H???Interaction between water and benzene using density-functional approaches: Effects of nonlocal exchange and long-range dispersion corrections in the true minimum. <b>2021</b> , 1206, 113464	1
55	Investigating the Role of Ammonia in Atmospheric Nucleation. 2007, 52-56	
54	Evaluation of Proton Transfer in DNA Constituents: Development and Application of Ab Initio Based Reaction Kinetics. <i>Challenges and Advances in Computational Chemistry and Physics</i> , <b>2010</b> , 187-211 <sup>0.7</sup>	
53	Quantum-Mechanical Investigations of Noncovalent Interactions of Carbon Materials. <b>2015</b> , 1-32	1
52	Chapter 4. Isotope Effects as Analytical Probes: Applications of Computational Theory. <i>RSC</i> Theoretical and Computational Chemistry Series, <b>2020</b> , 125-154	

51	Theoretical Study on Aluminum Oxide Cluster Anions A12Ox[(x=2B)) with Rhombus Structure. <i>ChemistrySelect</i> , <b>2020</b> , 5, 15137-15147	1.8	
50	Synthesis of azido-dienediols by enzymatic dioxygenation of benzylazides: an experimental and theoretical study. <i>European Journal of Organic Chemistry</i> ,	3.2	
49	XNgNSi (X = HCC, F; Ng = Kr, Xe, Rn): A New Class of Metastable Insertion Compounds Containing Ng-C/F and Ng-N Bonds and Possible Isomerization therein. <i>Journal of Physical Chemistry A</i> , <b>2021</b> ,	2.8	0
48	An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> ,	3.6	1
47	Bromination of carbon nanohorns to improve sodium-ion storage performance. <i>Applied Surface Science</i> , <b>2022</b> , 580, 152238	6.7	1
46	Unveiling the synthesis of spirocyclic, tricyclic, and bicyclic triazolooxazines from intramolecular [3 + 2] azide-alkyne cycloadditions with a molecular electron density theory perspective. <i>Structural Chemistry</i> , <b>2022</b> , 33, 555	1.8	1
45	A chemical dynamics study of the reaction of the methylidyne radical (CH, XI) with dimethylacetylene (CHCCCH, XA) <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 24, 578-593	3.6	4
44	Computational insight into networking H-bonds in open and cyclic forms of galactose. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1255, 132432	3.4	
43	Theoretical evidence for the formation of perfluorocarboxylic acids form atmospheric oxidation degradation of fluorotelomer acrylates <i>Environmental Science and Pollution Research</i> , <b>2022</b> , 1	5.1	O
42	Computational investigation of thermal decomposition mechanism of 5-nitro-5-R-1,3-dioxane compounds. <i>Structural Chemistry</i> , 1	1.8	
41	Ability of Boron to Act as a Nucleophile and an Electrophile in Boryl Shift Reactions Unveiled by Electron Density Distribution Analysis <i>Journal of Organic Chemistry</i> , <b>2022</b> ,	4.2	0
40	Non-energetic Formation of Ethanol via CCH Reaction with Interstellar HO Ices. A Computational Chemistry Study <i>ACS Earth and Space Chemistry</i> , <b>2022</b> , 6, 496-511	3.2	1
39	Effect of hydrogen bonds and CF group on the regioselectivity and mechanism of [3 + 2] cycloaddition reactions between nitrile oxide and 2,4-disubstituted cyclopentenes. A MEDT study <i>Journal of Molecular Modeling</i> , <b>2022</b> , 28, 104	2	0
38	Open-Shell Variant of the London Dispersion-Corrected Hartree-Fock Method (HFLD) for the Quantification and Analysis of Noncovalent Interaction Energies <i>Journal of Chemical Theory and Computation</i> , <b>2022</b> ,	6.4	2
37	Quantum mechanical studies of 2D nanobiohybrids (Review Article). <i>Low Temperature Physics</i> , <b>2022</b> , 48, 278-285	0.7	
36	Table_1.pdf. <b>2020</b> ,		
35	Data_Sheet_1.pdf. <b>2019</b> ,		
34	Data_Sheet_2.zip. <b>2019</b> ,		

33	A quantum chemistry study on CH homolytic bond dissociation enthalpies of five-membered and six-membered heterocyclic compounds. <i>Journal of the Indian Chemical Society</i> , <b>2022</b> , 100527		O
32	Effect of Water Molecule on the Complete Series Reactions of Chlorothiobenzenes with H/ĐOH: A Theoretical Study. <i>Atmosphere</i> , <b>2022</b> , 13, 849	2.7	
31	Conformational influence on the thermal rate constants and product distributions of 2-butanone + H abstraction reactions. <i>Chemical Physics Letters</i> , <b>2022</b> , 139723	2.5	O
30	The Homogeneous Gas-Phase Formation Mechanism of PCNs from Cross-Condensation of Phenoxy Radical with 2-CPR and 3-CPR: A Theoretical Mechanistic and Kinetic Study. <i>International Journal of Molecular Sciences</i> , <b>2022</b> , 23, 5866	6.3	
29	Hetero-porphyrin based channel for separation of proton isotope: A density functional theory study. <i>Microporous and Mesoporous Materials</i> , <b>2022</b> , 339, 111995	5.3	О
28	Non-Covalent Interactions Atlas benchmark data sets 5: London dispersion in an extended chemical space. <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> , 24, 14780-14793	3.6	1
27	Theoretical studies on excited-state properties and luminescence mechanism of a CarbeneMetalAmide Au(I) complex with thermally activated delayed fluorescence. <i>Journal of the Chinese Chemical Society</i> ,	1.5	
26	Hydrogen-bond acidity of silanols: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , <b>2022</b> , 1266, 133505	3.4	O
25	Long-bonding and effects of carbon hybridization on the bonding of M ? Ng ? C compounds (MI=ICu, Ag, Au). <i>International Journal of Quantum Chemistry</i> ,	2.1	
24	A Non-coded <b>2</b> ,2-Amino Acid with Isoxazoline Core Able to Stabilize Peptides Folding Through an Unprecedented Hydrogen Bond. <i>European Journal of Organic Chemistry</i> ,	3.2	
23	Desorption of organic molecules from interstellar ices, combining experiments and computer simulations: Acetaldehyde as a case study. <i>Astronomy and Astrophysics</i> ,	5.1	1
22	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> ,	2.8	O
21	Prediction of acute toxicity to Daphnia magna and interspecific correlation: a global QSAR model and a Daphnia-minnow QTTR model. <i>SAR and QSAR in Environmental Research</i> , 1-18	3.5	О
20	Unveiling the [3+2] cycloaddition between difluoromethyl diazomethane and 3-ylideneoxindole from the perspective of molecular electron density theory.		2
19	Antioxidant and anticancer properties of plant-based bioactive flavonoids cardamonin and alpinetin: A theoretical insight from IDOH antiradical and Cu (II) chelation mechanisms.		O
18	The performance of exchangedorrelation functionals in describing electron density parameters of saddle point structures along chemical reactions. <b>2022</b> , 43, 1830-1838		O
17	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.		2
16	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.		10

15	Synthesis of eugenol derivative by the ring opening of epoxide eugenol and its analysis through chemical reactivity: a DFT approach. 1-9	О
14	Porphyrin based channel for separation of proton isotope: A density functional theory study. <b>2022</b> , 171, 111032	0
13	Polyaromatic hydrocarbons with an imperfect aromatic system as catalysts of interstellar H2 formation.	O
12	A comprehensive benchmark investigation of quantum chemical methods for carbocations.	O
11	Testing of Exchange-Correlation Functionals of DFT for a Reliable Description of the Electron Density Distribution in Organic Molecules. <b>2022</b> , 23, 14719	1
10	How a Chromium Tricarbonyl Complex Catalyzes the [3 + 2] Cycloaddition Reaction of N-Substituted Phenylnitrones with Styrene: A Molecular Electron Density Theory Analysis. <b>2022</b> , 41, 3:	809-3822 <sup>O</sup>
9	CRYSTAL23: A Program for Computational Solid State Physics and Chemistry.	1
8	The Highly Exothermic Hydrogen Abstraction Reaction H2Te + OH -> H2O + TeH: Comparison with Analogous Reactions for H2Se and H2S.	O
7	Understanding the mechanism and regio- and stereo selectivity of [3 + 2] cycloaddition reactions between substituted azomethine ylide and 3,3,3- trifluoro -1-nitroprop-1-ene, within the molecular electron density theory.	0
6	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. <b>2023</b> , 13,	O
5	Insights into the CO 2 Capture Capacity of Covalent Organic Frameworks.	0
4	Electrophilicity and nucleophilicity scales at different DFT computational levels.	O
3	Structure and stability of a new set of noble gas insertion compounds, XNgOPO(OH)2 (X = F, Cl, Br; Ng = Kr, Xe, Rn): an in silico investigation. <b>2023</b> , 142,	О
2	On the Nature of the Partial Covalent Bond between Noble Gas Elements and Noble Metal Atoms. <b>2023</b> , 28, 3253	O
1	Regio- and stereoselectivity of [3+2] cycloaddition reactions between (Z)-1-(anthracen-9-yl)-N-methyl nitrone and analogs of trans-Ehitrostyrene on the basis of MEDT computational study.	0