Harmonic Vibrational Frequencies:Â An Evaluation of H Quadratic Configuration Interaction, Density Functiona Factors

The Journal of Physical Chemistry

100, 16502-16513

DOI: 10.1021/jp960976r

Citation Report

#	Article	IF	Citations
25	Relative Stabilities and Hydride Affinities of Silatropylium and Silabenzyl Cations and Their Isomers. Comparison with the Carbon Analogues Tropylium and Benzyl Cations. Journal of the American Chemical Society, 1996, 118, 10561-10570.	6.6	38
26	Hydrogen Transfer between Ethyl Radical and Ethylene:Â An Example Where Kinetics Does Not Follow Thermodynamics. The Journal of Physical Chemistry, 1996, 100, 17087-17089.	2.9	25
27	The spectroscopy of hexafluorothioacetone, a blue gas. Journal of Chemical Physics, 1997, 106, 7479-7490.	1.2	13
28	Spectroscopic studies of the BÌƒâ€‰2Aâ€²â€²-XÌƒâ€‰2Aâ€²â€² system of the jet-cooled vinoxy radical. Journal of Chemical Physics, 1997, 106, 10048-10065.	1.2	56
29	Density functional crystal orbital study on the normal vibrations of polyacetylene and polymethineimine. Journal of Chemical Physics, 1997, 107, 10075-10084.	1.2	66
30	The electron affinities of the perfluorocarbons C2Fn, n=1â€“6. Journal of Chemical Physics, 1997, 107, 8536-8544.	1.2	38
31	Predicting electron affinities with density functional theory: Some positive results for negative ions. Journal of Chemical Physics, 1997, 107, 2529-2541.	1.2	114
32	An ab initio study of OCCN and OCCN+. Journal of Chemical Physics, 1997, 107, 3840-3844.	1.2	30
33	Quantitative Analyses of Cieplakvs.Felkin-Anh Effects in Hydride Reduction of Cyclohexanone. Chemistry Letters, 1997, 26, 431-432.	0.7	10
34	Identification of the Borirene Molecule, (CH)2BH:Â Matrix Isolation FTIR and DFT Calculations for Five Vibrational Modes of Six Isotopic Molecules. Journal of the American Chemical Society, 1997, 119, 12402-12403.	6.6	23
35	Some Interstellar Reactions Involving Electrons and Neutral Species: Attachment and Isomerization. Astrophysical Journal, 1997, 491, 210-215.	1.6	70
36	13C and15N Kinetic Isotope Effects on the Decarboxylation of 3-Carboxybenzisoxazole. Theory vs Experiment. Journal of Organic Chemistry, 1997, 62, 7305-7309.	1.7	11
37	Infrared spectroscopic evidence for an attractive intramolecular 1,5-CHÂ·Â·Â·O interaction in 1-methoxy-2-(methylthio)ethane. Chemical Communications, 1997, , 2213-2214.	2.2	9
38	A comparison of two methods for direct tunneling dynamics: Hydrogen exchange in the glycolate anion as a test case. Journal of Chemical Physics, 1997, 106, 3956-3964.	1.2	29
39	Reactions of Laser-Ablated Mg, Ca, Sr, and Ba Atoms with Hydrogen Cyanide in Excess Argon. Matrix Infrared Spectra and Density Functional Calculations on Novel Isocyanide Products. Journal of Physical Chemistry A, 1997, 101, 9666-9672.	1.1	32
40	Gas Phase Reactions of Cysteine with Charged Electrophiles:Â Regioselectivities of the Dimethylchlorinium Ion and the Methoxymethyl Cationâ€‚1. Journal of Organic Chemistry, 1997, 62, 6112-6120.	1.7	28
41	Conjugated Dual Hydrogen Bonds Mediating 2-Pyridone/2-Hydroxypyridine Tautomerism. Journal of Physical Chemistry B, 1997, 101, 9119-9126.	1.2	73
42	Theoretical Study of Thermal Decomposition Mechanism of Oxalic Acid. Journal of Physical Chemistry A, 1997, 101, 2702-2708.	1.1	79

#	Article	IF	Citations
43	A Comparison of the Properties of Various Fused-Ring Quinones and Their Radical Anions Using Hartreeâ^'Fock and Hybrid Hartreeâ^'Fock/Density Functional Methods. Journal of Physical Chemistry A, 1997, 101, 7154-7166.	1.1	54
44	Ab Initio Prediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory:Â Î±-Pinene. Journal of Physical Chemistry A, 1997, 101, 9912-9924.	1.1	124
45	Distinctive Normal Harmonic Vibrations of [2.2]Paracyclophane. Journal of Physical Chemistry A, 1997, 101, 8233-8241.	1.1	32
46	Ab InitioPrediction of Vibrational Absorption and Circular Dichroism Spectra of Chiral Natural Products Using Density Functional Theory:Â Camphor and Fenchone. Journal of Physical Chemistry A, 1997, 101, 6322-6333.	1.1	99
47	Proton-Transport Catalysis:Â A Systematic Study of the Rearrangement of the Isoformyl Cation to the Formyl Cation. Journal of the American Chemical Society, 1997, 119, 7573-7578.	6.6	95
48	Thermal and Magnetic Properties of Coronene and Related Molecules. Journal of Physical Chemistry A, 1997, 101, 9176-9179.	1.1	55
49	The Lowest Excited Singlet States of 1-Azaadamantane and 1-Azabicyclo[2.2.2]octane:Â Fluorescence Excitation Spectroscopy and Density Functional Calculations. Journal of the American Chemical Society, 1997, 119, 11523-11533.	6.6	21
50	Theoretical Investigation of the Reaction between Aluminum and Propene. Comparison between Calculated and Experimental ESR Results. Journal of Physical Chemistry A, 1997, 101, 4814-4820.	1.1	5
51	Translational Activation of the SN2 Nucleophilic Displacement Reactions Cl-+ CH3Cl (CD3Cl) â†' ClCH3(ClCD3) + Cl-:Â A Guided Ion Beam Study. Journal of Physical Chemistry A, 1997, 101, 5969-5986.	1.1	119
52	Ring Opening of Substituted Cyclopropylidenes to Cyclic Allenes. Journal of Organic Chemistry, 1997, 62, 9267-9275.	1.7	38
53	Substituent Effects on Site Selectivity (CC vs CN) in Heterocumuleneâ^'Heterodiene [4 + 2] Cycloadditions:Â Density Functional and Semiempirical AM1 Molecular Orbital Calculations. Journal of Organic Chemistry, 1997, 62, 8497-8502.	1.7	6
54	Mechanistic Aspects of the Alternating Copolymerization of Propene with Carbon Monoxide Catalyzed by Pd(II) Complexes of Unsymmetrical Phosphineâ^'Phosphite Ligands. Journal of the American Chemical Society, 1997, 119, 12779-12795.	6.6	183
55	Ab Initio Study of the Structures and Vibrational Spectra of Some Diamine Radical Cations. Journal of Physical Chemistry A, 1997, 101, 3626-3633.	1.1	39
56	A DFT Study of the Simmonsâ^'Smith Cyclopropanation Reaction. Journal of the American Chemical Society, 1997, 119, 12300-12305.	6.6	59
57	Effects of Neutral Bases on the Isomerization of Conventional Radical Cations CH3Xâ€¢+to Their Distonic Isomersâ€¢CH2X+H (X = F, OH, NH2):Â Proton-Transport Catalysis and Other Mechanisms. Journal of the American Chemical Society, 1997, 119, 9831-9839.	6.6	80
58	Assessment of Modified Gaussian-2 (G2) and Density Functional Theories for Molecules Containing Third-Row Atoms Gaâ^'Krâ€. Journal of Physical Chemistry A, 1997, 101, 8701-8705.	1.1	50
59	Reactions of Laser-Ablated Beryllium Atoms with Hydrogen Cyanide in Excess Argon. FTIR Spectra and Quantum Chemical Calculations on BeCN, BeNC, HBeCN, and HBeNC. Journal of the American Chemical Society, 1997, 119, 6392-6398.	6.6	29
60	The Effect of Pressure on Deuterium-Hydrogen Fractionation in High-Temperature Water. Science, 1997, 277, 791-794.	6.0	84

#	Article	IF	Citations
61	Theoretical Study of Thermal Decomposition Mechanisms of Isoxazole. Journal of Physical Chemistry A, 1997, 101, 7231-7235.	1.1	14
62	Theoretical Study of Cation/Ether Complexes:Â The Alkali Metals and Dimethyl Ether. Journal of Physical Chemistry A, 1997, 101, 6125-6131.	1.1	58
63	Vibrational Analysis of 1,3,3-Trinitroazetidine Using Matrix Isolation Infrared Spectroscopy and Quantum Chemical Calculations. Journal of Physical Chemistry A, 1997, 101, 7742-7748.	1.1	14
64	Density-Functional Studies on the Structure and Vibrational Spectra of Transient Intermediates of p-Benzoquinone. Journal of Physical Chemistry A, 1997, 101, 4449-4459.	1.1	72
65	Understanding the activation energy trends for the C2H4+OHâ†'C2H4OH reaction by using canonical variational transition state theory. Journal of Chemical Physics, 1997, 107, 7266-7274.	1.2	50
66	Structures and Properties of Ubiquinone-1 and Its Radical Anion from Hybrid Hartreeâ^'Fock/Density Functional Studies. Journal of Physical Chemistry A, 1997, 101, 5799-5804.	1.1	36
67	Dimethylcarbene, Its Radical Cation and Dication. Journal of the American Chemical Society, 1997, 119, 9039-9041.	6.6	13
68	Conformational enthalpies, Î"HÂ° [axial/equatorial], of 3- and 4-methylcyclohexanone. Computational and Theoretical Chemistry, 1997, 419, 11-18.	1.5	5
69	Density functional study of hydrogen-bonded systems: Energetic and vibrational features of some gas-phase adducts of hydrogen fluoride. Computational and Theoretical Chemistry, 1997, 419, 227-238.	1.5	35
70	Computational chemistry predictions of reaction processes in organometallic vapor phase epitaxy. Progress in Crystal Growth and Characterization of Materials, 1997, 35, 117-149.	1.8	45
71	Molecular modeling. Current Opinion in Chemical Biology, 1997, 1, 392-398.	2.8	5
72	Ab initio derived spectroscopic quality force fields for molecular modeling and dynamics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1347-1363.	2.0	16
73	The gas-phase infrared spectra of phenanthrene-h10 and phenanthrene-d10. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1839-1851.	2.0	18
74	The vibrational spectrum of acenaphthylene: linear dichroism and ab initio model calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2095-2107.	2.0	6
75	Vibrational spectra and harmonic force fields of pyrrolidine derivatives: comparison between HF, MP2 and DFT force fields. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 2537-2551.	2.0	32
76	Ab initio study of the reaction C2H4+ â†' C2H3+ + H. International Journal of Mass Spectrometry and Ion Processes, 1997, 167-168, 149-160.	1.9	8
77	Ab initio prediction of the spectra of carbon cumulenes. Chemical Physics, 1997, 223, 149-158.	0.9	18
78	The ring-puckering motion in perfluorocyclobutane. Journal of Molecular Structure, 1997, 405, 159-167.	1.8	16

#	Article	IF	Citations
79	Conformational and vibrational analyses of 2-methoxyethanol and 2-(methylthio)ethanol by density functional theory. Journal of Molecular Structure, 1997, 413-414, 217-226.	1.8	11
80	On the Mechanism of the McMurry Reaction. Angewandte Chemie International Edition in English, 1997, 36, 2234-2237.	4.4	30
81	Isofulminic Acid â€“ Phantom or Reality?. Liebigs Annalen, 1997, 1997, 2505-2517.	0.8	15
82	On the Oxenoid Character of Alkylperoxy Anions and Their Lithium Compounds: A Combined Massâ€Spectrometric and Theoretical Investigation. Chemische Berichte, 1997, 130, 1085-1097.	0.2	21
83	Dimethyl Peroxide Radical Cation: A New Theoretical and Experimental Approach to the C₂H₆O^{â€¢+}₂ Potential Energy Surface. Chemistry - A European Journal, 1997, 3, 626-638.	1.7	17
84	A Study of the Gasâ€Phase Reactivity of Neutral Alkoxy Radicals by Mass Spectrometry: Î±â€Cleavages and Bartonâ€type Hydrogen Migrations. Chemistry - A European Journal, 1997, 3, 1866-1883.	1.7	47
85	Structure of 3-nitropyrazole in solution and in the solid state. , 1997, 10, 637-645.		22
86	Internal conrotation and disrotation in H2BCH2BH2 and diborylmethane 1,3 H exchange. Journal of Computational Chemistry, 1997, 18, 1792-1803.	1.5	12
87	Calculation of molecular vibrations: Selective scaling factors for semiempirical force constants. Journal of Computational Chemistry, 1997, 18, 2050-2059.	1.5	14
88	Computation of vibrational frequencies for adsorbates on surfaces. International Journal of Quantum Chemistry, 1997, 65, 827-838.	1.0	92
89	Double- or single-well potential for GSIPT in 1-hydroxy-2-acetonaphthone?. Chemical Physics Letters, 1997, 269, 151-155.	1.2	32
90	Computational density functional theory vibrational spectra of cubane. Chemical Physics Letters, 1997, 270, 376-381.	1.2	20
91	Investigation of the use of B3LYP zero-point energies and geometries in the calculation of enthalpies of formation. Chemical Physics Letters, 1997, 270, 419-426.	1.2	173
92	An ab initio study concerning the experimental observability of C3H62+ isomers. Chemical Physics Letters, 1997, 280, 244-250.	1.2	8
93	Relative stabilities of ortho-, meta- and para-tolyl cations. Chemical Physics Letters, 1997, 280, 260-265.	1.2	26
94	Methylated NF3. A G2MS theoretical study on the structure, stability, and interconversion of the CH3â€“NF3+ and CH3Fâ€“NF2+ isomers. Chemical Physics Letters, 1997, 281, 431-437.	1.2	20
95	Kinetics of the reaction of Cl atoms with FC(O)O and FC(O) OCl. Chemical Physics Letters, 1997, 266, 253-258.	1.2	9
96	The prediction of vibrational frequencies of inorganic molecules using density functional theory. Chemical Physics Letters, 1998, 282, 219-226.	1.2	168

#	Article	IF	Citations
97	MRMP study of radical photodissociation reaction thresholds for acetaldehyde and acetone. Chemical Physics Letters, 1998, 284, 19-23.	1.2	22
98	Ab initio determination of the nuclear relaxation contribution to the second hyperpolarizability of carbon disulfide. Chemical Physics Letters, 1998, 287, 185-188.	1.2	9
99	A symmetric structure of the gas-phase H3+(H2)9 cluster. Chemical Physics Letters, 1998, 287, 563-569.	1.2	33
100	Theoretical binding energies of lithium ions to short-chain alcohols. Chemical Physics Letters, 1998, 288, 408-412.	1.2	13
101	Theoretical investigation of the Ca+â€“N2 and Ca2+â€“N2 complexes. Chemical Physics Letters, 1998, 295, 204-210.	1.2	26
102	Structures and spectroscopic properties of SCnS (n=2â€“6): density functional theory study. Chemical Physics Letters, 1998, 297, 65-71.	1.2	21
103	Calculation of bond dissociation energies for large molecules using locally dense basis sets. Chemical Physics Letters, 1998, 297, 181-186.	1.2	35
104	The lowâ€lying singletâ€triplet transitions of phenylacetylene and styrene: Analysis of the vibronic structure. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 882-893.	0.9	6
105	Vibrational modes of isolated hydroxyls of silica computed ab initio in a cluster approach. Chemical Physics Letters, 1998, 294, 103-108.	1.2	49
106	The isomers of dichloromethane and its radical cation: an ab initio exploration of the neutral and charged CH2Cl2 potential energy surfaces. Computational and Theoretical Chemistry, 1998, 425, 207-226.	1.5	6
107	A density functional study of vibrational frequencies of diphenylbutadiene in the ground and transient states. Computational and Theoretical Chemistry, 1998, 453, 107-117.	1.5	5
108	Dimerization versus complexation of triethylaluminum and diethylaluminum chloride: an ab initio determination of structures, energies of formation, and vibrational spectra. Computational and Theoretical Chemistry, 1998, 454, 149-159.	1.5	11
109	Modelling the signatures of interstellar polycyclic aromatic hydrocarbons with quantum chemistry. Computational and Theoretical Chemistry, 1998, 458, 203-215.	1.5	18
110	The Formation of HAlX2 (X = Cl, Br) in the Thermolysis of Intramolecularly Coordinated Alanes Me2N(CH2)3AlX2: A Matrix Isolation Study. European Journal of Inorganic Chemistry, 1998, 1998, 1807-1810.	1.0	11
111	Matrix Isolation of 3,4-Benzocyclodeca-3,7,9-triene-1,5-diyne. , 1998, 1998, 799-803.		6
112	A Combined Neutralization-Reionization Mass Spectrometric and Theoretical Study of Oxyallyl and Other Elusive [C3, H4, O] Neutrals. European Journal of Organic Chemistry, 1998, 1998, 987-1009.	1.2	34
113	Theoretical study of reaction of trifluoromethyl radical with hydroxyl and hydrogen radicals. Journal of Computational Chemistry, 1998, 19, 277-289.	1.5	20
114	Automated molecular mechanics parameterization with simultaneous utilization of experimental and quantum mechanical data. Journal of Computational Chemistry, 1998, 19, 1146-1166.	1.5	99

#	Article	IF	Citations
115	Inexpensive vibrational anharmonicities from estimated derivatives: Diatomic molecules. Journal of Computational Chemistry, 1998, 19, 1315-1324.	1.5	7
116	Conformers of gaseous protonated glycine. Journal of Computational Chemistry, 1998, 19, 1862-1876.	1.5	40
117	Atmospheric chemistry of acetone: Kinetic study of the CH3C(O)CH2O2+NO/NO2 reactions and decomposition of CH3C(O)CH2O2NO2. International Journal of Chemical Kinetics, 1998, 30, 475-489.	1.0	32
118	Density functional study of chlorine-oxygen compounds related to the ClO self-reaction. International Journal of Quantum Chemistry, 1998, 66, 203-217.	1.0	18
119	Thermodynamic and kinetic analysis using AB initio calculations on dimethyl-ether radical+O2 reaction system. Proceedings of the Combustion Institute, 1998, 27, 201-209.	0.3	5
120	Anomeric amides â€" Structure, properties and reactivity. Tetrahedron, 1998, 54, 7229-7271.	1.0	102
121	A theoretical study of the electrochemical reduction of oxygen. Journal of Electroanalytical Chemistry, 1998, 448, 189-204.	1.9	31
122	Theoretical density functional and ab initio computational study of the tautomeric, vibrational and H-bond properties of 1,7-di-CH3-guanine: a comparison with FT-IR data from matrix isolation experiments. Journal of Molecular Structure, 1998, 442, 201-220.	1.8	15
123	Vibrational spectra and conformations of 1,4-cyclohexadiene and its oxygen analogues: ab initio and density functional calculations. Journal of Molecular Structure, 1998, 470, 265-275.	1.8	8
124	Rearrangement and dissociation of ionized 1,2-diaminoethane. International Journal of Mass Spectrometry, 1998, 179-180, 337-348.	0.7	6
125	A mass spectrometric and ab initio study of the pathways for dehydration of simple glycine and cysteine-containing peptide [M+H]+ ions. Journal of the American Society for Mass Spectrometry, 1998, 9, 945-956.	1.2	102
126	Role of the sulfhydryl group on the gas phase fragmentation reactions of protonated cysteine and cysteine containing peptides. Journal of the American Society for Mass Spectrometry, 1998, 9, 1275-1284.	1.2	60
127	Postâ€"Hartreeâ€"Fock MP2 and density functional theory derived structure and vibrations of 1,2-dithiole-2-thione and 1,2-dithiole-3-one. Vibrational Spectroscopy, 1998, 16, 77-83.	1.2	11
128	Vibrational spectroscopy and conformational studies of 1,4-benzodioxan: ab initio and density functional calculations. Vibrational Spectroscopy, 1998, 17, 173-182.	1.2	10
129	Ab initio calculations and supersonic jet studies on the geometry of 4-dimethylaminobenzonitrile (DMABN) and related compounds in the ground and excited state. Chemical Physics, 1998, 234, 35-57.	0.9	50
130	Protonated NF3O. A G2MS theoretical study on the structure, stability, and interconversion of the (NF3O)H+ isomers. International Journal of Mass Spectrometry and Ion Processes, 1998, 175, 317-324.	1.9	4
131	Characterization of an ambident electrophile: the gas phase reactivity of the methoxymethyl cation. International Journal of Mass Spectrometry and Ion Processes, 1998, 175, 107-122.	1.9	18
132	Advantages and drawbacks of the quantum chemistry methodology in predicting the thermochemical data of lanthanide trihalide molecules. Journal of Alloys and Compounds, 1998, 275-277, 934-939.	2.8	9

#	Article	IF	Citations
133	Reactivity and Regioselectivity of Hydroxyl Radical Addition to Halogenated Ethenes. Journal of Physical Chemistry A, 1998, 102, 1583-1594.	1.1	81
134	Study of the Hydrates of H2SO4 Using Density Functional Theory. Journal of Physical Chemistry A, 1998, 102, 6533-6539.	1.1	128
135	Stability and Three-Dimensional Aromaticity of closo-Monocarbaborane Anions, CBn-1Hn-, and closo-Dicarboranes, C2Bn-2Hn. Inorganic Chemistry, 1998, 37, 3454-3470.	1.9	245
136	Density-functional crystal orbital study on the structures and energetics of polyacetylene isomers. Physical Review B, 1998, 57, 11994-12001.	1.1	52
137	Comparison of the performance of local, gradient-corrected, and hybrid density functional models in predicting infrared intensities. Journal of Chemical Physics, 1998, 109, 10587-10593.	1.2	163
138	Structure and Nonrigidity of B9H92-and B9H10-. Comparisons of BnHn2-and BnHn+1-Systems. Inorganic Chemistry, 1998, 37, 1693-1703.	1.9	19
139	Unimolecular Chemistry of the Gaseous Cyclopropylamine Radical Cation. Journal of the American Chemical Society, 1998, 120, 152-160.	6.6	33
140	Reaction of Organic Sulfides with Singlet Oxygen. A Revised Mechanism. Journal of the American Chemical Society, 1998, 120, 4439-4449.	6.6	134
141	A High-Level Computational Study on the Thermochemistry and Thermal Decomposition of Sulfur Mustard (2,2â€˜-Dichloroethyl Sulfide):â€‰ A Chemical Warfare Agent. Journal of Physical Chemistry A, 1998, 102, 3438-3446.	1.1	14
142	Accurate Heats of Formation for SiFn and SiFn+, for n = 1â^'4. Journal of Physical Chemistry A, 1998, 102, 876-880.	1.1	37
143	Câ€“H Hyperconjugation in Î±-chlorocarbocations. Journal of the Chemical Society Perkin Transactions II, 1998, , 2371-2374.	0.9	6
144	Theoretical studies on mechanisms of the insertion of boron into methane and its consequent reactions. Molecular Physics, 1998, 93, 329-339.	0.8	5
145	Ab Initio Study of the Triple-Proton-Transfer Reactions of Ground and Excited States of 7-Hydroxyquinoline in Methanol Solution. Journal of the American Chemical Society, 1998, 120, 7568-7576.	6.6	66
146	Raman Spectroscopic Measurements and ab Initio Molecular Orbital Studies of Cadmium(II) Hydration in Aqueous Solution. Journal of Physical Chemistry B, 1998, 102, 3564-3573.	1.2	42
147	Structures, Vibrational Frequencies, Thermodynamic Properties, and Bond Dissociation Energies of the Bromomethanes and Bromomethyl Radicals:Â an Ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 6191-6199.	1.1	45
148	Reactions of Laser-Ablated Niobium, Tantalum, and Rhenium Atoms with Nitrogen Atoms and Molecules. Infrared Spectra and Density Functional Calculations of the Metal Nitride and Dinitride Molecules. Journal of Physical Chemistry A, 1998, 102, 9061-9071.	1.1	40
149	Matrix Infrared Spectra and Density Functional Calculations of Three Al, N, O Isomers. Journal of Physical Chemistry A, 1998, 102, 5019-5026.	1.1	12
150	An assessment of theoretical procedures for the calculation of reliable free radical thermochemistry: A recommended new procedure. Journal of Chemical Physics, 1998, 108, 604-615.	1.2	206

#	Article	IF	Citations
151	Ring Opening of the Cyclopropylcarbinyl Radical and ItsN- andO-Substituted Analogues:Â A Theoretical Examination of Very Fast Unimolecular Reactions. Journal of the American Chemical Society, 1998, 120, 10223-10233.	6.6	96
152	p-Phenylenebismethylene:Â Characterization, Calculation, and Conversion to a Conjugated Bis-Carbonyloxide. Journal of the American Chemical Society, 1998, 120, 11528-11529.	6.6	33
153	Influence of Bystander Substituents on the Rates of 1,2-H and 1,2-Ph Shifts in Singlet and Triplet Carbenes. Journal of Physical Chemistry A, 1998, 102, 8467-8476.	1.1	41
154	Theoretical Investigation of the Nature of Aluminum-Containing Species Present in Alkaline Solution. Journal of Physical Chemistry B, 1998, 102, 10372-10382.	1.2	41
155	Chemical and Thermodynamic Properties of Methyl Chloride Dimer Radical Cations in the Gas Phase. Journal of the American Chemical Society, 1998, 120, 1517-1522.	6.6	39
156	The Importance of Ionâ^'Neutral Complexes in Gas-Phase Ionic Reactions:Â Fragmentation of [CH3CH2OCH2]+as a Prototypical Case. Journal of the American Chemical Society, 1998, 120, 8430-8437.	6.6	23
157	Density Functional Study of the Conformations and Vibrations of 1,2-Dimethoxyethane. Journal of Physical Chemistry A, 1998, 102, 2691-2699.	1.1	56
158	Structural and Thermochemical ab Initio Studies of Lanthanide Trihalide Molecules with Pseudopotentials. Inorganic Chemistry, 1998, 37, 1984-1991.	1.9	47
159	Hydrogen Bonding of Methanol with Bridged OH Groups of Zeolites:Â Ab Initio Calculation,1H NMR and FTIR Studies. Journal of Physical Chemistry B, 1998, 102, 2454-2463.	1.2	37
160	Density Functional Calculations of Thermochemical Equilibria. Journal of Physical Chemistry A, 1998, 102, 1568-1575.	1.1	7
161	Spectroscopic determination of Î”HÂ° for axial/equatorial and ethyl rotor conformations in 4-methyl and 4-ethyl cyclohexanone cooled in a supersonic jet. Journal of Chemical Physics, 1998, 108, 869-875.	1.2	13
162	Experimental and ab initio study of the infrared spectra of ionic species derived from SF6 and SF4 and trapped in solid neon. Journal of Chemical Physics, 1998, 108, 9639-9650.	1.2	32
163	Pericyclic versus Pseudopericyclic 1,5-Electrocyclization of Iminodiazomethanes. An ab Initio and Density Functional Theory Study. Journal of Organic Chemistry, 1998, 63, 5801-5805.	1.7	83
164	The Prototype Geâ^'H Insertion Reaction of Germylene with Germane. Absolute Rate Constants, Temperature Dependence, RRKM Modeling and the Potential Energy Surface. Journal of the American Chemical Society, 1998, 120, 12657-12665.	6.6	64
165	Substituent Effects in Mixed Trihalobenzenes. Journal of Physical Chemistry A, 1998, 102, 3532-3536.	1.1	6
166	The OÂ·Â·Â·Hâ^'O Hydrogen Bond in the Gas Phase. Microwave Structure of Ethylene Oxideâ^'Water. Journal of the American Chemical Society, 1998, 120, 11144-11148.	6.6	38
167	Mechanism of Dioxirane Oxidation of CH Bonds:Â Application to Homo- and Heterosubstituted Alkanes as a Model of the Oxidation of Peptides. Journal of Organic Chemistry, 1998, 63, 5413-5422.	1.7	59
168	Direct Observation and Characterization ofp-Phenylenebisnitrene. A Labile Quinoidal Diradical. Journal of the American Chemical Society, 1998, 120, 11530-11531.	6.6	33

#	Article	IF	Citations
169	Structures and Energetics of Some Potential Intermediates in Titanium Nitride Chemical Vapor Deposition:Â TiClm(NH2)n, TiClm(NH2)nNH, and TiClm(NH2)nN. An ab Initio Molecular Orbital Study. Journal of Physical Chemistry B, 1998, 102, 5152-5157.	1.2	19
170	Reactions of Manganese and Rhenium Atoms with NO. Infrared Spectra and Density Functional Calculations of Î·1and Î·2Addition and Insertion Reaction Products. Journal of Physical Chemistry A, 1998, 102, 10041-10050.	1.1	17
171	Isotope Exchange in Ionized O3/O2Mixtures:Â The Role of O5+, a Unique On+Complex. Inorganic Chemistry, 1998, 37, 1398-1400.	1.9	11
172	Heat of Formation of thetert-Butyl Radical. Journal of Physical Chemistry A, 1998, 102, 10787-10790.	1.1	28
173	Proton Affinities of Dicyanogen Isomers:â€‰ Is There a Preferred Site of Protonation for CNCN?. Journal of Physical Chemistry A, 1998, 102, 7835-7840.	1.1	13
174	Oxidative Damage to and by Cysteine in Proteins:â€‰ An ab Initio Study of the Radical Structures, Câ^'H, Sâ^'H, and Câ^'C Bond Dissociation Energies, and Transition Structures for H Abstraction by Thiyl Radicals. Journal of the American Chemical Society, 1998, 120, 8848-8855.	6.6	108
175	A Theoretical Study of Propagation Rate Coefficients for Methacrylonitrile and Acrylonitrile. Macromolecules, 1998, 31, 5175-5187.	2.2	52
176	Vibrational Spectroscopic and ab Initio Studies on Conformations of the Chemical Species in a Reaction of Aqueous 2-(N,N-Dimethylamino)ethanol Solutions with Carbon Dioxide. Importance of Strong NH+Â·Â·Â·O Hydrogen Bonding. Journal of Physical Chemistry A, 1998, 102, 8056-8062.	1.1	18
177	Anomalous Change of Bond Energies in the Cluster Ion N2H+(H2)n. Journal of Physical Chemistry A, 1998, 102, 1214-1218.	1.1	17
178	Proton Affinity of Dimethyl Sulfoxide and Relative Stabilities of C2H6OS Molecules and C2H7OS+Ions. A Comparative G2(MP2) ab Initio and Density Functional Theory Study. Journal of Physical Chemistry A, 1998, 102, 4703-4713.	1.1	131
179	Infrared Spectra and Density Functional Calculations for OScCO, Sc-(Î·2-OC)O, OSc-(Î·2-CO), and Three OScCO+Cation Isomers in Solid Argon. Journal of the American Chemical Society, 1998, 120, 13230-13239.	6.6	70
180	Thermochemistry of Aluminum Halides:â€‰ A Theoretical Appraisal. Journal of Physical Chemistry A, 1998, 102, 7828-7834.	1.1	19
181	Radical Cation ofN,N-Dimethylpiperazine:Â Dramatic Structural Effects of Orbital Interactions through Bonds. Journal of the American Chemical Society, 1998, 120, 3748-3757.	6.6	31
182	The Three Isomers of Protonated Ethane, C2H7+. Journal of Physical Chemistry A, 1998, 102, 10903-10911.	1.1	27
183	Ground-State Tautomerism and Excited-State Proton-Transfer Processes in 4,5-Dimethyl-2-(2â€˜-hydroxyphenyl)imidazole in Solution:Â Fluorescence Spectroscopy and Quantum Mechanical Calculations. Journal of Physical Chemistry A, 1998, 102, 10736-10745.	1.1	49
184	Inversion Processes in Phosphines and Their Radical Cations:â€‰ When Is a Pseudo-Jahnâ^'Teller Effect Operative?. Journal of Physical Chemistry A, 1998, 102, 6549-6557.	1.1	37
185	Pitfalls for the Frozen-Core Approximation:Â Gaussian-2 Calculations on the Sodium Cation Affinities of Diatomic Fluorides. Journal of Physical Chemistry A, 1998, 102, 6138-6151.	1.1	36
186	Full Longitudinal Acoustic Mode (LAM) Spectrum of an N-Alkane:â€‰ Comparison of Observed and Computed Incoherent Inelastic Neutron Scattering Spectrum of N-Octadecane. Journal of Physical Chemistry B, 1998, 102, 5955-5956.	1.2	19

#	Article	IF	Citations
187	Comment on â€œIR Matrix Spectroscopy of Pentachlorocyclopentadienyl Cation C5Cl5+â€• Journal of Physical Chemistry A, 1998, 102, 8437-8438.	1.1	3
188	Direct Scaling of Primitive Valence Force Constants:Â An Alternative Approach to Scaled Quantum Mechanical Force Fields. Journal of Physical Chemistry A, 1998, 102, 1412-1424.	1.1	495
189	Degenerate Lithiumâ^'Hydrogen Exchange Reactions:â€‰ An Alternative Mechanism for Metalation of CH4 in Gas Phase and Tetrahydrofuran Solution. Journal of Physical Chemistry A, 1998, 102, 8369-8376.	1.1	14
190	The Largecloso-Borane Dianions, BnHn2-(n= 13â^'17) Are Aromatic, Why Are They Unknown?â€. Inorganic Chemistry, 1998, 37, 6765-6772.	1.9	157
191	Theoretical and Experimental Studies of Molecular Geometry, Orbitals, and Vibrational Spectra of Bioactive 3,7-Dinitrodibenzobromolium Cation. Journal of Physical Chemistry A, 1998, 102, 9261-9266.	1.1	2
192	High-Level Computational Study of the Stereoelectronic Effects of Substituents on Alkene Epoxidations with Peroxyformic Acid. Journal of the American Chemical Society, 1998, 120, 9902-9910.	6.6	65
193	Thermochemistry of CH3CN, CH3NC, and Their Cyclic Isomers and Related Radicals, Cations, and Anions:â€‰ Some Curious Discrepancies between Theory and Experiment. Journal of Physical Chemistry A, 1998, 102, 7074-7080.	1.1	45
194	Alkynes, Allenes, and Alkenes in [3,3]-Sigmatropy:â€‰ Functional Diversity and Kinetic Monotony. A Theoretical Analysis. Journal of the American Chemical Society, 1998, 120, 5622-5627.	6.6	55
195	The Nature of the Transition Structure for the Oxidation of Alkanes with Dioxiranes. Journal of the American Chemical Society, 1998, 120, 10528-10533.	6.6	60
196	Molecular Mechanics (MM3*) Parameters for Ruthenium(II)â^'Polypyridyl Complexes. Inorganic Chemistry, 1998, 37, 4120-4127.	1.9	67
197	Theoretical Studies of the Structure, Tautomerism, and Vibrational Spectra of 3-Amino-5-nitro-1,2,4-triazole. Journal of Physical Chemistry A, 1998, 102, 10348-10357.	1.1	33
198	Experimental and Theoretical Investigation of the Geometry and Vibrational Frequencies of 1,2,3-Triazole, 1,2,4-Triazole, and Tetrazole Anions. Journal of Physical Chemistry A, 1998, 102, 620-629.	1.1	45
199	Radical Addition to Alkenes:Â Further Assessment of Theoretical Procedures. Journal of Physical Chemistry A, 1998, 102, 2237-2245.	1.1	147
200	An Evaluation of Density Functional Theory and ab Initio Predictions for Bridge-Bonded Aluminum Compounds. Journal of Physical Chemistry A, 1998, 102, 2613-2623.	1.1	64
201	A Computational Study on the Reaction Mechanism of the Boultonâ^'Katritzky Rearrangement. Journal of the American Chemical Society, 1998, 120, 13478-13484.	6.6	48
202	Oxidation of Alkenes, Sulfides, Amines, and Phosphines with Peroxynitrous Acid:Â Comparison with Other Oxidants Such as Peroxyformic Acid and Dimethyldioxirane. Journal of the American Chemical Society, 1998, 120, 775-783.	6.6	57
203	Gas-Phase RNA and DNA Ions. 1. H/D Exchange of the [M â^' H]-Anions of Nucleoside 5â€˜-Monophosphates (GMP, dGMP, AMP, dAMP, CMP, dCMP, UMP, dTMP), Ribose 5-Monophosphate, and 2-Deoxyribose 5-Monophosphate with D2O and D2S. Journal of the American Chemical Society, 1998, 120, 10187-10193.	6.6	59
204	Solvation of the Li+â€“Clâ^'â€“Li+ triple ion in the gas phase. Journal of Chemical Physics, 1998, 109, 4258-4266.	1.2	7

#	Article	IF	Citations
205	Femtosecond dynamics of photoinduced molecular detachment from halogenated alkanes. I. Transition state dynamics and product channel coherence. Journal of Chemical Physics, 1998, 109, 4415-4427.	1.2	32
206	Vibrational spectra of charged defects in a series of Î±,Î±â€²-dimethyl end-capped oligothiophenes induced by chemical doping with iodine. Journal of Chemical Physics, 1998, 109, 10419-10429.	1.2	107
207	Vibrational structure in the carbon 1s ionization of hydrocarbons: Calculation using electronic structure theory and the equivalent-cores approximation. Journal of Chemical Physics, 1998, 109, 1041-1051.	1.2	86
208	High-resolution carbon1sphotoelectron spectrum of ethene:â€ƒAb initiocalculation of vibrational structure with dynamic localization of the core hole. Physical Review A, 1998, 57, 157-161.	1.0	40
209	B3LYP-DFT characterization of the potential energy surface of the CH(Xâ€‰2Î)+C2H2 reaction. Journal of Chemical Physics, 1998, 108, 1068-1080.	1.2	73
210	Experimental and ab initio study of the infrared spectra of ionic species derived from PF5, PF3, and F3PO and trapped in solid neon. Journal of Chemical Physics, 1998, 108, 8381-8393.	1.2	21
211	Density functional crystal orbital study on the normal vibrations and phonon dispersion curves of all-trans polyethylene. Journal of Chemical Physics, 1998, 108, 7901-7908.	1.2	34
212	Remarkable Changes in the (N)CH3Stretching Wavenumbers of Amines on Protonation. Chemistry Letters, 1998, 27, 531-532.	0.7	6
213	[14] Determining transition states from kinetic isotope effects. Methods in Enzymology, 1999, 308, 355-397.	0.4	43
214	Molecular modelling study of solid acidity in molybdenum oxide supported on silica-alumina. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 459-478.	0.8	6
215	Intermolecular bonding and vibrations of phenolâ‹…oxirane. Journal of Chemical Physics, 1999, 110, 1463-1474.	1.2	18
216	Fourier transform microwave spectroscopy of jet-cooled ZrO2 produced by laser vaporization. Journal of Chemical Physics, 1999, 111, 3526-3535.	1.2	40
217	Benchmark enthalpies of formation and binding energies of proton-bound pairs between HCN and HCN, NH3, H2O, and HF. Journal of Chemical Physics, 1999, 110, 7779-7788.	1.2	16
218	Infrared spectra of the CO2â^’ and C2O4â^’ anions isolated in solid argon. Journal of Chemical Physics, 1999, 110, 2414-2422.	1.2	82
219	Molecular-field splitting and vibrational structure in the phosphorus 2p photoelectron spectrum of PF3. Journal of Chemical Physics, 1999, 111, 4472-4477.	1.2	18
220	Infrared spectra and density functional calculations of Cu(CO)1â€“4+, Cu(CO)1â€“3, and Cu(CO)1â€“3â^’ in solid neon. Journal of Chemical Physics, 1999, 111, 4548-4557.	1.2	73
221	Vibrational study of a wellâ€“barrierâ€“well thiopheneâ€“based oligomer in relation to the effective Ï€-conjugation length. Journal of Chemical Physics, 1999, 110, 6907-6915.	1.2	26
222	Inelastic neutron scattering spectra of the longitudinal acoustic modes of the normal alkanes from pentane to pentacosane. Journal of Chemical Physics, 1999, 111, 429-437.	1.2	46

#	Article	IF	Citations
223	Electronic spectra of carbon chain anions: C2nHâ¯â€‰(n=5â€“12). Journal of Chemical Physics, 1999, 111, 9280-9286.	1.2	21
224	Inductive Effects in Neutral Pentacoordinated Silicon Compounds Containing a Si â†•N Dative Bond. A Theoretical Study. Organometallics, 1999, 18, 5584-5593.	1.1	69
225	Infrared spectra of cyclic-O6+ and trans-O6+ in solid neon and argon. Journal of Chemical Physics, 1999, 110, 9450-9456.	1.2	40
226	Mass analyzed threshold ionization of phenolâ‹…CO: Intermolecular binding energies of a hydrogen-bonded complex. Journal of Chemical Physics, 1999, 111, 1947-1954.	1.2	67
227	Exchange and insertion reactions involving borane adducts of phosphirane and phosphirene: a G2(MP2) ab initio investigation. Journal of Organometallic Chemistry, 1999, 580, 320-327.	0.8	12
228	The CO2 with dimethylamine reaction: ab initio predicted vibrational spectra. Journal of Molecular Structure, 1999, 482-483, 633-637.	1.8	8
229	Conformational study of 1,2-diaminoethane by combined ab initio MO calculations and Raman spectroscopy. Journal of Molecular Structure, 1999, 482-483, 639-646.	1.8	42
230	Infrared-induced rotational isomerization of 1,2-ethanediamine in argon matrices and conformational analysis by DFT calculation. Journal of Molecular Structure, 1999, 479, 41-52.	1.8	35
231	The assignment of the vibrations of substituted mercaptotetrazoles based on quantum chemical calculations. Journal of Molecular Structure, 1999, 482-483, 231-235.	1.8	7
232	Theoretical and experimental 1H, 13C, 15N, and 17O NMR spectra of 5-nitro, 5-amino, and 5-carboxy uracils. Journal of Molecular Structure, 1999, 482-483, 333-337.	1.8	23
233	An ab initio and density functional theory study of the structure and vibrational frequencies of the CH 2 FO and CHF 2 O radicals. Journal of Molecular Structure, 1999, 485-486, 67-71.	1.8	2
234	Theoretical verification and extension of the McKean relationship between bond lengths and stretching frequencies. Journal of Molecular Structure, 1999, 485-486, 385-407.	1.8	41
235	Molecular and vibrational structure of 2,2â€²-dihydroxybenzophenone: infrared linear dichroism and quantum chemical calculations. Journal of Molecular Structure, 1999, 509, 153-163.	1.8	20
236	Conformational analysis of alkylamino chains using isolated Câ€“D stretching vibrations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 2231-2246.	2.0	10
237	New infrared spectra and the tautomeric studies of purine and Î±l-alanine with an innovative sampling technique. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 2329-2342.	2.0	50
238	Gas phase and condensed phase SNi reactions. The competitive five and six centre cyclisations of the 4,5-epoxypentoxide anion: a joint experimental and theoretical study. International Journal of Mass Spectrometry, 1999, 185-187, 327-341.	0.7	0
239	A theoretical study of the isomerization and dissociation processes of the HOâ€“Cî—»O+ ion: interstate crossing in the formation of Hâ€“Cî—»O++O. International Journal of Mass Spectrometry, 1999, 185-187, 291-305.	0.7	1
240	Calculated energy barriers for the identity SN2 reaction H2O + CH3OH2+ â†' +H2OCH3 + OH2 in the gas phase, in water clusters, and in aqueous solution. International Journal of Mass Spectrometry, 1999, 182-183, 13-22.	0.7	10

#	Article	IF	Citations
241	Characterization of [Mâ€“H] cations, radicals and anions of glycine in the gas phase: a combined experimental and ab initio study. International Journal of Mass Spectrometry, 1999, 182-183, 203-211.	0.7	34
242	A density functional theory study of the catalytic role of Ar, Kr, Xe, and N2 in the CH3OHÂ·+ to CH2OH2Â·+ isomerization reaction. International Journal of Mass Spectrometry, 1999, 190-191, 181-194.	0.7	17
243	Ethene loss kinetics of methyl 2-methyl butanoate ions studied by threshold photoelectron-photoion coincidence: The enol ion of methyl propionate heat of formation. Journal of the American Society for Mass Spectrometry, 1999, 10, 200-208.	1.2	2
244	Infrared absorption and Raman scattering of (Z)-3-hydroxypropenal. A density functional theoretical study. Chemical Physics, 1999, 240, 51-61.	0.9	34
245	Theoretical study of interstellar hydroxylamine chemistry: protonation and proton transfer mediated by H3+. Chemical Physics, 1999, 244, 163-174.	0.9	21
246	Kinetics of the recombination reactions of CClF with CF2 and with CClF. Chemical Physics, 1999, 246, 157-166.	0.9	6
247	The relative stabilities of benzotriazole tautomers determined by a rotational band contour analysis of the Nâ€“H stretching vibration. Chemical Physics, 1999, 248, 17-25.	0.9	36
248	The 3.2-3.5 Âm region revisited -- I. A theoretical study of the effects of aliphatic substitution on some model PAHs. Monthly Notices of the Royal Astronomical Society, 1999, 304, 241-253.	1.6	22
249	A computational study of proton and electron affinities. Tetrahedron, 1999, 55, 10013-10026.	1.0	24
250	Ground-state density-matrix algorithm for excited-state adiabatic surfaces: application to polyenes. Chemical Physics Letters, 1999, 302, 77-84.	1.2	23
251	Infrared spectra of Dewar 2-picoline in low-temperature argon matrices. Chemical Physics Letters, 1999, 308, 403-407.	1.2	7
252	Thermochemistry of hydrochlorofluoromethanes revisited: a theoretical study with the Gaussian-3 (G3) procedure. Chemical Physics Letters, 1999, 311, 275-280.	1.2	22
253	Performance of a kinetic energy density-dependent functional (VSXC) for predicting vibrational frequencies. Chemical Physics Letters, 1999, 312, 269-276.	1.2	32
254	Binding energies of nitrile-containing proton-bound clusters: the performance of HF, MP2 and B3-LYP vs. G2. Chemical Physics Letters, 1999, 314, 311-316.	1.2	7
255	ISOEFF98. A program for studies of isotope effects using Hessian modifications. Journal of Mathematical Chemistry, 1999, 26, 75-86.	0.7	144
256	Theoretical Study of Xâ^'H Bond Energetics (X = C, N, O, S):Â Application to Substituent Effects, Gas Phase Acidities, and Redox Potentials. Journal of Physical Chemistry A, 1999, 103, 1653-1661.	1.1	243
257	Cluster model study of methoxy radical adsorption on the Cu (111) surface. Computational and Theoretical Chemistry, 1999, 463, 163-168.	1.5	18
258	Ab initio HF and DFT calculations of geometric structures and vibrational spectra of electrically conducting doped oligothiophenes. Computational and Theoretical Chemistry, 1999, 463, 211-216.	1.5	22

#	Article	IF	Citations
259	The effect of remote substituents in free radical addition reactions: new evidence for the penultimate unit effect. Computational and Theoretical Chemistry, 1999, 461-462, 91-96.	1.5	29
260	An ab initio study of protonation of B12H122â^'. Structure and non-rigidity of B12H13â^' and formation of B12H11â^' and B24H233â^'. Computational and Theoretical Chemistry, 1999, 461-462, 187-202.	1.5	22
261	Ab initio and density functional theory study on the geometries, energies, and vibrational spectra of the conformations of 3-methyl-3-penten-2-one. Computational and Theoretical Chemistry, 1999, 467, 85-93.	1.5	8
262	Density functional calculations of enthalpies of hydrogenation, isomerization, and formation of small cyclic hydrocarbons. Computational and Theoretical Chemistry, 1999, 468, 59-66.	1.5	20
263	Computation of adsorbate vibrational frequencies: methyl, methylidyne and methoxy adsorbed on the Al(111) surface. Computational and Theoretical Chemistry, 1999, 464, 153-162.	1.5	6
264	Copolymers of carbon dioxide and nitrogen: an AM1 and ab initio computational study. Computational and Theoretical Chemistry, 1999, 469, 77-102.	1.5	12
265	Theoretical study on infrared vibrational spectra of boric-acid in gas-phase using density functional methods. Computational and Theoretical Chemistry, 1999, 469, 223-227.	1.5	15
266	Inter-relationships between the geometrical parameters of the amino group in several para -substituted anilines. Computational and Theoretical Chemistry, 1999, 493, 171-177.	1.5	22
267	High-Resolution Fourier Transform Infrared Spectroscopy of Vinyl Alcohol: Rotational Analysis of the Î½13 CH2 Wagging Fundamental at 817 cmâ^'1. Journal of Molecular Spectroscopy, 1999, 197, 68-75.	0.4	23
268	Theoretical Study of Intermediates in the Urate Oxidase Reaction. Bioorganic Chemistry, 1999, 27, 351-362.	2.0	17
269	Characterization of Fermi resonances in adsorbate vibrational spectra using cluster calculations: Methoxy adsorption on Al(111) and Cu(111). International Journal of Quantum Chemistry, 1999, 75, 815-820.	1.0	20
270	Compatibility of correlation-consistent basis sets with a hybrid Hartree-Fock/density functional method. Journal of Computational Chemistry, 1999, 20, 207-216.	1.5	37
271	The Reduction of Î±-X-Acetophenones (X = PhO, Br, Cl) in Hydrogen-Donating Solvents at Elevated Temperatures. European Journal of Organic Chemistry, 1999, 1999, 607-616.	1.2	8
273	The Structures and Energies of Phosphaalkyne Trimers, (HCP)3. European Journal of Organic Chemistry, 1999, 1999, 3291-3303.	1.2	40
275	Density Functional Studies on Conjugate Addition of (Me2CuLi)2 to Cyclohexenone: Stereoselectivity and Rate-Determining Step. Chemistry - A European Journal, 1999, 5, 1534-1543.	1.7	70
276	Comparison study of the prediction of Raman intensities using electronic structure methods. Journal of Chemical Physics, 1999, 111, 8819-8824.	1.2	137
277	Adsorption of pyrrole derivatives in alkali metal cation-exchanged faujasites: comparative studies by surface vibrational techniques, X-ray diffraction and temperature-programmed desorption augmented with theoretical studies Part I. Pyrrole as probe molecule. Physical Chemistry Chemical Physics, 1999, 1, 593-603.	1.3	48
278	Production of HCl in the OH + ClO Reaction:â€‰ Laboratory Measurements and Statistical Rate Theory Calculations. Journal of Physical Chemistry A, 1999, 103, 6540-6551.	1.1	25

#	Article	IF	Citations
279	A Theoretical and Experimental Study of the Molecular Rearrangement of 5-Methyl-4-nitrobenzofuroxan. Journal of the American Chemical Society, 1999, 121, 6700-6711.	6.6	40
280	Kinetic and Thermodynamic Analysis on OH Addition to Ethylene:Â Adduct Formation, Isomerization, and Isomer Dissociations. Journal of Physical Chemistry A, 1999, 103, 7646-7655.	1.1	49
281	Calculation of dipole moment functions with density functional theory: application to vibrational band intensities. Molecular Physics, 1999, 96, 1125-1138.	0.8	36
283	Poly Methoxy Phenols in Solution:Â Oâˆ'H Bond Dissociation Enthalpies, Structures, and Hydrogen Bonding. Journal of Organic Chemistry, 1999, 64, 6969-6975.	1.7	165
284	Ab Initio Calculations of Vibronic Spectra and Dynamics for Small Polyatomic Molecules:Â Role of Duschinsky Effect. Journal of Physical Chemistry A, 1999, 103, 10674-10690.	1.1	139
285	Isomerization and Dissociation in Competition:Â The Two-Component Dissociation Rates of Methyl Propionate Ions. Journal of Physical Chemistry A, 1999, 103, 1221-1227.	1.1	8
286	Allyl Zincation of Vinyl Metals:â€‰ A Computational Study. Organic Letters, 1999, 1, 929-931.	2.4	28
287	Mechanism of the Gas-Phase HO + H2O â†' H2O + OH Reaction and Several Associated Isotope Exchange Reactions:â€‰ A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053.	1.1	34
288	A study of FeCO+ with correlated wavefunctions. Physical Chemistry Chemical Physics, 1999, 1, 967-975.	1.3	31
289	Density functional study of configurational, conformational, energetic, electronic and spectroscopic properties of fluorohydroxyformaldoxime and its dehydration products. Physical Chemistry Chemical Physics, 1999, 1, 4541-4547.	1.3	5
290	An assessment of theoretical procedures for the calculation of reliable radical stabilization energiesâ€Šâ€¡. Journal of the Chemical Society Perkin Transactions II, 1999, , 2305-2313.	0.9	121
291	An ab initio quasi-classical direct dynamics investigation of the F+C2H4â†'C2H3F+H product energy distributions. Physical Chemistry Chemical Physics, 1999, 1, 999-1011.	1.3	32
292	Î³-Dissociations of 3-alkylbicyclo[1.1.1]pent-1-yl radicals into [1.1.1]propellane and alkyl radicals: verification of a theoretical prediction. Physical Chemistry Chemical Physics, 1999, 1, 1399-1404.	1.3	5
293	Structure, conformation, anomeric effects and rotational barriers in the HERON amides, N,Nâ€Šâ€²-diacyl-N,Nâ€Šâ€²-dialkoxyhydrazines. Journal of the Chemical Society Perkin Transactions II, 1999, , 2053-2058.	0.9	32
294	Poly(3â€²,4â€²-[bis(N,Nâ€²-ethyloxamyl)]terthiophene): A new functionalized conductive polymer with tunable pendent ethyloxamyl substituents. Physical Chemistry Chemical Physics, 1999, 1, 2755-2760.	1.3	7
295	Ab initio study of the n-Ï€* electronic transition in acetone: Symmetry-forbidden vibronic spectra. Journal of Chemical Physics, 1999, 111, 205-215.	1.2	58
296	An ab initio molecular dynamics study of the SN2 reaction Clâ^'+CH3Brâ†'CH3Cl+Brâ^'. Journal of Chemical Physics, 1999, 111, 10887-10894.	1.2	34
297	Infrared spectra of the C2O4+ cation and C2O4â^' anion isolated in solid neon. Journal of Chemical Physics, 1999, 110, 6820-6826.	1.2	54

#	Article	IF	Citations
298	Formation of CF3Oâˆ™ in the gas phase. Journal of Chemical Physics, 1999, 110, 8436-8442.	1.2	11
299	The thermal unimolecular decomposition rate constants of ethoxy radicals. Physical Chemistry Chemical Physics, 1999, 1, 2935-2944.	1.3	91
300	Gas phase and condensed phase SNi reactions. The competitive six and seven centre cyclisations of the 5,6-epoxyhexoxide anion. A joint experimental and ab initio study. A comparison with SNi reactions of homologous epoxyalkoxide anionsâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 457-464.	0.9	4
301	Use of a radical clock to study the photodecarboxylation of amino acidatocobalt(III) complexesâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1999, , 3565-3571.	1.1	6
302	Glycine radicals in the gas phaseâ€Šâ€â€¡. Journal of the Chemical Society Perkin Transactions II, 1999, , 2315-2323.	0.9	43
304	Phenoxyl, (Methylthio)phenoxyl, and (Methylthio)cresyl Radical Models for the Structures, Vibrations, and Spin Properties of the Cysteine-Linked Tyrosyl Radical in Galactose Oxidase. Journal of Physical Chemistry B, 1999, 103, 4764-4772.	1.2	22
305	Theoretical Investigation of the Role of Intramolecular Hydrogen Bonding in Î²-Hydroxyethoxy and Î²-Hydroxyethylperoxy Radicals in the Tropospheric Oxidation of Ethene. Journal of Physical Chemistry A, 1999, 103, 1768-1775.	1.1	70
306	Computational Study of the Mechanisms for the Reaction of O2(3Î£g) with Aromatic Radicals. Journal of Physical Chemistry A, 1999, 103, 8108-8117.	1.1	59
307	Analysis of Tertiary Butyl Radical + O2, Isobutene + HO2, Isobutene + OH, and Isobuteneâˆ™OH Adducts + O2:Â A Detailed Tertiary Butyl Oxidation Mechanism. Journal of Physical Chemistry A, 1999, 103, 9731-9769.	1.1	62
308	Gas-phase reactions of the dichlorocarbene radical cation. Journal of the Chemical Society Perkin Transactions II, 1999, , 2267-2272.	0.9	11
309	Of Ortho-Conjugatively Linked Reactive Intermediates:Â The Cases of Ortho-Phenylene-(Bis)Nitrene, -Carbenonitrene, and -(Bis)Carbene. Journal of the American Chemical Society, 1999, 121, 10563-10572.	6.6	30
310	Vibrational spectra and ab initio dft calculations of 3,3â€²-and 4,4â€²-dimethyl substituted 2,2â€²-bithiophene.. Synthetic Metals, 1999, 101, 590-591.	2.1	4
311	Calculation of OH-stretching band intensities of the water dimer and trimer. Journal of Chemical Physics, 1999, 110, 9104-9115.	1.2	171
312	Gaussian-3 theory using density functional geometries and zero-point energies. Journal of Chemical Physics, 1999, 110, 7650-7657.	1.2	1,606
313	A Systematic Application of Density Functional Theory to Some Carbon-Containing Molecules and Their Anions. Journal of Physical Chemistry A, 1999, 103, 4065-4077.	1.1	86
314	Calculation of Vibrational Spectra of Linear Tetrapyrroles. 1. Global Sets of Scaling Factors for Force Fields Derived by ab Initio and Density Functional Theory Methods. Journal of Physical Chemistry A, 1999, 103, 289-303.	1.1	39
315	Quantum Mechanical Tunneling in the Unimolecular Dissociation of the Propargyl Bromide Molecular Ion. Journal of Physical Chemistry A, 1999, 103, 4602-4608.	1.1	7
316	A quantum chemical approach to the water assisted neutral hydrolysis of ethyl acetate and its derivatives. Physical Chemistry Chemical Physics, 1999, 1, 1025-1030.	1.3	30

#	Article	IF	Citations
317	Proposed Mechanism of 1,1-Diamino-Dinitroethylene Decomposition:Â A Density Functional Theory Study. Journal of Physical Chemistry A, 1999, 103, 11045-11051.	1.1	125
318	Experimental Proof of the Non-Least-Motion Cycloadditions of Dichlorocarbene to Alkenes:Â Kinetic Isotope Effects and Quantum Mechanical Transition States. Journal of the American Chemical Society, 1999, 121, 3933-3938.	6.6	77
319	Ab Initio Calculations of Absolute pKaValues in Aqueous Solution I. Carboxylic Acids. Journal of Physical Chemistry A, 1999, 103, 11194-11199.	1.1	165
320	Vibrational Frequencies. , 1999, , 219-234.		0
321	Oxidative Aromatic Substitutions:â€‰ Hartreeâ^'Fock/Density Functional and ab Initio Molecular Orbital Studies of Benzene and Toluene Nitrosation. Journal of Physical Chemistry A, 1999, 103, 4261-4269.	1.1	42
322	Study of the Electrocyclization of (Z)-Hexa-1,3,5-triene and Its Heterosubstituted Analogues Based on Ab Initio and DFT Calculations. Journal of Organic Chemistry, 1999, 64, 6842-6848.	1.7	54
323	Reactions of Laser-Ablated Mo and W Atoms with Dinitrogen:Â Infrared Spectra of Metal Nitrides, Dinitrides, and Complexes in Solid Argon and Nitrogen. Journal of Physical Chemistry A, 1999, 103, 4649-4658.	1.1	19
324	Infrared Spectroscopic and Density Functional Theoretical Investigation of the Reaction Products of Laser-Ablated Zr, Hf, and Th Atoms with Nitric Oxide. Journal of Physical Chemistry A, 1999, 103, 4836-4844.	1.1	35
325	Infrared Spectral, Structural, and Conformational Studies of Zwitterionicl-Tryptophan. Journal of Physical Chemistry A, 1999, 103, 9995-10003.	1.1	100
326	Hydrogen Migration in the Phenylethen-2-yl Radical. Journal of Physical Chemistry A, 1999, 103, 7127-7135.	1.1	48
327	Adsorption of the Phosphate Groups on Silica Hydroxyls:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 1228-1238.	1.1	70
328	Conformational Dependence of the Penultimate Unit Effect in Free-Radical Copolymerization. Macromolecules, 1999, 32, 5270-5276.	2.2	50
329	Energetics and Structures of the Carbonyl Chloride Radical, Oxalyl Chloride, and Their Cations. Journal of Physical Chemistry A, 1999, 103, 7918-7922.	1.1	16
330	Reaction of OH Radical with C2H3Cl:Â Rate Constant and Reaction Pathway Analysis. Journal of Physical Chemistry A, 1999, 103, 7800-7810.	1.1	20
331	Theoretical Characterization of the Structures and Reactivity of 7-Hydroxyquinolineâ^'(H2O)n(n= 1â^'3) Complexes. Journal of Physical Chemistry A, 1999, 103, 5567-5573.	1.1	22
332	Mechanism and Kinetics of the Reaction of Acetylene and Nitric Oxide. Journal of Physical Chemistry A, 1999, 103, 5015-5022.	1.1	5
333	2-Chloroallyl Cation. Structure, FT-IR Spectra, and Matrix Isolation. Journal of Organic Chemistry, 1999, 64, 4931-4934.	1.7	6
334	Origins of Stereoselectivity in the Coreyâ^'Chaykovsky Reaction. Insights from Quantum Chemistry. Journal of Organic Chemistry, 1999, 64, 4596-4606.	1.7	41

#	Article	IF	Citations
335	Reaction of Aqueous 2-(N-Methylamino)ethanol Solutions with Carbon Dioxide. Chemical Species and Their Conformations Studied by Vibrational Spectroscopy and ab Initio Theories. Journal of Physical Chemistry A, 1999, 103, 4283-4292.	1.1	35
336	Magnesium Dicyanide:â€‰ Three Isomers or Seven?. Journal of Physical Chemistry A, 1999, 103, 2107-2116.	1.1	6
337	Vibrational Analysis and Ring-Puckering Inversion Barrier of Perfluorocyclopentene. Journal of Physical Chemistry A, 1999, 103, 3726-3731.	1.1	4
338	Infrared Spectra of OMCO (M = Crâ^'Ni), OMCO- (M = Crâ^'Cu), and MCO2- (M = Coâ^'Cu) in Solid Argon. Journal of Physical Chemistry A, 1999, 103, 2013-2023.	1.1	58
339	Electronic Spectra of the Carbon Chain Anions C2n-1H-(n= 5â^'8) in the Gas Phase. Journal of Physical Chemistry A, 1999, 103, 9712-9716.	1.1	18
340	Experimental and Theoretical Investigations of Ring-Expansion in 1-Methylcyclopropylcarbene. Journal of Organic Chemistry, 1999, 64, 5886-5895.	1.7	16
341	Infrared Spectra and Density Functional Calculations of Small Vanadium and Titanium Carbonyl Molecules and Anions in Solid Neon. Journal of Physical Chemistry A, 1999, 103, 5259-5268.	1.1	48
342	Preference ofnpÏ€â^'npÏ€Bonding (n= 3, 4) over Purely Ïƒ-Bonded Species in M42+(M = S, Se):Â Geometries, Bonding, and Energetics of Several M42+Isomersâ€‚â€¡. Inorganic Chemistry, 1999, 38, 5203-5211.	1.9	38
343	Infrared Spectra and Density Functional Calculations for OMCO, OMâ^'(Î·2-CO), OMCO+, and OMOC+ (M) Tj ETQq0 0 0 rgBT /Overlock	1.1	50
344	Intramolecular Solvation of Carboxylate Anions in the Gas Phase. Journal of Physical Chemistry A, 1999, 103, 7008-7016.	1.1	15
345	In Vivo, in Vitro, and Calculated Vibrational Spectra of Plastoquinone and the Plastosemiquinone Anion Radical. Journal of Physical Chemistry B, 1999, 103, 9790-9800.	1.2	38
346	Differential Adsorption of Phenol Derivatives onto a Polymeric Sorbent:â€‰ A Combined Molecular Modeling and Experimental Study. Journal of Physical Chemistry B, 1999, 103, 9879-9887.	1.2	26
347	Scaling Factors for the Prediction of the Frequencies of the Ring Modes in Benzene Derivatives. Journal of Physical Chemistry A, 1999, 103, 11366-11377.	1.1	36
348	Unimolecular Reactions of Proton-Bound Cluster Ions:Â Competition between Dissociation and Isomerization in the Methanolâ^'Acetonitrile Dimer. Journal of Physical Chemistry A, 1999, 103, 3687-3692.	1.1	20
349	Ab Initio Calculations of Enthalpies of Hydrogenation, Isomerization, and Formation of Cyclic C6 Hydrocarbons. Benzene Isomers. Journal of Physical Chemistry A, 1999, 103, 426-430.	1.1	34
350	Structures and Binding Energies of Proton-Bound Pairs of HCN and CH3CN with NH3, H2O, HF, CH3NH2, CH3OH, and CH3F. Journal of Physical Chemistry A, 1999, 103, 5905-5909.	1.1	17
351	Decomposition of Î²-Hydroxypropoxy Radicals in the OH-Initiated Oxidation of Propene. A Theoretical and Experimental Study. Journal of Physical Chemistry A, 1999, 103, 4693-4702.	1.1	57
352	Photochemical Reaction of Ozone and Benzene:Â An Infrared Matrix Isolation Study. Journal of the American Chemical Society, 1999, 121, 4271-4277.	6.6	29

#	Article	IF	Citations
353	An ab Initio Investigation of the Reactions of 1,1- and 1,2-Dichloroethane with Hydroxyl Radical. Journal of Physical Chemistry A, 1999, 103, 10874-10883.	1.1	182
354	Density functional calculation of structure and vibrational spectra of polyenes. Journal of Chemical Physics, 1999, 110, 3241-3250.	1.2	35
355	Using Raman Spectroscopy To Monitor the Solvent-Exposed and â€œBuriedâ€•Forms of Flavin in p-Hydroxybenzoate Hydroxylase. Biochemistry, 1999, 38, 16727-16732.	1.2	52
356	Propyne Pyrolysis in a Flow Reactor:Â An Experimental, RRKM, and Detailed Kinetic Modeling Study. Journal of Physical Chemistry A, 1999, 103, 5889-5899.	1.1	116
357	New Molecular Mechanics (MM3*) Force Field Parameters for Calculations on (Î·3-Allyl)palladium Complexes with Nitrogen and Phosphorus Ligands. Organometallics, 1999, 18, 2884-2895.	1.1	38
358	Dynamics of Endoergic Bimolecular Proton Transfer Reactions:Â F-+ ROH â†' HF + RO-(R = H, CH3, CH3CH2,) Tj ETQq1 1 0.784314 rg	1.1	23
359	Rationalization of Product Selectivities in Asymmetric Hornerâ^'Wadsworthâ^'Emmons Reactions by Use of a New Method for Transition-State Modeling. Journal of Organic Chemistry, 1999, 64, 5845-5852.	1.7	36
360	Influence of Electronic Correlation on Structural, Dynamic, and Elastic Properties of Mg2Si. Journal of Physical Chemistry B, 1999, 103, 2601-2606.	1.2	25
361	Effect of Angle Strain in Conjugated Cycloalkenylidenes. Singletâ^'Triplet Splitting of Cyclobutenylidene and Its Ground-State Intramolecular Rearrangements. Journal of Organic Chemistry, 1999, 64, 3299-3305.	1.7	16
362	Modulating Electron Density in the Bound Product, 4-Hydroxybenzoyl-CoA, by Mutations in 4-Chlorobenzoyl-CoA Dehalogenase Near the 4-Hydroxy Groupâ€. Biochemistry, 1999, 38, 4198-4206.	1.2	26
363	Gas-Phase Nuclear Magnetic Resonance Study of (15N)Trifluoroacetamide:â€‰ Comparison of Experimental and Computed Kinetic Parameters. Journal of the American Chemical Society, 1999, 121, 4478-4484.	6.6	8
364	Structures, Vibrational Frequencies and Polarizabilities of Diazaborinines, Triazadiborinines, Azaboroles, and Oxazaboroles. Journal of Physical Chemistry A, 1999, 103, 2141-2151.	1.1	33
365	Structure and Energetics of Vinoxide and the X(2Aâ€˜Ââ€˜) and A(2Aâ€˜) Vinoxy Radicals. Journal of Physical Chemistry A, 1999, 103, 9190-9194.	1.1	32
366	Surface-Enhanced Raman Scattering of a Cu/Pd Alloy Colloid Protected by Poly(N-vinyl-2-pyrrolidone). Langmuir, 1999, 15, 7980-7992.	1.6	83
367	A Computational Study on the Mechanism and Kinetics of the Pyrolysis of 2-Nitrophenyl Azide. Journal of Physical Chemistry A, 1999, 103, 9086-9092.	1.1	38
368	Direct Observation of Hydrogen Atom Adducts to Nitromethane and Methyl Nitrite. A Variable-Time Neutralizationâ^'Reionization Mass Spectrometric and ab Initio/RRKM Study. Journal of Physical Chemistry A, 1999, 103, 9241-9251.	1.1	15
369	An ab Initio Study of Intramolecular Hydrogen Bondings in Î±-Hydroxy Ketomethylene Dipeptide Isostereâ€. Journal of Organic Chemistry, 1999, 64, 5036-5041.	1.7	7
370	Vibrational Spectroscopic Study of a Series of Î±,Î±â€˜-Diethyl End-Capped Oligothiophenes with Different Chain Lengths in the Neutral State. Journal of Physical Chemistry A, 1999, 103, 816-822.	1.1	34

#	Article	IF	Citations
371	Competitive Gas-Phase Solvation of Alkali Metal Ions by Water and Methanol. Journal of Physical Chemistry A, 1999, 103, 9891-9898.	1.1	42
372	Effect of the Penultimate Unit on Radical Stability and Reactivity in Free-Radical Polymerization. Macromolecules, 1999, 32, 2935-2940.	2.2	61
373	A Density Functional Theory Study of the Hydrates of NH3Â·H2SO4 and Its Implications for the Formation of New Atmospheric Particles. Journal of Physical Chemistry A, 1999, 103, 2801-2811.	1.1	53
374	Feâ''Catecholate and Feâ''Oxalate Vibrations and Isotopic Substitution Shifts from DFT Quantum Chemistry. Journal of Physical Chemistry A, 1999, 103, 256-264.	1.1	41
375	Ab Initio Study of Unimolecular Decomposition of Nitroethylene. Journal of Physical Chemistry A, 1999, 103, 11040-11044.	1.1	37
376	An Infrared Spectroscopic and Density Functional Theoretical Investigation of the Reaction Products of Laser-Ablated Scandium and Titanium Atoms with Nitric Oxide. Journal of Physical Chemistry A, 1999, 103, 1115-1125.	1.1	36
377	Contribution of Pyrone-Type Structures to Carbon Basicity:Â An ab Initio Study. Langmuir, 1999, 15, 3897-3904.	1.6	54
378	Acid Ionization of HBr in a Small Water Cluster. Israel Journal of Chemistry, 1999, 39, 273-281.	1.0	37
379	Adsorption of Poly(Î³-Substituted Î±-, L-Glutamate) on Aluminum Surface: Atr and Mo Approaches. Molecular Crystals and Liquid Crystals, 2000, 349, 155-158.	0.3	0
380	Ultrafast Charge Transfer Studied by Femtosecond IRâ€Spectroscopy and ab Initio Calculations. Journal of the Chinese Chemical Society, 2000, 47, 721-728.	0.8	20
381	Electronic absorption, resonance Raman and excited-state resonance Raman spectroscopy of rhenium(I) and copper(I) complexes, with substituted dipyrido[3,2-a : 2â€²,3â€²-c]phenazine ligands, and their electron reduced products. Journal of Raman Spectroscopy, 2000, 31, 243-253.	1.2	40
382	All-atom empirical force field for nucleic acids: I. Parameter optimization based on small molecule and condensed phase macromolecular target data. Journal of Computational Chemistry, 2000, 21, 86-104.	1.5	1,460
383	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O2 reaction system. International Journal of Chemical Kinetics, 2000, 32, 435-452.	1.0	33
384	Do branched structures exist for cyanide-containing magnesium compounds? Computational studies on a range of mixed-ligand compounds XMg(CN) (X = F, Cl, OH, SH, NH2, CH3, CN). International Journal of Quantum Chemistry, 2000, 76, 626-642.	1.0	7
385	A vibrational analysis with Fermi resonances for methoxy adsorption on Cu(111) using ab initio cluster calculations. International Journal of Quantum Chemistry, 2000, 77, 350-357.	1.0	19
386	Scaling factors for the prediction of vibrational spectra. I. Benzene molecule. International Journal of Quantum Chemistry, 2000, 77, 661-684.	1.0	405
387	Proton affinity of peroxyacetyl nitrate. A computational study of topical proton affinities. Journal of Mass Spectrometry, 2000, 35, 1351-1359.	0.7	9
388	Fluorinated methyl cation (CF3+, CFH2+)-alkyl nitrile cluster ions. Journal of Mass Spectrometry, 2000, 35, 1407-1415.	0.7	5

#	Article	IF	Citations
389	A Theoretical Study of the Properties and Reactivities of Ketene, Thioketene, and Selenoketene. European Journal of Organic Chemistry, 2000, 2000, 1411-1421.	1.2	23
390	Dissociation dynamics of propargyl chloride molecular ion near the reaction threshold: manifestation of quantum mechanical tunneling. Rapid Communications in Mass Spectrometry, 2000, 14, 1110-1115.	0.7	6
391	Infrared and Raman spectra of a new radical cation charged defect created on a well-barrier-well thiophene-based oligomer. Journal of Raman Spectroscopy, 2000, 31, 565-570.	1.2	23
392	Fourier transform Raman spectrum andab initio and density functional computations of the vibrational spectrum, molecular geometry, atomic charges and some molecular properties of the anticarcinogenic drug 5-fluorouracil. Journal of Raman Spectroscopy, 2000, 31, 595-603.	1.2	50
393	Vibrational analysis and excited-state geometric changes of betaine-30 derived from Raman and infrared spectra combined withab initio calculations. Journal of Raman Spectroscopy, 2000, 31, 797-803.	1.2	34
394	FTIR and FT-Raman spectra of 5-methyluracil (thymine). Journal of Raman Spectroscopy, 2000, 31, 1005-1012.	1.2	48
395	ab initio calculations and thermochemical analysis on C1 atom abstractions of chlorine from chlorocarbons and the reverse alkyl abstractions: Cl2 + Rï¿½ ? Clï¿½ + RCl. International Journal of Chemical Kinetics, 2000, 32, 548-565.	1.0	6
396	Hemispiroalkaplanes: Hydrocarbon Cage Systems with a Pyramidal-Tetracoordinate Carbon Atom and Remarkable Basicity. Chemistry - A European Journal, 2000, 6, 2470-2483.	1.7	40
397	Torquoselectivity in the Cationic Cyclopentannelation of (2Z)-Hexa-2,4,5-trienal Acetals. Chemistry - A European Journal, 2000, 6, 4021-4033.	1.7	13
398	Theoretical Study of 1,3-Dipolar Cycloaddition Reactions with Inverse Electron Demand â^' A DFT Study of the Lewis Acid Catalyst and Solvent Effects in the Reaction of Nitrones with Vinyl Ethers. European Journal of Organic Chemistry, 2000, 2000, 2265-2272.	1.2	66
399	Stereochemical Aspects of a Two-Step Staudinger Reaction â^' Asymmetric Synthesis of Chiral Azetidine-2-ones. European Journal of Organic Chemistry, 2000, 2000, 2379-2390.	1.2	29
400	Conformational properties of thiophene oligomers. Journal of Heterocyclic Chemistry, 2000, 37, 847-853.	1.4	26
401	Stability and infrared spectra of mono-, di-, and trichloromethanol. Chemical Physics Letters, 2000, 322, 97-102.	1.2	46
402	Infrared spectra of Dewar 4-picoline in low-temperature argon matrices and vibrational analysis by DFT calculation. Chemical Physics Letters, 2000, 322, 363-370.	1.2	38
403	Density functional vibrational analysis using wavenumber-linear scale factors. Chemical Physics Letters, 2000, 325, 477-483.	1.2	208
404	The alternative thermal decomposition mode of 2-oxetanone and 2-azetidinone: a DFT and PES study. Chemical Physics Letters, 2000, 325, 433-439.	1.2	15
405	Ab initio studies toward understanding photoisomerization of acrylic acid in the gas phase. Chemical Physics Letters, 2000, 325, 683-692.	1.2	10
406	Computational studies on the ring openings of cyclopropyl radical and cyclopropyl cation. Chemical Physics Letters, 2000, 328, 90-96.	1.2	39

#	Article	IF	Citations
407	Reaction mechanism of CO2 with Ca atom: A theoretical study. Chemical Physics Letters, 2000, 331, 526-532.	1.2	12
408	The infrared vibrational spectra of the two major C84 isomers. Chemical Physics Letters, 2000, 332, 35-42.	1.2	17
409	A theoretical study of [Be,(H2O)n]2+, [BeOH,(H2O)nâˆ’1]+ and [Be(OH)2,(H2O)nâˆ’2] aggregates (n=1â€“6). Incidence of the first hydration shells on the hydrolysis reactions of Be2+ and BeOH+ systems. Chemical Physics Letters, 2000, 332, 367-374.	1.2	20
410	Theoretical studies of the reduction of ethylene carbonate. Chemical Physics Letters, 2000, 317, 421-429.	1.2	66
411	Heterocyclic quinones as core units for redox switches: UVâ€“vis/NIR, FTIR spectroelectrochemistry and DFT calculations on the vibrational and electronic structure of the radical anions. Journal of Electroanalytical Chemistry, 2000, 484, 24-32.	1.9	66
412	Anharmonicity in anisotropic displacement parameters. Acta Crystallographica Section A: Foundations and Advances, 2000, 56, 425-435.	0.3	47
413	35 Cl NQR spectra of phosphorus chlorides and their molecular conformations in crystals. Part 1. Phosphorus (III) chlorides RPCl 2. Journal of Molecular Structure, 2000, 550-551, 167-175.	1.8	3
414	Vibrational spectroscopic and theoretical calculation studies on conformational behavior of simple sodium 1-alkanesulfonates. Journal of Molecular Structure, 2000, 553, 49-59.	1.8	5
415	Polarized IR and DFT study of the fundamental vibrations of xanthone. Journal of Molecular Structure, 2000, 553, 235-241.	1.8	5
416	A gradient-corrected density functional study of structure, harmonic vibrational frequencies and charge distribution of benzenesulfonate anion on the ground-state potential energy surface. Journal of Molecular Structure, 2000, 555, 341-349.	1.8	13
417	G3(MP2) calculation of the enthalpies of formation, isomerization and hydrogenation of cubane and cyclooctatetraene. Journal of Molecular Structure, 2000, 556, 207-215.	1.8	15
418	Medium effects on the ionization of the acidic sites of bifunctional organic molecules: the case of 4-hydroxybenzoic acid. Journal of Molecular Structure, 2000, 556, 245-252.	1.8	8
419	Are cumulenones kinked? A systematic high-level ab initio study of H 2 CCCO, H 2 CCCCO and H 2 CCCCCO. Journal of Molecular Structure, 2000, 556, 253-261.	1.8	16
420	Molecular mechanics (MM3) calculations on phosphonamidate compounds. Journal of Molecular Structure, 2000, 556, 283-291.	1.8	1
421	Molecular structure of trans -azoxybenzene determined by gas electron diffraction combined with ab initio calculations. Journal of Molecular Structure, 2000, 554, 203-210.	1.8	16
422	The vibrational spectra and normal coordinates analysis of bromofluoromethane, CH 2 BrF. Journal of Molecular Structure, 2000, 517-518, 197-208.	1.8	14
423	The infrared spectra and molecular structure of zwitterionic l-Î²-phenylalanine. Journal of Molecular Structure, 2000, 519, 153-163.	1.8	37
424	Molecular structures, conformations, and vibrational spectra of bicyclo[3.1.0]hexane and its oxygen analogues. Journal of Molecular Structure, 2000, 519, 75-84.	1.8	16

#	Article	IF	Citations
425	Vibrational spectroscopic and quantum chemical studies of the trioxatriangulenium carbocation. Journal of Molecular Structure, 2000, 520, 63-73.	1.8	12
426	Density functional study on the structures and vibrational spectra of the radical cation and dication of Î±,Î±â€²-bis(aminomethyl)quaterthiophene. Journal of Molecular Structure, 2000, 521, 249-260.	1.8	6
427	Asymmetric aldol reaction of 2-cyanopropionates catalyzed by a trans-chelating chiral diphosphineâ€“rhodium(I) complex: highly enantioselective construction of quaternary chiral carbon centers at Î±-positions of nitriles. Journal of Organometallic Chemistry, 2000, 603, 18-29.	0.8	38
428	Structures and vibrational frequencies of pyruvic acid: density functional theory study. Vibrational Spectroscopy, 2000, 23, 181-186.	1.2	54
429	Theoretical IR and Raman spectra of diketene and its 3-methylene isomer. Vibrational Spectroscopy, 2000, 22, 19-28.	1.2	16
430	Ab initio HF, density functional and experimental studies on the IR spectra and structure of 1,2-benzisothiazol-3-(2H)-thione-1,1-dioxide (thiosacchanin) and its nitranion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2000, 56, 1949-1956.	2.0	30
431	The involvement of ionâ€“neutral complexes in ethylene loss from [PhC(CH3)2]+ and its isomers. International Journal of Mass Spectrometry, 2000, 199, 29-40.	0.7	7
432	A density functional theory study of methyl shifts and methylcyclopropanol ion formation in C4H8O+Â· ions. International Journal of Mass Spectrometry, 2000, 199, 41-57.	0.7	5
433	Ab initio calculated gas-phase basicities of polynuclear aromatic hydrocarbons. International Journal of Mass Spectrometry, 2000, 201, 283-295.	0.7	33
434	Unimolecular reaction dynamics from kinetic energy release distributions. VI. Energy-selected ions. International Journal of Mass Spectrometry, 2000, 201, 59-67.	0.7	16
435	Mediators for hydrogenation of carbon monoxide: theoretical study of addition of H2 to HCO+ in the presence of CO or H2O. International Journal of Mass Spectrometry, 2000, 201, 179-185.	0.7	2
436	Landmarks in the theory of mass spectra. International Journal of Mass Spectrometry, 2000, 200, 43-56.	0.7	51
437	Rearrangement and fragmentation pathways of [C3H7Z]+ ions (Z = NH and S): are ionâ€“neutral complexes important?. International Journal of Mass Spectrometry, 2000, 194, 181-196.	0.7	9
438	Identifying ylide ions and methyl migrations in the gas phase: the decarbonylation reactions of simple ionized N-heterocycles. International Journal of Mass Spectrometry, 2000, 195-196, 71-83.	0.7	17
439	Mechanisms of reactions between ammonia and methylene oxonium ions: immonium ion formation versus transfer of the oxygen substituent. International Journal of Mass Spectrometry, 2000, 195-196, 171-184.	0.7	14
440	Thiosulfoxides (X2S˜...S) and disulfanes (XSSX):. International Journal of Mass Spectrometry, 2000, 195-196, 239-249.	0.7	20
441	Protonation sites in methyl nitrate and the formation of transient CH4NO3 radicals. A neutralizationâ€”reionization mass spectrometric and computational study. Journal of the American Society for Mass Spectrometry, 2000, 11, 380-392.	1.2	9
442	The fragmentation pathways of protonated glycine: A computational study. Journal of the American Society for Mass Spectrometry, 2000, 11, 687-696.	1.2	62

#	Article	IF	Citations
443	Proton affinity of uracil. A computational study of protonation sites. Journal of the American Society for Mass Spectrometry, 2000, 11, 1065-1071.	1.2	74
444	Leaving group and gas phase neighboring group effects in the side chain losses from protonated serine and its derivatives. Journal of the American Society for Mass Spectrometry, 2000, 11, 1047-1060.	1.2	91
445	Derivatization of protonated peptides via gas phase ionâ€"molecule reactions with acetone. Journal of the American Society for Mass Spectrometry, 2000, 11, 244-256.	1.2	23
446	Silylcyanides and silylisocyanides: a comparative theoretical study. Chemical Physics, 2000, 254, 187-202.	0.9	8
447	Infrared spectra of monomeric l-alanine and l-alanine-N-d3 zwitterions isolated in a KBr matrix. Chemical Physics, 2000, 255, 195-204.	0.9	26
448	Gas-phase measurement of Î"H0 between axial and equatorial conformations of 3-methylcyclopentanone. Chemical Physics, 2000, 256, 251-258.	0.9	24
449	Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide. Chemical Physics, 2000, 256, 169-176.	0.9	39
450	About the vacuum UV photoabsorption spectrum of methyl fluoride (CH3F): the fine structure and its vibrational analysis. Chemical Physics, 2000, 257, 283-299.	0.9	37
451	Photodissociation dynamics of CH2BrCl at 234 nm. Chemical Physics, 2000, 260, 143-150.	0.9	46
452	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. Chemical Physics, 2000, 261, 189-203.	0.9	39
453	The inelastic incoherent neutron spectrum of crystalline oxamide: experiment and simulation of a solid. Chemical Physics, 2000, 261, 249-260.	0.9	9
454	Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonucleosides. Chemical Physics, 2000, 260, 317-325.	0.9	42
455	Protonation of archetypal aromatic and antiaromatic systems â€" G2 studies of benzene and cyclobutadiene. Chemical Physics, 2000, 253, 59-71.	0.9	26
456	The attractive quartet potential energy surface for the CH3C()+CO reaction. Chemical Physics, 2000, 252, 17-23.	0.9	2
457	Kinetics of the reactions of FC(O)O2 radicals with F atoms and F2. Chemical Physics, 2000, 253, 205-217.	0.9	14
458	The EVA spectral descriptor. European Journal of Medicinal Chemistry, 2000, 35, 367-375.	2.6	45
459	Gas-phase acidity and Câ€"H bond energy of diacetylene. Chemical Physics Letters, 2000, 318, 149-154.	1.2	22
460	Density functional studies of phenoxylâ€"Na+ ion complexes: implications for tyrosyl free radical interactions in vitro. Chemical Physics Letters, 2000, 325, 69-72.	1.2	12

#	Article	IF	Citations
461	Ab initio study of the alkaline hydrolysis of a thio-Î²-lactam structure. Chemical Physics Letters, 2000, 326, 304-310.	1.2	10
462	An isomeric study of N5+, N5, and N5â^': a Gaussian-3 investigation. Chemical Physics Letters, 2000, 329, 483-489.	1.2	54
463	AB initio study of naphthalene formation by addition of vinylacetylene to phenyl. Proceedings of the Combustion Institute, 2000, 28, 2563-2568.	2.4	35
464	The electronic and vibrational structures of ironâ€"oxo porphyrin with a methoxide or cysteinate axial ligand. Journal of Inorganic Biochemistry, 2000, 82, 141-152.	1.5	28
465	Infrared and Raman spectra of 4-(dimethylamino)benzonitrile and isotopomers in the ground state and vibrational analysis. Chemical Physics, 2000, 260, 193-214.	0.9	52
466	Intramolecular hydrogen-bonding in 2-nitroresorcinol. A combined FT-IR, FT-Raman and computational study. Chemical Physics, 2000, 253, 193-204.	0.9	39
467	Geometrical structures, energies and vibrational frequencies of phenylthiyl, p -aminophenylthiyl and their disulfides by using quantum chemical calculations. Computational and Theoretical Chemistry, 2000, 531, 51-64.	1.5	2
468	The cyclooctatetraenoquinones, a computational study. Computational and Theoretical Chemistry, 2000, 531, 181-192.	1.5	6
469	A theoretical study of the hydrates of (H 2 SO 4) 2 and its implications for the formation of new atmospheric particles. Computational and Theoretical Chemistry, 2000, 497, 19-37.	1.5	56
470	A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. Computational and Theoretical Chemistry, 2000, 497, 105-113.	1.5	9
471	Density functional vibrational analysis of N -methylthiourea and three deuterated analogues. Computational and Theoretical Chemistry, 2000, 499, 175-183.	1.5	3
472	An ab initio study of the interaction of alkali metals with the HCN/HNC system. Computational and Theoretical Chemistry, 2000, 505, 133-148.	1.5	2
473	Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. Computational and Theoretical Chemistry, 2000, 505, 109-116.	1.5	4
474	Vibrational spectroscopic study of pyrrole and its deuterated derivatives: comparison of the quality of the applicability of the DFT/Becke3P86 and the DFT/Becke3LYP functionals. Computational and Theoretical Chemistry, 2000, 507, 75-87.	1.5	28
475	Ab initio and density functional calculations of mean-square amplitudes of vibration for benzene and cubane. Computational and Theoretical Chemistry, 2000, 507, 111-118.	1.5	4
476	Pyramidane 2. Further computational studies: potential energy surface, basicity and acidity, electron-withdrawing and electron-donating power, ionization energy and electron affinity, heat of formation and strain energy, and NMR chemical shifts. Computational and Theoretical Chemistry, 2000, 507, 165-184.	1.5	31
477	Dimers, trimers and oligomers of sulfur oxides: an ab initio and density functional study. Computational and Theoretical Chemistry, 2000, 530, 265-279.	1.5	13
478	Evaluation of the accuracy of PM3, AM1 and MNDO/d as applied to zinc compounds. Computational and Theoretical Chemistry, 2000, 505, 289-301.	1.5	39

#	Article	IF	Citations
479	Title is missing!. Journal of Solution Chemistry, 2000, 29, 1047-1060.	0.6	126
480	Title is missing!. International Journal of Thermophysics, 2000, 21, 1439-1461.	1.0	6
481	On the Relative Importance of Oâ€“H/Ï€ Interactions in 7-Norbornenols. Structural Chemistry, 2000, 11, 241-244.	1.0	5
482	Density functional theory predictions for small radicals containing boron and aluminium: broken symmetry problems and solutions. Molecular Physics, 2000, 98, 961-966.	0.8	6
483	Toward an Understanding of the Mechanisms of the Intramolecular [5 + 2] Cycloaddition Reaction of Î³-Pyrones Bearing Tethered Alkenes. A Theoretical Study. Journal of Organic Chemistry, 2000, 65, 5480-5486.	1.7	22
484	Mechanisms of reactions between > Si=O groups and CO2, N2O, and HCâ‰¡CH molecules: An experimental and quantum chemical study. Kinetics and Catalysis, 2000, 41, 415-428.	0.3	1
485	Theoretical Study of the Heats of Formation of SF, FSO, FSO2 and HSO Radicals. Zeitschrift Fur Physikalische Chemie, 2000, 214, .	1.4	9
486	Theoretical characterization of the structures and properties of phenol-(H[sub 2]O)[sub 2] complexes. Journal of Chemical Physics, 2000, 113, 5253.	1.2	13
487	Nonequilibrium formulation of infrared frequencies and intensities in solution: Analytical evaluation within the polarizable continuum model. Journal of Chemical Physics, 2000, 113, 11270-11279.	1.2	69
488	Evidence for [sup 1]L[sub a] fluorescence from jet-cooled 3-methylindole-polar solvent complexes. Journal of Chemical Physics, 2000, 113, 5235.	1.2	40
489	Analysis of the intramolecular charge transfer in donorâ€“acceptor Î±,Î±â€²-substituted oligothiophenes from their vibrational spectra. Journal of Chemical Physics, 2000, 112, 5105-5112.	1.2	36
490	Thermochemistry of gas phase CF2 reactions: A density functional theory study. Journal of Chemical Physics, 2000, 113, 4103-4108.	1.2	30
491	Isomeric structures and energies of Hn+ clusters (n=13, 15, and 17). Journal of Chemical Physics, 2000, 113, 4230-4237.	1.2	44
492	Modeling proton mobility in acidic zeolite clusters. I. Convergence of transition state parameters from quantum chemistry. Journal of Chemical Physics, 2000, 112, 6779-6786.	1.2	33
493	Refinements on solvation continuum models: Hydrogen-bond effects on the OH stretch in liquid water and methanol. Journal of Chemical Physics, 2000, 112, 5382-5392.	1.2	44
494	Chemical Reactions in Ionic Molecular Aggregates. An ab initio and R2PI-Study of the Halogenbenzene/Ammonia System. Zeitschrift Fur Physikalische Chemie, 2000, 214, .	1.4	1
495	Calculation of aqueous proton dissociation constants of quinoline and hydroxyquinolines: A comparison of solvation models. Physical Chemistry Chemical Physics, 2000, 2, 5383-5388.	1.3	11
496	Towards nanostructured arrays of single molecule magnets: new Fe19 oxyhydroxide clusters displaying high ground state spins and hysteresisâ€Šâ€. Dalton Transactions RSC, 2000, , 1835-1840.	2.3	200

#	Article	IF	Citations
497	Radiative Association Reactions of Na+, Mg+, and Al+ with Abundant Interstellar Molecules. Variational Transition State Theory Calculations. Journal of Physical Chemistry A, 2000, 104, 4480-4488.	1.1	52
498	Excited-State Amineâ^'Imine Double Proton Transfer in 7-Azaindoline. Journal of Physical Chemistry B, 2000, 104, 7818-7829.	1.2	159
499	Benzooxirene, naphthooxirenes, and anthraceneoxirenes: the stabilization of the oxirene system by bond fixation in acenes. A comparison of ab initio and DFT in the investigation of annelated oxirenes. Canadian Journal of Chemistry, 2000, 78, 297-306.	0.6	21
500	Conformation and Proton Configuration of Pyrimidine Deoxynucleoside Oxidation Damage Products in Water. Chemical Research in Toxicology, 2000, 13, 462-470.	1.7	66
501	Oxygen and hydrogen isotope fractionation by hydration complexes of Li+, Na+, K+, Mg2+, Fâ^', Clâ^', and Brâ^': a theoretical study. Geochimica Et Cosmochimica Acta, 2000, 64, 3007-3033.	1.6	42
502	Experimental and simulation study of salt effects and pressure/density effects on oxygen and hydrogen stable isotope liquid-vapor fractionation for 4â€“5 molal aqueous NaCl and KCl solutions to 400Â°C. Geochimica Et Cosmochimica Acta, 2000, 64, 1773-1784.	1.6	90
503	Theoretical investigation on the conformational preferences of sulfinimines. Perkin Transactions II RSC, 2000, , 43-50.	1.1	58
504	Isotope Effects and the Mechanism of Chlorotrimethylsilane-Mediated Addition of Cuprates to Enones. Journal of the American Chemical Society, 2000, 122, 3288-3295.	6.6	73
505	Formation of Anti-Bredt Olefins from Bridgehead Carbene Precursors:Â A Computational Study. Journal of the American Chemical Society, 2000, 122, 5861-5865.	6.6	13
506	Seâ€“N interactions in selenohydroxylamine: a theoretical study. Perkin Transactions II RSC, 2000, , 2469-2474.	1.1	11
507	Experimental and Theoretical Analysis of the Vibrational Spectra and Theoretical Study of the Structures of 3,6-Dichloropyridazine and 3,4,5-Trichloropyridazine. Journal of Physical Chemistry A, 2000, 104, 2599-2612.	1.1	13
508	IR and Raman assignments for zinc phthalocyanine from DFT calculations. Physical Chemistry Chemical Physics, 2000, 2, 3949-3955.	1.3	129
509	Photochemical Reactions of Oxygen Atoms with Toluene, m-Xylene, p-Xylene, and Mesitylene:â€‰ An Infrared Matrix Isolation Investigation. Journal of Physical Chemistry A, 2000, 104, 4108-4114.	1.1	9
510	Reactions of Laser-Ablated Fe, Co, and Ni with NO:â€‰ Infrared Spectra and Density Functional Calculations of MNO+ and M(NO)x (M = Fe, Co, x = 1â^'3; M = Ni, x = 1, 2), and M(NO)x- (M = Co, Ni; x = 1, 2). Journal of Physical Chemistry A, 2000, 104, 3915-3925.	1.1	50
511	Ab initio study of (NH3)2: Accurate structure and energetics. Journal of Chemical Physics, 2000, 112, 230-237.	1.2	64
512	Anharmonic Vibrational Spectroscopy of Hydrogen-Bonded Systems Directly Computed from ab Initio Potential Surfaces:Â (H2O)n,n= 2, 3; Cl-(H2O)n,n= 1, 2; H+(H2O)n,n= 1, 2; H2Oâ^'CH3OH. Journal of Physical Chemistry A, 2000, 104, 2772-2779.	1.1	174
513	Nucleophile-Induced Intramolecular Dipole 1,5-Transfer and 1,6-Cyclization:Â Experimental and ab Initio Studies of Formation, Thermolysis, and Molecular and Electronic Structures of 3,6-Diphenyl-1-propanesulfenimido-1,2,4,5-tetrazine. Journal of the American Chemical Society, 2000, 122, 2087-2095.	6.6	11
514	A DFT Study on the Câ^'H Bond Dissociation Enthalpies of Haloalkanes:Â Correlation between the Bond Dissociation Enthalpies and Activation Energies for Hydrogen Abstraction. Journal of Physical Chemistry A, 2000, 104, 9244-9249.	1.1	74

#	Article	IF	Citations
515	A direct-dynamics study of the zwitterion-to-neutral interconversion of glycine in aqueous solution. Journal of Chemical Physics, 2000, 113, 9714-9721.	1.2	94
516	Theoretical characterization of the excited-state structures and properties of phenol and its one-water complex. Journal of Chemical Physics, 2000, 112, 1204-1211.	1.2	54
517	Is SH4, the simplest 10-S-4 sulfurane, observable?. Physical Chemistry Chemical Physics, 2000, 2, 2239-2244.	1.3	7
518	Effect of heat treatment on boron impurity in Vycor. Part I. Near infrared spectra and ab initio calculations of the vibrations of model molecules for surface boranols. Physical Chemistry Chemical Physics, 2000, 2, 1747-1755.	1.3	7
519	Theoretical studies of unimolecular reactions of C2â€“C5 alkoxy radicals. Part I. Ab initio molecular orbital calculations. Physical Chemistry Chemical Physics, 2000, 2, 1899-1905.	1.3	51
520	Computational Study of the Electronic Structure of Substituted Phenylcarbene in the Gas Phase. Journal of Organic Chemistry, 2000, 65, 8348-8356.	1.7	72
521	Theoretical Study on the Reaction Mechanism of Nickel Atoms with Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 11622-11627.	1.1	30
522	Photodissociation of HN3 at 248 nm and Longer Wavelength:â€‰ A CASSCF Study. Journal of Physical Chemistry A, 2000, 104, 4045-4050.	1.1	12
523	Theoretical study of the reaction of CH3C(Xìƒ 2Aâ€³, Ã£4A2) with N2. Physical Chemistry Chemical Physics, 2000, 2, 5560-5565.	1.3	1
524	Theoretical study of the solvent effect on the hydrogen abstraction reaction of the methyl radical with hydrogen peroxideâ€Šâ€. Perkin Transactions II RSC, 2000, , 977-981.	1.1	15
525	Near infrared and ab initio study of the vibrational modes of isolated silanol on silica. Physical Chemistry Chemical Physics, 2000, 2, 3217-3226.	1.3	51
526	Theoretical studies of unimolecular reactions of C2â€“C5 alkoxy radicals. Part II. RRKM dynamical calculations. Physical Chemistry Chemical Physics, 2000, 2, 1907-1918.	1.3	61
527	The loss of CO from the ortho, meta and para forms of deprotonated methyl benzoate in the gas phase. Perkin Transactions II RSC, 2000, , 1665-1673.	1.1	14
528	Ab initio study of the vibrational properties of acetic acid monomers and dimers. Physical Chemistry Chemical Physics, 2000, 2, 5020-5029.	1.3	68
529	The cyclization of N-butylpent-4-enylaminyl revisited: a combined theoretical and experimental studyâ€Šâ€. Perkin Transactions II RSC, 2000, , 425-431.	1.1	16
530	The Î² Câ€“C bond scission in alkoxy radicals: thermal unimolecular decomposition of t-butoxy radicals. Physical Chemistry Chemical Physics, 2000, 2, 1677-1683.	1.3	82
531	Addition complex formation vs. direct abstraction in the OH+C2H4 reaction. Physical Chemistry Chemical Physics, 2000, 2, 3591-3596.	1.3	46
532	Enthalpy of formation of selected carbonyl radicals from theory and comparison with experiment. Physical Chemistry Chemical Physics, 2000, 2, 5430-5436.	1.3	22

#	Article	IF	Citations
533	Homolysis of allyloxy(hydroxy)carbene. A density functional theory and ab initio study. Perkin Transactions II RSC, 2000, , 1980-1983.	1.1	12
534	Potential Energy Surface of SCl3-. Journal of Physical Chemistry A, 2000, 104, 2958-2961.	1.1	23
535	Unimolecular Reactions of Proton-Bound Cluster Ions:â€‰ Competition between Dissociation and Isomerization in the Ethanolâ^'Acetonitrile Dimer. Journal of Physical Chemistry A, 2000, 104, 8505-8511.	1.1	15
536	Molecular Complexes between Sodium and Carbonyl Compounds:Â Photoionization and ab Initio Molecular Orbital Studies. Journal of Physical Chemistry A, 2000, 104, 10825-10833.	1.1	6
537	Evidence of Dynamical Jahnâ^'Teller Effect on Triphenylene Radical Cation:Â Resonance Raman Spectrum and ab Initio Quantum-Chemical Calculations. Journal of Physical Chemistry A, 2000, 104, 9121-9129.	1.1	19
538	A Combined Spectroscopic and Theoretical Study of a Series of Aminomethyl End-Capped Oligothiophenes with Potential Applications in Thin Film Devices. Journal of Physical Chemistry A, 2000, 104, 735-740.	1.1	24
539	Ab Initio Calculations on Reactions of CHF3with Its Fragments. Journal of Physical Chemistry A, 2000, 104, 2729-2733.	1.1	11
540	Spectroscopic Studies of 12-Oxo-5(12H)-naphthacenylidene and 7H-Benz[de]anthracen-7-ylidene in Shpolskii Matrixes at 5 K. Journal of Physical Chemistry A, 2000, 104, 3391-3397.	1.1	8
541	A Computational Review of an Experimental Hint at Unusual Hydrogen Bonding in o-Cresol Cation Radical. Journal of Physical Chemistry A, 2000, 104, 5298-5301.	1.1	14
542	The Low-Lying Excited States of Pyridine. Journal of Physical Chemistry A, 2000, 104, 8389-8408.	1.1	125
543	An Ab Initio and Density Functional Theory Investigation of the Structures and Energetics of Halide Ionâ^'Alcohol Complexes in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 7871-7880.	1.1	16
544	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. Journal of Physical Chemistry A, 2000, 104, 5351-5357.	1.1	62
545	Unimolecular Reactions of Protonated Hydrogen Peroxide:â€‰ A Quantum Chemical Survey. Journal of Physical Chemistry A, 2000, 104, 8382-8388.	1.1	24
546	Theoretical Study of the Tautomeric/Conformational Equilibrium of Aspartic Acid Zwitterions in Aqueous Solution. Journal of Physical Chemistry A, 2000, 104, 6834-6843.	1.1	38
547	Theoretical Study of the Formation of Acetone in the OH-Initiated Atmospheric Oxidation of Î±-Pinene. Journal of Physical Chemistry A, 2000, 104, 11140-11146.	1.1	54
548	Computational Study of the Unimolecular Decomposition Pathways of Phenylperoxy Radical. Journal of Physical Chemistry A, 2000, 104, 3004-3011.	1.1	62
549	Matrix-Isolation and Mass-Spectrometric Studies of the Thermolysis of [Me2N(CH2)3]GaMe2. Characterization of the Monomeric Organogallanes Me2GaH, MeGaH2, and MeGaâ€. Journal of Physical Chemistry A, 2000, 104, 3627-3634.	1.1	14
550	Organic Thermochemistry at High ab Initio Levels. 3. A G3 Study of Cyclic Saturated and Unsaturated Hydrocarbons (Including Aromatics). Journal of Organic Chemistry, 2000, 65, 4298-4302.	1.7	82

#	Article	IF	Citations
551	Ab Initio Study of Peroxyacetic Nitric Anhydride and Peroxyacetyl Radical:Â Characteristic Infrared Band of Peroxyacetyl Radical. Journal of Physical Chemistry A, 2000, 104, 2613-2617.	1.1	9
552	Ring Expansion in Methylene Pyrrole Radicals. Quantum Chemical Calculations. Journal of Physical Chemistry A, 2000, 104, 530-538.	1.1	13
553	Oâˆ'O Bond Dissociation Enthalpy in Di(trifluoromethyl) Peroxide (CF3OOCF3) as Determined by Very Low Pressure Pyrolysis. Density Functional Theory Computations on Oâˆ'O and Oâˆ'H Bonds in (Fluorinated) Derivatives. Journal of Physical Chemistry A, 2000, 104, 10713-10720.	1.1	57
554	Ab Initio and Density Functional Study of the Activation Barrier for Ethane Cracking in Cluster Models of Zeolite H-ZSM-5. Journal of Physical Chemistry B, 2000, 104, 1944-1949.	1.2	106
555	Time-Resolved Resonance Raman and Density Functional Study of the Radical Cation of Chlorpromazine. Journal of Physical Chemistry A, 2000, 104, 4140-4148.	1.1	23
556	Rearrangement Pathways of Arylperoxy Radicals. I. The Azabenzenes. Journal of Physical Chemistry A, 2000, 104, 6088-6094.	1.1	11
557	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. 2. Studies of Xâˆ'X and Xâˆ'Y (X, Y = C, N, O, S, Halogen) Bondsâ€. Journal of Physical Chemistry A, 2000, 104, 1938-1943.	1.1	64
558	Ground State of 1,6-Bridged [10] Annulenes:â€‰ Infrared and Raman Spectra and Density Functional Calculations. Journal of Physical Chemistry A, 2000, 104, 3110-3116.	1.1	24
559	Matrix Infrared Spectra and Density Functional Calculations for GaNO, InNO, and TlNO. Journal of Physical Chemistry A, 2000, 104, 8475-8479.	1.1	15
560	Carbonâˆ'Oxygen Bond Dissociation Enthalpies in Peroxyl Radicals. Journal of Physical Chemistry A, 2000, 104, 915-921.	1.1	33
561	The Atmospheric Chemistry of the Acetonoxy Radical. Journal of Physical Chemistry A, 2000, 104, 11578-11588.	1.1	75
562	Will an Î·3-Si3H3Ligand Form Sandwich Compounds with Main Group Elements?. Journal of the American Chemical Society, 2000, 122, 1725-1728.	6.6	26
563	Kinetic Analysis for HO2Addition to Ethylene, Propene, and Isobutene, and Thermochemical Parameters of Alkyl Hydroperoxides and Hydroperoxide Alkyl Radicals. Journal of Physical Chemistry A, 2000, 104, 4997-5012.	1.1	62
564	Molecular Orbital Studies of Titanium Nitride Chemical Vapor Deposition:Â Gas Phase Complex Formation, Ligand Exchange, and Elimination Reactions. Chemistry of Materials, 2000, 12, 2466-2474.	3.2	24
565	Theoretical Studies of the Radiation Products of Hydroxyproline. Journal of Physical Chemistry A, 2000, 104, 8583-8592.	1.1	20
566	Combined Theoretical and Vibrational Study of Dihexylbithienoquinonoid Derivatives with Regioregular Head-to-Head, Head-to-Tail, and Tail-to-Tail Orientations. Journal of Physical Chemistry A, 2000, 104, 661-672.	1.1	30
567	Theoretical Investigation of the Neutral/Zwitterionic Equilibrium of Î³-Aminobutyric Acid (GABA) Conformers in Aqueous Solution. Journal of Physical Chemistry A, 2000, 104, 6844-6854.	1.1	41
568	Equilibrium Isotope Effects in Cationic Transition-Metal(I) Ethene Complexes M(C2X4)+with M = Cu, Ag, Au and X = H, D. Organometallics, 2000, 19, 2608-2615.	1.1	58

#	Article	IF	Citations
569	Conformational Study of 3-Methyltetrahydropyran by (2+1) Resonance-Enhanced Multiphoton Ionization Spectroscopy. Journal of Physical Chemistry A, 2000, 104, 509-513.	1.1	6
570	Vibrational Analysis of a Chemisorbed Polyatomic Molecule:Â Methoxy on Cu(100). Journal of Physical Chemistry B, 2000, 104, 2448-2459.	1.2	40
571	Computational and Experimental Infrared Spectra of 1,4-Dinitropiperazine and Vibrational Mode Assignment. Journal of Physical Chemistry A, 2000, 104, 8898-8907.	1.1	2
572	Structures, Rotational Barriers, and Thermodynamic Properties of C2Vinyl and Chlorovinyl Alcohols and Additivity Groups. Journal of Physical Chemistry A, 2000, 104, 9197-9206.	1.1	20
573	Theoretical Study of the Alkaline Hydrolysis of a Bicyclic Aza-Î²-lactam. Journal of Physical Chemistry B, 2000, 104, 11389-11394.	1.2	21
574	Matrix Infrared Spectroscopic Study of Magnesium Carbene and Carbenoid Radicals and Analysis of Their Bonding with Density Functional Calculations. Inorganic Chemistry, 2000, 39, 1204-1215.	1.9	24
575	A Density Functional Theory Study of the Radiation Products of Glycine. Journal of Physical Chemistry A, 2000, 104, 5080-5086.	1.1	36
576	Mechanism of Peroxynitrite Oxidation of Aliphatic CH Bonds in Saturated and Unsaturated Hydrocarbons. A Theoretical Model for the CH Oxidation of Lipids. Journal of the American Chemical Society, 2000, 122, 1191-1199.	6.6	26
577	Unimolecular Reaction Dynamics from Kinetic Energy Release Distributions. 7. Average Translational Energy Release. Journal of Physical Chemistry A, 2000, 104, 5422-5429.	1.1	9
578	C6F6 and sym-C6F3H3:â€‰ Ab Initio and DFT Studies of Structure, Vibrations, and Inelastic Neutron Scattering Spectra. Journal of Physical Chemistry A, 2000, 104, 982-989.	1.1	25
579	(N,N-Dimethylaminoxy)trifluorosilane:Â Strong, Dipole Moment Driven Changes in the Molecular Geometry Studied by Experiment and Theory in Solid, Gas, and Solution Phases. Journal of the American Chemical Society, 2000, 122, 4471-4482.	6.6	83
580	Theoretical Studies of the Reactivity of Cyclopentadienyl Nitrosyl Alkyl Species of Molybdenum and Tungsten. Organometallics, 2000, 19, 2858-2867.	1.1	17
581	Structures, Rotation Barrier, and Thermodynamic Properties Î”HfÂ°298, SÂ°298, and Cp(T) of Chloromethyl Hypochlorites CH3OCl, CH2ClOCl, CHCl2OCl, and CCl3OCl. Journal of Physical Chemistry A, 2000, 104, 9581-9590.	1.1	23
582	Kinetics of Hydrogen Abstraction from Chloromethanes by the Hydroxyl Radical:â€‰ A Computational Study. Journal of Physical Chemistry A, 2000, 104, 8535-8539.	1.1	30
583	Ab Initio Study of Radical Addition Reactions: Addition of a Primary Ethylbenzene Radical to Ethene (I). Journal of Physical Chemistry A, 2000, 104, 10939-10950.	1.1	139
584	Conformational Distribution of Gas-phase Glycerol. Journal of Physical Chemistry A, 2000, 104, 11220-11222.	1.1	32
585	Condensation Reactions between 1,3-Butadiene Radical Cation and Acetylene in the Gas Phase. Journal of Physical Chemistry A, 2000, 104, 5778-5786.	1.1	34
586	Cheletropic Decomposition of Cyclic Nitrosoamines Revisited:â€‰ The Nature of the Transition States and a Critical Role of the Ring Strain. Journal of Organic Chemistry, 2000, 65, 3612-3619.	1.7	4

#	Article	IF	Citations
587	Mechanistic Aspects of Stannole Formation Catalyzed by the Phosphine-Coordinated Transition-Metal Complexes M(PR3)2:Â An ab Initio MO Study. Organometallics, 2000, 19, 5661-5670.	1.1	15
588	Thermochemical Property, Pathway and Kinetic Analysis on the Reactions of Allylic Isobutenyl Radical with O2:â€‰ an Elementary Reaction Mechanism for Isobutene Oxidation. Journal of Physical Chemistry A, 2000, 104, 9715-9732.	1.1	58
589	Temperature Dependence of Cluster Ion Decomposition in a Quadrupole Ion Trapâ€. Journal of Physical Chemistry A, 2000, 104, 10280-10287.	1.1	24
590	Gas-Phase Nuclear Magnetic Resonance Study of Berry Pseudorotation of SF4. Comparison of Experimental and Calculated Kinetic Parameters and Falloff Kinetics. Journal of Physical Chemistry A, 2000, 104, 3341-3348.	1.1	16
591	Conformers of n-Si6Me14:â€‰ Ab Initio, Molecular Mechanics, and Additive Increment Methods. Journal of Physical Chemistry A, 2000, 104, 3367-3380.	1.1	27
592	Calculated Vibrational Spectra for CHnOHmSpecies. Journal of Physical Chemistry A, 2000, 104, 34-44.	1.1	14
593	Nuclear Dynamics Discrete Variable Representation Study of the Equilibrium Isotope Effect on H2Binding in M(Î·2-H2)LnComplexes:Â An Effective Theoretical Way To Account for Anharmonicity. Journal of Physical Chemistry A, 2000, 104, 7898-7905.	1.1	19
594	Mechanism of the Reaction of CH3SO with NO2 in Relation to Atmospheric Oxidation of Dimethyl Sulfide:â€‰ Experimental and Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 935-946.	1.1	41
595	Theoretical Study on the Reaction Mechanism of CO2with Mg. Journal of Physical Chemistry A, 2000, 104, 7646-7650.	1.1	22
596	Solvation of Li+ by Acetone, THF, and Diethyl Ether in the Gas Phase and the Ionâ^'Molecule Association Mechanism. Journal of Physical Chemistry A, 2000, 104, 2230-2237.	1.1	36
597	Surface-Enhanced Raman Spectra of Phthalimide. Interpretation of the SERS Spectra of the Surface Complex Formed on Silver Islands and Colloids. Journal of Physical Chemistry A, 2000, 104, 9500-9505.	1.1	83
598	REFLECTIONABSORPTIONINFRAREDSPECTROSCOPY AND THESTRUCTURE OFMOLECULARADSORBATES ONMETALSURFACES. Annual Review of Physical Chemistry, 2000, 51, 381-403.	4.8	76
599	An ab Initio Post-Hartreeâ^'Fock Comparative Study of 5-Azacytosine and Cytosine and Their Dimers with Guanine. Journal of Physical Chemistry A, 2000, 104, 9964-9970.	1.1	34
600	Modification of Regioselectivity in Cycloadditions to C70under Microwave Irradiation. Journal of Organic Chemistry, 2000, 65, 2499-2507.	1.7	84
601	Ab Initio Calculations of Absolute pKa Values in Aqueous Solution II. Aliphatic Alcohols, Thiols, and Halogenated Carboxylic Acids. Journal of Physical Chemistry A, 2000, 104, 2402-2409.	1.1	152
602	Assessment of Gaussian-3 and density functional theories for a larger experimental test set. Journal of Chemical Physics, 2000, 112, 7374-7383.	1.2	711
603	Hydrogen Atom Adducts to Nitrobenzene:Â Formation of the Phenylnitronic Radical in the Gas Phase and Energetics of Wheland Intermediates. Journal of the American Chemical Society, 2000, 122, 9511-9524.	6.6	62
604	Can Hydrocarbon Chains Be Disrupted by Fast O(3P) Atoms?. Journal of Physical Chemistry A, 2000, 104, 9976-9982.	1.1	28

#	Article	IF	Citations
605	Influence of Compression upon Kinetic Isotope Effects for SN2 Methyl Transfer:Â A Computational Reappraisal. Journal of the American Chemical Society, 2000, 122, 10895-10902.	6.6	29
606	Reaction Rate Prediction via Group Additivity Part 1:â€‰ H Abstraction from Alkanes by H and CH3. Journal of Physical Chemistry A, 2001, 105, 6910-6925.	1.1	136
607	Computational Analysis of the Potential Energy Surfaces of Glycerol in the Gas and Aqueous Phases:Â Effects of Level of Theory, Basis Set, and Solvation on Strongly Intramolecularly Hydrogen-Bonded Systems. Journal of the American Chemical Society, 2001, 123, 11743-11754.	6.6	133
608	Carborane-Containing Liquid Crystals:Â Synthesis and Structural, Conformational, Thermal, and Spectroscopic Characterization of Diheptyl and Diheptynyl Derivatives ofp-Carboranesâ€. Inorganic Chemistry, 2001, 40, 6622-6631.	1.9	62
609	Theoretical Study of [2 + 1] Cycloaddition of CO and CS to Acetylenes Forming Cyclopropenones and Cyclopropenethiones. Journal of Organic Chemistry, 2001, 66, 4316-4326.	1.7	33
610	A Theoretical Study of the Molecular Mechanism of the Reaction betweenN,N-Dimethylmethyleneammonium Cation and Cyclopentadiene. Journal of Organic Chemistry, 2001, 66, 3211-3214.	1.7	51
611	Ab Initio Calculation of Amide Carbonyl Stretch Vibrational Frequencies in Solution with Modified Basis Sets. 1. N-Methyl Acetamide. Journal of Physical Chemistry A, 2001, 105, 10922-10928.	1.1	184
612	(V2O5)n Gas-Phase Clusters (n = 1â˜’12) Compared to V2O5 Crystal:â€‰ DFT Calculations. Journal of Physical Chemistry A, 2001, 105, 8588-8598.	1.1	135
613	CF2XCF2X and CF2XCF2â€¢ Radicals (X = Cl, Br, I):â€‰ Ab Initio and DFT Studies and Comparison with Experiments. Journal of Physical Chemistry A, 2001, 105, 3623-3632.	1.1	40
614	Stereochemistry of Radical Halogenation Reactions. An ab Initio Molecular Orbital Study. Journal of Physical Chemistry A, 2001, 105, 10890-10898.	1.1	10
615	Classical and Quantum-Mechanical Studies of Crystalline FOX-7 (1,1-Diamino-2,2-dinitroethylene). Journal of Physical Chemistry A, 2001, 105, 5010-5021.	1.1	121
616	Basicity of Some Organic Superbases in Acetonitrile. Organic Letters, 2001, 3, 1523-1526.	2.4	175
617	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties:Â Ethanol, Î±-Monoethanols, Dichloroethanols, and Corresponding Radicals Derived from H Atom Loss. Journal of Physical Chemistry A, 2001, 105, 9543-9552.	1.1	23
618	An ab Initio Study of the Structure and Properties of Aluminum Hydroxide:Â Gibbsite and Bayerite. Journal of Physical Chemistry B, 2001, 105, 10236-10242.	1.2	86
619	Nucleophilic Substitution at the Imidoyl Carbon Atom: Intermediate Mechanistic and Reactivity Behavior between Carbonyl and Vinyl Carbon Substitution. Journal of the American Chemical Society, 2001, 123, 2326-2333.	6.6	24
620	On the Choice of Optimal Methodology for Calculation of 13C and 1H NMR Isotropic Chemical Shifts in Cagelike Systems. Case Studies of Adamantane, 2-Adamantanone, and 2,4-Methano-2,4-dehydroadamantane. Journal of Chemical Information and Computer Sciences, 2001, 41, 1478-1487.	2.8	19
621	The Ozonolysis of AcetyleneA Quantum Chemical Investigation. Journal of the American Chemical Society, 2001, 123, 6127-6141.	6.6	51
622	An Experimental and Computational Study of 1,2-Hydrogen Migrations in 2-Hydroxycyclopentylidene and Its Conjugate Base. Journal of Organic Chemistry, 2001, 66, 1600-1606.	1.7	18

#	Article	IF	Citations
623	Spectroscopic and Theoretical Investigations of Vibrational Frequencies in Binary Unsaturated Transition-Metal Carbonyl Cations, Neutrals, and Anions. Chemical Reviews, 2001, 101, 1931-1962.	23.0	427
624	Kinetics of hydrogen abstraction reactions of CF3CHO, CF2ClCHO, CFCl2CHO and CCl3CHO with OH Radicals: An ab initio study. Physical Chemistry Chemical Physics, 2001, 3, 3961-3966.	1.3	10
625	Calculation of Optical Rotation Using Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 5356-5371.	1.1	351
626	The insertion reaction of germylene into the Siâ€“H bond of silane: absolute rate constants, temperature dependence, RRKM modelling, and quantum chemical (ab initio and DFT) calculations. Physical Chemistry Chemical Physics, 2001, 3, 184-192.	1.3	39
627	Variational Transition State Calculations of the CH2F2 + OH Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2001, 105, 10553-10561.	1.1	21
628	Gaussian-3X (G3X) theory: Use of improved geometries, zero-point energies, and Hartreeâ€“Fock basis sets. Journal of Chemical Physics, 2001, 114, 108.	1.2	477
629	A Mechanistic Study of the Reactions of H, O (3P), and OH with Monocyclic Aromatic Hydrocarbons by Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 140-152.	1.1	66
630	(15N5)-Labeled Adenine Derivatives:Â Synthesis and Studies of Tautomerism by15N NMR Spectroscopy and Theoretical Calculations. Journal of Organic Chemistry, 2001, 66, 5463-5481.	1.7	119
631	Bond Dissociation Energies and Radical Stabilization Energies Associated with Substituted Methyl Radicals. Journal of Physical Chemistry A, 2001, 105, 6750-6756.	1.1	265
632	A Study of the Mechanism of the Reaction between Ozone and the Chlorine Atom Using Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 4065-4070.	1.1	18
633	Detailed Kinetic Study of the Growth of Small Polycyclic Aromatic Hydrocarbons. 1. 1-Naphthyl + Ethyneâ€. Journal of Physical Chemistry A, 2001, 105, 1561-1573.	1.1	97
634	Reaction Rate Prediction via Group Additivity, Part 2:Â H-Abstraction from Alkenes, Alkynes, Alcohols, Aldehydes, and Acids by H Atoms. Journal of Physical Chemistry A, 2001, 105, 8969-8984.	1.1	103
635	p-Phenylenecarbenonitrene and Its Halogen Derivatives: How Does Resonance Interaction between a Nitrene and a Carbene Center Affect the Overall Electronic Configuration?. Journal of the American Chemical Society, 2001, 123, 2628-2636.	6.6	30
636	Ab Initio Structures and Vibrational Spectra of Li[C(CF3SO2)3] and Li[CH(CF3SO2)2]. Journal of Physical Chemistry A, 2001, 105, 9258-9264.	1.1	9
637	Ab initio studies of dissociation pathways on the ground- and excited-state potential energy surfaces for formyl chloride (HClCO). Journal of Chemical Physics, 2001, 115, 10431.	1.2	13
638	The Theoretical Prediction of Molecular Radical Species:â€‰ a Systematic Study of Equilibrium Geometries and Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2001, 105, 9736-9747.	1.1	142
639	The Elusive Benzocyclobutenylidene:Â A Combined Computational and Experimental Attempt. Journal of the American Chemical Society, 2001, 123, 2870-2876.	6.6	24
640	The Vibrational Spectrum of Fullerene C60. Journal of Physical Chemistry A, 2001, 105, 11192-11196.	1.1	126

#	Article	IF	Citations
641	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in HypericinÂ¶. Photochemistry and Photobiology, 2001, 74, 157.	1.3	10
642	Nitrobenzene Isomers. Journal of Physical Chemistry A, 2001, 105, 995-1010.	1.1	20
643	Tertiary cyclohexyl cations. Definitive evidence for the existence of isomeric structures (hyperconjomers). Perkin Transactions II RSC, 2001, , 869-874.	1.1	38
644	A detailed experimental and theoretical study on the decomposition of methoxy radicals. Physical Chemistry Chemical Physics, 2001, 3, 2450-2458.	1.3	55
645	Amidolithium-mediated enolization: does proton transfer occur via a dimer intermediate with bridging carbonyls?. New Journal of Chemistry, 2001, 25, 262-267.	1.4	10
646	Theoretical studies on thiocarbonyl group transfer reactions. New Journal of Chemistry, 2001, 25, 859-863.	1.4	3
647	Theoretical study of cyanophosphapropyne (NCCP), isocyanophosphapropyne (CNCP) and their isomers: stability and properties. Physical Chemistry Chemical Physics, 2001, 3, 1588-1597.	1.3	5
648	Theoretical study of the thermal decomposition of several Î²-chloroalkoxy radicals. Physical Chemistry Chemical Physics, 2001, 3, 175-178.	1.3	13
649	Some recent aspects of unimolecular gas phase ion chemistry. Chemical Society Reviews, 2001, 30, 186-192.	18.7	36
650	The role of the ground and excited potential energy surfaces in the O(1Dâ€Šandâ€Š3P)+SiH4 reactions: A theoretical study. Journal of Chemical Physics, 2001, 114, 10816-10834.	1.2	13
651	The effects of the presence of an alkaline atomic cation in a molecular hydrogen environment. Journal of Chemical Physics, 2001, 114, 2213-2218.	1.2	57
652	Excited state photoelectron spectroscopy of anisoleDedicated to Professor F. DÃ¶rr on the occasion of his 80th birthday.. Physical Chemistry Chemical Physics, 2001, 3, 5358-5368.	1.3	28
653	Ab initio studies of the gas-phase thermodynamic properties and bond dissociation energies for haloethanes and halomethyl radicals. Physical Chemistry Chemical Physics, 2001, 3, 811-818.	1.3	20
654	Structure and infrared (IR) assignments for the OLED material: N,Nâ€²-diphenyl-N,Nâ€²-bis(1-naphthyl)-1,1â€²-biphenyl-4,4â€³-diamine (NPB). Physical Chemistry Chemical Physics, 2001, 3, 2131-2136.	1.3	60
655	Theoretical studies of the thermal and chemically activated decomposition of CF3CY2O (Y = F, H) radicals. Physical Chemistry Chemical Physics, 2001, 3, 2352-2364.	1.3	28
656	The retro-ene reaction of gaseous immonium ions revisitedElectronic supplementary information (ESI) available: Table s1 [G2(MP2) total energies of the involved species] and Table s2 [archive entries for MP2(full)/6-31G(d) optimised geometries]. See http://www.rsc.org/suppdata/p2/b1/b105386h. Perkin Transactions II RSC, 2001, , 2324-2328.	1.1	7
657	Central metal dependence of the NO+â€“NO- isomerism in pentacoordinate MX(CO)(NO)(PR3)2 complexes. New Journal of Chemistry, 2001, 25, 981-984.	1.4	1
658	Calculation of reaction rate constants for hydrogenâ€“deuterium exchange reactions of methane catalysed by acid zeolites. Chemical Communications, 2001, , 1108-1109.	2.2	10

#	Article	IF	Citations
659	A Theoretical Study of the Effect of a Tetraalkylammonium Counterion on the Hydrogen Bond Strength inZ-Hydrogen Maleate. Journal of the American Chemical Society, 2001, 123, 7134-7145.	6.6	35
660	Theoretical Analysis of Heteroaromatic Thioaminyl Radicals. Part 1:â€‰ A Comparison of Ab Initio and Density Functional Methods in Calculations of Molecular Geometry and Isotropic Hyperfine Coupling Constants. Journal of Physical Chemistry A, 2001, 105, 7615-7625.	1.1	35
661	Energetics of Uracil Cation Radical and Anion Radical Ionâ'Molecule Reactions in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 8740-8747.	1.1	18
662	Molecular Structure and Torsional Potential oftrans-Azobenzene. A Gas Electron Diffraction Study. Journal of Physical Chemistry A, 2001, 105, 9347-9353.	1.1	89
663	Theoretical study of cyclopropenones and cyclopropenethiones: decomposition via intermediates. Perkin Transactions II RSC, 2001, , 898-905.	1.1	19
664	Ground-state tautomerism and rotational isomerization in 4,5-dimethyl-2-(2-hydroxyphenyl)imidazole in the gas phase and in polar solvents: a theoretical study of the aromaticity, intramolecular hydrogen-bond strength and differential soluteâ€"solvent interactions. Physical Chemistry Chemical Physics, 2001, 3, 3569-3579.	1.3	24
665	Theoretical Investigation of Steric and Electronic Effects in Coenzyme B12Models. Organometallics, 2001, 20, 550-556.	1.1	58
666	The Photobleaching Sequence of a Short-Wavelength Visual Pigmentâ€. Biochemistry, 2001, 40, 7832-7844.	1.2	49
667	Cyclizations of 4-Pentenyl, 5-Hexenyl, 6-Heptenyl, and 7-Octenyl Fluorinated Radicals:Â A Density Functional Theory Theoretical Study. Journal of Organic Chemistry, 2001, 66, 6074-6082.	1.7	5
668	Double proton transfer in the complex of acetic acid with methanol: Theory versus experiment. Journal of Chemical Physics, 2001, 114, 1567-1574.	1.2	38
669	Conrotatory Photochemical Ring Opening of Alkylcyclobutenes in Solution. A Test of the Hot Ground-State Mechanism. Journal of the American Chemical Society, 2001, 123, 5188-5193.	6.6	9
670	Chromophore Protonation States and the Proton Shuttle Mechanism in Green Fluorescent Protein:Â Inferences Drawn from ab Initio Theoretical Studies of Chemical Structures and Vibrational Spectraâ€. Journal of Physical Chemistry B, 2001, 105, 2850-2857.	1.2	26
671	Addition vs Abstraction Reactions of the Methyl Radical with Nitrones, Alkenes, Aldehydes, and Imines. Journal of Physical Chemistry A, 2001, 105, 7096-7105.	1.1	23
672	Experimental Techniques in Gas-Phase Ion Thermochemistry. Chemical Reviews, 2001, 101, 391-444.	23.0	222
673	How Persistent Is Cyclopropyl upon Nucleophilic Substitution, and Is Frontside Displacement Possible? A Model Study. Journal of Organic Chemistry, 2001, 66, 7084-7089.	1.7	8
674	The Reaction of Protonated Dimethyl Ether with Dimethyl Ether:Â Temperature and Isotope Effects on the Methyl Cation Transfer Reaction Forming Trimethyloxonium Cation and Methanol. Journal of the American Chemical Society, 2001, 123, 3980-3985.	6.6	14
675	Conversion of CO to Formaldehyde Catalyzed by BeO:Â A Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 10433-10438.	1.1	7
676	Binding Energy in and Equilibrium Constant of Formation for the Dodecahedrane Compounds He@C20H20 and Ne@C20H20. Journal of Physical Chemistry A, 2001, 105, 1315-1319.	1.1	63

#	Article	IF	Citations
677	Isomerization of Indole. Quantum Chemical Calculations and Kinetic Modeling. Journal of Physical Chemistry A, 2001, 105, 3605-3614.	1.1	18
678	Is the H2OCl+Ion a Viable Intermediate for the Hydrolysis of ClONO2on Ice Surfaces?. Journal of Physical Chemistry A, 2001, 105, 3132-3139.	1.1	17
679	Resonance Raman Scattering by the Green Fluorescent Protein and an Analogue of Its ChromophoreâŠ¥. Journal of Physical Chemistry B, 2001, 105, 5316-5322.	1.2	82
680	Synthesis of Silicon-Based Infrared Semiconductors in the Geâ^'Sn System Using Molecular Chemistry Methods. Journal of the American Chemical Society, 2001, 123, 10980-10987.	6.6	25
681	A Gaussian-2 ab Initio Study of the [C2H5S]- Potential Energy Surface:â€‰ I. Structures and Energetics of [C2H5S]- Anions and Fragmentation Pathways of the Thioethoxide Anion. Journal of Physical Chemistry A, 2001, 105, 7651-7664.	1.1	4
682	Nitrous Oxide as a 1,3-Dipole:Â A Theoretical Study of Its Cycloaddition Mechanism. Journal of Organic Chemistry, 2001, 66, 6096-6103.	1.7	55
683	Ab Initio MO Study of the Structures of N2, NO, and CO Molecules Coordinated to the Pdn (n = 1, 2, 5,) Tj ETQq0 0 0 rgBT /Overlock 10	1.2	5
684	S0 and S1 States of Monochlorophenols:â€‰ Ab Initio CASSCF MO Study. Journal of Physical Chemistry A, 2001, 105, 9252-9257.	1.1	10
685	Probing Inhibitors Binding to Human Urokinase Crystals by Raman Microscopy:Â Implications for Compound Screeningâ€. Biochemistry, 2001, 40, 9751-9757.	1.2	22
686	Reactions in the Alâ^'Hâ^'Cl System Studied by ab Initio Molecular Orbital and Density Functional Methods. Journal of Physical Chemistry A, 2001, 105, 264-273.	1.1	20
687	Structure, Torsional Potentials, and Thermodynamic Properties Î"HÂ°f298, SÂ°298, andCp(T) of Chloro-Dimethyl Ethers:Â CH2ClOCH3, CHCl2OCH3, and CCl3OCH3. Density Functional and ab Initio Calculations. Journal of Physical Chemistry A, 2001, 105, 5420-5430.	1.1	8
688	A Fourier Transform Ion Cyclotron Resonance Study of theTemperature and Isotope Effects on the Kinetics of Low-Pressure Association Reactions of Protonated Dimethyl Ether with Dimethyl Ether. Journal of Physical Chemistry A, 2001, 105, 1011-1019.	1.1	10
689	Molecular Orbital Studies of Titanium Nitride Chemical Vapor Deposition:Â Imido Dimer Formation and Elimination Reactions. Chemistry of Materials, 2001, 13, 1095-1100.	3.2	5
690	Ab Initio Molecular Orbital Study of the Reaction of GeH2 with H2O and Decomposition Reactions of H3GeOH. Journal of Physical Chemistry A, 2001, 105, 4988-4991.	1.1	5
691	Synthesis, Decomposition, and Structural Studies in the Gas Phase and Solid State of N,N-Dimethylaminoxygermane. Inorganic Chemistry, 2001, 40, 661-666.	1.9	15
692	A Theoretical Investigation of the Triplet Carbon Atom C(3P) + Vinyl Radical C2H3(2Aâ€˜) Reaction and Thermochemistry of C3Hn(n= 1â^'4) Species. Journal of Physical Chemistry A, 2001, 105, 3284-3299.	1.1	55
693	Modeling the Action of an Antitumor Drug:Â A Density Functional Theory Study of the Mechanism of Tirapazamine. Journal of the American Chemical Society, 2001, 123, 7320-7325.	6.6	23
694	UV-Induced Photoisomerization of Acetylacetone and Identification of Less-Stable Isomers by Low-Temperature Matrix-Isolation Infrared Spectroscopy and Density Functional Theory Calculation. Journal of Physical Chemistry A, 2001, 105, 10832-10838.	1.1	61

#	Article	IF	Citations
695	Conformational Studies of Methyl 3-O-Methyl-Î±-d-arabinofuranoside:â€‰ An Approach for Studying the Conformation of Furanose Rings. Journal of the American Chemical Society, 2001, 123, 8811-8824.	6.6	36
696	First Principles Calculation of pKa Values for 5-Substituted Uracils. Journal of Physical Chemistry A, 2001, 105, 274-280.	1.1	185
697	Inelastic Neutron Scattering:Â A Tool in Molecular Vibrational Spectroscopy and a Test of ab Initio Methods. Journal of Physical Chemistry A, 2001, 105, 3949-3960.	1.1	70
698	Direct Dynamic Studies on Tropospheric Reactivity of Fluorinated Ethanes:â€‰ Scope and Limitations of the General Reaction Parameter Method. Journal of Physical Chemistry A, 2001, 105, 1968-1978.	1.1	11
699	Triplet Organometallic Reactivity under Ambient Conditions:Â An Ultrafast UV Pump/IR Probe Study. Journal of the American Chemical Society, 2001, 123, 2255-2264.	6.6	82
700	First ab Initio and Density Functional Study on the Structure, Bowl-to-Bowl Inversion Barrier, and Vibrational Spectra of the Elusive C3v-Symmetric Buckybowl:â€‰ Sumanene, C21H12. Journal of Physical Chemistry A, 2001, 105, 4488-4494.	1.1	81
701	Consecutive Photolyses of Naphthalenedicarboxylic Anhydrides in Low Temperature Matrixes:â€‰ Experimental and Computational Studies on Naphthynes and Benzocyclopentadienylideneketenes. Journal of Physical Chemistry A, 2001, 105, 7790-7798.	1.1	26
702	Ab Initio Study of Radical Reactions: Cyclization Pathways for the Butylbenzene Radical (II). Journal of Physical Chemistry A, 2001, 105, 7713-7723.	1.1	23
703	Revisiting the Hammond Postulate:Â The Role of Reactant and Product Ionic States in Regulating Barrier Heights, Locations, and Transition State Frequenciesâ€. Journal of Physical Chemistry A, 2001, 105, 1489-1497.	1.1	56
704	Theoretical Investigation on Stability of the CÂ·H2OCl Radical. Journal of Physical Chemistry A, 2001, 105, 3941-3946.	1.1	7
705	Crystal Structure of [PPN+][Cr(CO)4NO-]:Â Calculations and Comparisons of Cr(CO)4NO-with Mn(CO)5-. Organometallics, 2001, 20, 3613-3616.	1.1	7
706	Theoretical Studies of Mechanisms and Kinetic Isotope Effects on the Decarboxylation of Orotic Acid and Derivatives. Journal of the American Chemical Society, 2001, 123, 12067-12073.	6.6	34
707	Hydrogen Atom Adducts to the Amide Bond. Generation and Energetics of the Amino(hydroxy)methyl Radical in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 11144-11155.	1.1	47
708	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Radicals Derived from H Atom Loss in Mono-, Di-, and Trichloromethanol and Parent Chloromethanols. Journal of Physical Chemistry A, 2001, 105, 4504-4516.	1.1	43
709	On the Direction and Magnitude of Radical Substituent Effects:Â The Role of Polar Interaction on Thermodynamic Stabilities of Benzylic Câˆ’H Bonds and Related Carbon Radicals. Journal of Organic Chemistry, 2001, 66, 1466-1472.	1.7	40
710	Carbon-to-Carbon Identity Proton Transfer from Allene, Ketene, Ketenimine, and Thioketene to Their Respective Conjugate Anions in the Gas Phase. Anab InitioStudy. Journal of the American Chemical Society, 2001, 123, 7146-7153.	6.6	16
711	Hydroxyl Radical Adducts to Pyridine. The Generation and Properties of the Elusive N-Hydroxypyridyl Radical. Journal of Physical Chemistry A, 2001, 105, 9130-9141.	1.1	14
712	Protonation of an H2O Dimer by a Zeolitic BrÃ¸nsted Acid Site. Journal of Physical Chemistry B, 2001, 105, 3034-3038.	1.2	29

#	Article	IF	Citations
713	Unimolecular Reaction Dynamics from Kinetic Energy Release Distributions. 8. Protonated Fluorobenzene and Structure of the Phenyl Ion. Journal of Physical Chemistry A, 2001, 105, 3719-3724.	1.1	13
714	Chlorine Kinetic Isotope Effects on the Haloalkane Dehalogenase Reaction. Journal of the American Chemical Society, 2001, 123, 4550-4555.	6.6	49
715	Carbomethoxychlorocarbene:Â Spectroscopy, Theory, Chemistry and Kinetics. Journal of the American Chemical Society, 2001, 123, 6061-6068.	6.6	31
716	Synthesis, X-ray Structure, and Properties of 2-(1â€˜-Pyridin-2â€˜-one)Benzimidazole. Journal of Physical Chemistry B, 2001, 105, 12759-12770.	1.2	9
717	Internal Bond Rotation in Substituted Methyl Radicals, H2Bâ”CH2, H3Câ”CH2, H2Nâ”CH2, and HOâ”CH2:â€‰ Hardness Profiles. Journal of Physical Chemistry A, 2001, 105, 1343-1353.	1.1	20
718	Polarity of the Transition State Controls the Reactivity of Related Charged Phenyl Radicals Toward Atom and Group Donors. Journal of Organic Chemistry, 2001, 66, 2726-2733.	1.7	40
719	Unimolecular and Photoinduced Dissociations of Aromatic C8H10+â€¢Molecular Ions. Journal of Physical Chemistry A, 2001, 105, 5751-5758.	1.1	25
720	First-Principles Theoretical Study of Molecular HCl Adsorption on a Hexagonal Ice (0001) Surface. Journal of Physical Chemistry A, 2001, 105, 7037-7046.	1.1	37
721	Transition from Hydrogen Bonding to Ionization in (HCl)n(NH3)n and (HCl)n(H2O)n Clusters:â€‰ Consequences for Anharmonic Vibrational Spectroscopy. Journal of Physical Chemistry A, 2001, 105, 8323-8332.	1.1	94
722	Ion Pairs in Polymer Electrolytes Revisited:â€‰ An Ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 8504-8509.	1.1	44
723	Theoretical Analysis of Heteroaromatic Thioaminyl Radicals. Part 2: A Comparison of Ab Initio and Density Functional Methods in the Description of Redox Processes. Journal of Physical Chemistry A, 2001, 105, 7626-7633.	1.1	45
724	The Effect of Alkylation of N- and O-Donor Atoms on Their Strength of Coordination to Silver(I). Journal of Physical Chemistry A, 2001, 105, 6567-6574.	1.1	30
725	Catalytic Chain Transfer in Free-Radical Polymerizations. Chemical Reviews, 2001, 101, 3611-3660.	23.0	360
726	Ab Initio Study of Hydrolysis of Amino Malononitrile:Â Formation of Amino Acetonitrile. Journal of Physical Chemistry A, 2001, 105, 6543-6551.	1.1	11
727	Carbon-to-Carbon Identity Proton Transfers from Propyne, Acetimide, Thioacetaldehyde, and Nitrosomethane to Their Respective Conjugate Anions in the Gas Phase. An ab Initio Study. Journal of Organic Chemistry, 2001, 66, 968-979.	1.7	23
728	CO Desorption from Oxygen Species on Carbonaceous Surface:Â 1. Effects of the Local Structure of the Active Site and the Surface Coverage. Journal of Physical Chemistry A, 2001, 105, 6757-6764.	1.1	120
729	Considerations on the Molecular Structures and Electronic Properties of 1-Methyl-2(1H)-pyridinimine in the Ground and Lowest Excited Singlet States.. Nippon Kagaku Kaishi / Chemical Society of Japan - Chemistry and Industrial Chemistry Journal, 2001, 2001, 401-413.	0.1	0
730	Radiation chemistry: from the early days to the next millennium. Studies in Physical and Theoretical Chemistry, 2001, 87, 1-19.	0.0	0

#	Article	IF	Citations
731	Ion Rearrangement at the Beginning of Cluster Formation: Methyl Substitution Effects on the Internal SN2 Reaction in the Proton-Bound Dimers of Acetonitrile and Alcohols. European Journal of Mass Spectrometry, 2001, 7, 267-277.	0.5	12
732	Quinones and quinoidal radicals in photosynthesis. Theoretical and Computational Chemistry, 2001, , 655-690.	0.2	5
733	The infrared spectra and structures of the valyl-glycine zwitterion isolated in a KBr matrix. Chemical Physics, 2001, 263, 243-253.	0.9	8
734	The vacuum UV photoabsorption spectrum of methyl chloride (CH3Cl) and its perdeuterated isotopomer CD3Cl. Chemical Physics, 2001, 272, 277-292.	0.9	23
735	Coupling between lattice and intramolecular modes in 9,10-dimethylanthracene: Raman spectra under pressure and quasi-harmonic lattice dynamics calculations. Chemical Physics, 2001, 273, 197-206.	0.9	5
736	The 3.2-3.5Î¼m region revisited - II. A theoretical study of the effects of hydrogenation on some model PAHs. Monthly Notices of the Royal Astronomical Society, 2001, 324, 355-366.	1.6	39
737	Ab initio calculation of the rate coefficient for short-chain branching in free-radical polymerizations. Polymer, 2001, 42, 1915-1920.	1.8	38
738	Computational studies of the reaction of the hydroxyl radical with hydrofluorocarbons (HFCs) and hydrofluoroethers (HFEs). Journal of Fluorine Chemistry, 2001, 109, 113-121.	0.9	25
739	Vibrational and theoretical DFT study of two regioregular methyl-disubstituted bithiophenes. Journal of Molecular Structure, 2001, 563-564, 539-544.	1.8	3
740	Vibrational spectroscopy and mode assignments for an analog of the green fluorescent protein chromophore. Journal of Molecular Structure, 2001, 569, 25-41.	1.8	43
741	Vibrational spectra and scaled quantum-mechanical molecular force fields. Journal of Molecular Structure, 2001, 567-568, 217-230.	1.8	52
742	The gas-phase molecular structure and quadratic force field of bis(dimethylamino)hydroborane, [(CH) Tj ETQq1 1 0.784314 rgBT /Ove Structure, 2001, 567-568, 247-268.	1.8	4
743	Asymmetric Dielsâ€“Alder reactions of optically active oxazolidinone-derived vinylsulfonamides. Tetrahedron: Asymmetry, 2001, 12, 1811-1815.	1.8	18
744	Theoretical IR, Raman and NMR spectra of 1,2- and 1,3-dimethylenecyclobutane. Vibrational Spectroscopy, 2001, 25, 133-149.	1.2	15
745	Quantum chemistry predicted correlations between geometric isomerism (conformation) of î—¸OH and î˜…NH substituents and typical group frequencies of nucleic acid bases: cytosine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 55-72.	2.0	5
746	Experimental and ab initio MO studies on the IR spectra and structure of pyridinium dicyanomethylide and trimethylammonium dicyanomethylide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 95-103.	2.0	10
747	Fragment mode analysis and its application to the vibrational normal modes of boron trichlorideâ€“ammonia and boron trichlorideâ€“pyridine complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 521-534.	2.0	5
748	Optimization of force constants with an Ureyâ€“Bradley force field avoiding normal mode crossings. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 535-544.	2.0	3

#	Article	IF	Citations
749	Surface-enhanced Raman scattering of p-nitrothiophenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1009-1016.	2.0	100
750	Looking for the PC bond in space: HPCO and HPCS as possible tracers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 859-873.	2.0	20
751	Calculated gas-phase infrared spectra of 2,2,5,5,8,8-hexamethylhexahydroimidazo[1,2-a]-pyrazine-3,6-dione: relative performance of Hartreeâ€“Fock and hybrid density functional theory methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1271-1282.	2.0	7
752	Raman and infrared spectra, conformational stability, ab initio calculations and assignment of fundamentals for 1-bromo-3-fluoropropane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1567-1586.	2.0	7
753	Ab initio calculations, FTIR and Raman spectra of 2,3-difluorobenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 2373-2389.	2.0	19
754	Quantum mechanical investigation of the inner-sphere reorganization energy of cyclooctatetraene/cyclooctatetraene radical anion. Part I. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 1959-1969.	2.0	11
755	Ion/molecule reaction kinetics using a modified Finnigan GCQ ion trap mass spectrometer: the energetics of the dehydration of proton-bound alcohol dimers. International Journal of Mass Spectrometry, 2001, 207, 183-193.	0.7	12
756	Beta cleavages of distonic ions, alpha cleavages of enol ions, isomerizations of distonic and enol ions and corresponding reactions of free radicals. International Journal of Mass Spectrometry, 2001, 210-211, 417-428.	0.7	8
757	Influence of fluorine substitution on the structures and thermochemistry of chloride ionâ€“ether complexes in the gas phase. International Journal of Mass Spectrometry, 2001, 210-211, 387-402.	0.7	9
758	Loss of CO2 from the ortho isomer of deprotonated methyl phenyl carbonate involves a methyl migration. International Journal of Mass Spectrometry, 2001, 210-211, 557-562.	0.7	2
759	Do all b2 ions have oxazolone structures? Multistage mass spectrometry and ab initio studies on protonated N-acyl amino acid methyl ester model systems. International Journal of Mass Spectrometry, 2001, 210-211, 71-87.	0.7	96
760	A mechanistic investigation of the reactions between the tert-butyl methylene oxonium ion [CH2OC(CH3)3+] and ammonia: competition between substitution, addition-elimination, and elimination. International Journal of Mass Spectrometry, 2001, 210-211, 459-468.	0.7	5
761	Side-chain involvement in the fragmentation reactions of the protonated methyl esters of histidine and its peptides. International Journal of Mass Spectrometry, 2001, 209, 99-112.	0.7	72
762	The methylene chloride radical cation and its distonic isomers in the gas phase. International Journal of Mass Spectrometry, 2001, 210-211, 403-415.	0.7	8
763	Large structural effects in neutral and protonated species: a computational study. Journal of Physical Organic Chemistry, 2001, 14, 839-845.	0.9	2
764	An ab initio post-Hartree-Fock study of vibrational infrared spectra of 5-azacytosine and cytosine. International Journal of Quantum Chemistry, 2001, 83, 203-212.	1.0	6
765	Substituent effects on inversion motion of 4-silatriafulvene derivatives: An ab initio MO study. International Journal of Quantum Chemistry, 2001, 84, 198-207.	1.0	21
766	Three conformers observed and characterized in 1-hexyne. International Journal of Quantum Chemistry, 2001, 85, 514-519.	1.0	16

#	Article	IF	Citations
767	Computational chemistry: A useful (sometimes mandatory) tool in mass spectrometry studies. Mass Spectrometry Reviews, 2001, 20, 195-245.	2.8	160
768	A quantum Monte Carlo study of energy differences in C4H3 and C4H5 isomers. International Journal of Chemical Kinetics, 2001, 33, 808-820.	1.0	18
769	Molecular hydrogen elimination from 2,5-dihydrofuran, 2,3-dihydrofuran, and 2-methyl-2,5-dihydrofuran: Quantum chemical and kinetics calculations. International Journal of Chemical Kinetics, 2001, 33, 685-697.	1.0	7
770	A new mechanism for initiation of free-radical chain reactions during high-temperature, homogeneous oxidation of unsaturated hydrocarbons: Ethylene, propyne, and allene. International Journal of Chemical Kinetics, 2001, 33, 698-706.	1.0	28
771	Vibrational Spectra, DFT Calculations, and Assignments of the syn and the gauche Forms of Vinylphosphine. Journal of Molecular Spectroscopy, 2001, 205, 252-260.	0.4	12
772	Quantum chemical characterization of the cytosine: 2-Aminopurine base pair. Journal of Computational Chemistry, 2001, 22, 1167-1179.	1.5	16
773	Reaction of OH radical with mono-, di-, and trichloroacetaldehyde: anab initio study. Journal of Computational Chemistry, 2001, 22, 1509-1521.	1.5	2
774	Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. Journal of Computational Chemistry, 2001, 22, 1666-1678.	1.5	21
775	Solvated CH5+ in Liquid Superacid. Chemistry - A European Journal, 2001, 7, 1936-1943.	1.7	31
776	Characterisation of Zeolitic Materials with a HEU-Type Structure Modified by Transition Metal Elements: Definition of Acid Sites in Nickel-Loaded Crystals in the Light of Experimental and Quantum-Chemical Results. Chemistry - A European Journal, 2001, 7, 3705-3721.	1.7	25
777	Thermal Rearrangements of 2-Vinylcyclopropylidene to Cyclopentadiene and Vinylallene: A Theoretical Investigation. Chemistry - A European Journal, 2001, 7, 3951-3960.	1.7	8
778	Factors Controlling the Addition of Carbon-Centered Radicals to Alkenesâ€"An Experimental and Theoretical Perspective. Angewandte Chemie - International Edition, 2001, 40, 1340-1371.	7.2	640
779	The Câ€"H bond dissociation enthalpies of haloethers and its correlation with the activation energies for hydrogen abstraction by OH radical: A DFT study. Chemical Physics Letters, 2001, 334, 200-206.	1.2	39
780	Structures, energetics and vibrational spectra of the valence isomers of phosphinine. An ab initio and DFT study. Chemical Physics Letters, 2001, 336, 343-348.	1.2	14
781	Intensity of the â†' symmetry-forbidden electronic transition in acetone by direct vibronic coupling mechanism. Chemical Physics Letters, 2001, 337, 331-334.	1.2	15
782	An ab initio and DFT study of the valence isomers of pyridine. Chemical Physics Letters, 2001, 337, 361-367.	1.2	17
783	A Gaussian-3 investigation of N7 isomers. Chemical Physics Letters, 2001, 338, 367-374.	1.2	29
784	Molecular orbital studies of titanium nitride chemical vapor deposition: gas phase Î²-elimination. Chemical Physics Letters, 2001, 340, 343-347.	1.2	13

#	Article	IF	Citations
785	Theoretical evaluation of Raman spectra and enhancement factors for a molecule adsorbed on a complex-shaped metal particle. Chemical Physics Letters, 2001, 342, 135-140.	1.2	50
786	The infrared spectroscopy of HNCCC: matrix isolation and density functional theory study. Chemical Physics Letters, 2001, 344, 625-630.	1.2	36
787	Ab initio and density functional study of the 5-pentacyclo[6.2.1.13,6.02,7.04,10]dodecyl cation. A symmetrical Î¼-hydride bridged carbocation. Chemical Physics Letters, 2001, 345, 189-194.	1.2	7
788	A theoretical re-evaluation of the heat of formation of phenylcarbene. Chemical Physics Letters, 2001, 349, 571-577.	1.2	16
789	Ab initio study of ammonia adsorption states on an ice surface II: theoretical characterization of the surface bound state. Chemical Physics Letters, 2001, 350, 141-146.	1.2	6
790	Transient resonance Raman and density functional theory investigation of the ultraviolet photolysis of dibromoacetonitrile in the solution phase. Chemical Physics Letters, 2001, 350, 78-85.	1.2	0
791	Nitromethyl Radical, Cation, and Anion. A Neutralization and Electron Photodetachmentâ^'Reionization Mass Spectrometric and ab Initio Computational Study of [C,H2,N,O2] Isomers. Journal of Physical Chemistry A, 2001, 105, 1371-1382.	1.1	15
792	Origin of Diastereofacial Selectivity in Tertiary 2-Adamantyl Cations. Journal of the American Chemical Society, 2001, 123, 6396-6403.	6.6	12
793	Solvent effects on the absorption spectrum and recombination kinetics of diphenylcarbonyl oxide. Russian Chemical Bulletin, 2001, 50, 793-797.	0.4	0
794	Title is missing!. Russian Journal of General Chemistry, 2001, 71, 1225-1232.	0.3	10
795	Calculated molecular properties for different alkanoic acidâ€“alkylamine complexes: A comparison with measured FTIR and Raman spectra. Chemical Physics, 2001, 263, 127-138.	0.9	13
796	Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole. Chemical Physics, 2001, 270, 67-78.	0.9	30
797	Hydrogen bonding effects on the conformational changes of polyglutamates containing long flexible side chains. Polymer, 2001, 42, 09915-09920.	1.8	22
798	Proton tunneling in calix[4]arenes: a theoretical investigation. Chemical Physics Letters, 2001, 343, 627-632.	1.2	14
799	Ab initio MO and experimental studies on the vibrational spectra and structure of 4-hydroxybenzonitrile and of its anion. Computational and Theoretical Chemistry, 2001, 535, 93-101.	1.5	28
800	Ground state vibrational spectra of corannulene: a theoretical study. Computational and Theoretical Chemistry, 2001, 538, 51-58.	1.5	2
801	Thermochemical analysis of the OH+C2H4â†'C2H4OH reaction using accurate theoretical methods. Computational and Theoretical Chemistry, 2001, 537, 199-212.	1.5	17
802	Charge transfer complexes between 4,4â€²-disubstituted diphenyldiacetylenes: experimental and theoretical study. Computational and Theoretical Chemistry, 2001, 540, 123-130.	1.5	8

#	Article	IF	Citations
803	Highlevel ab initio and hybrid density functional theory study of the energy profile for the 1 CO+ 2 CO + reaction. Computational and Theoretical Chemistry, 2001, 540, 101-112.	1.5	1
804	Protonation study of some enamine systems. Computational and Theoretical Chemistry, 2001, 541, 111-117.	1.5	12
805	Ab initio/density functional study of vibrational frequencies of acridine in the ground and excited states. Computational and Theoretical Chemistry, 2001, 542, 189-198.	1.5	0
806	The adsorption of ethylene on the (100) surfaces of platinum, palladium and nickel: a DFT study. Computational and Theoretical Chemistry, 2001, 542, 263-271.	1.5	44
807	Solvent effects on vibrational modes: ab-initio calculations, scaling and solvent functions with applications to the carbonyl stretch of dialkyl ketones. Computational and Theoretical Chemistry, 2001, 544, 191-203.	1.5	23
808	A theoretical investigation of tautomeric equilibria and proton transfer in isolated and hydrated thiocytosine. Computational and Theoretical Chemistry, 2001, 549, 101-109.	1.5	14
809	Vibrational frequencies and infrared intensities of the hydrogen-bonded H3Nâ‹¯HONO2 complex: an ab initio prediction. Computational and Theoretical Chemistry, 2001, 548, 113-121.	1.5	7
810	Complexes of lithium cation with nitrogen trifluoride: a computational investigation on the structure and stability of Li+â€“(NF3) isomers. Computational and Theoretical Chemistry, 2001, 574, 185-193.	1.5	14
811	The Adsorption of Acetylene and Ethylene on Transition Metal Surfaces. Progress in Theoretical Chemistry and Physics, 2001, , 217-240.	0.2	8
812	The reactions CHnD4âˆ’n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I.. Journal of Chemical Physics, 2001, 114, 2154-2165.	1.2	44
813	Glutathione radical: Intramolecular H abstraction by the thiyl radical. Canadian Journal of Chemistry, 2001, 79, 405-417.	0.6	28
814	The performance of density functional theory for equilibrium molecular properties of symmetry breaking molecules. Journal of Chemical Physics, 2001, 114, 8257-8269.	1.2	39
815	The reactions CHnD4âˆ’n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526.	1.2	29
816	A crystalline orbital study of polydiacetylenes. Journal of Chemical Physics, 2001, 114, 9130-9141.	1.2	24
817	A theoretical study of Si4H2 cluster with ab initio and density functional theory methods. Journal of Chemical Physics, 2001, 114, 1278-1285.	1.2	9
818	Problematic p-benzyne: Orbital instabilities, biradical character, and broken symmetry. Journal of Chemical Physics, 2001, 114, 10638-10650.	1.2	161
819	Ambident EthylN-Nitrosocarbamate Anion:Â Experimental and Computational Studies of Alkylation and Thermal Stability. Journal of the American Chemical Society, 2002, 124, 14115-14126.	6.6	6
820	Selectivity of the Î± and Î² bond fissions for bromoacetyl chloride upon nâ†'Ï€* excitation: A combined complete-active-space self-consistent field and multireference configuration interaction study. Journal of Chemical Physics, 2002, 117, 8745-8753.	1.2	16

#	Article	IF	Citations
821	Vibronic coupling in excited states of acetone. Journal of Chemical Physics, 2002, 116, 547-560.	1.2	25
822	Efficiency of the Ï€ conjugation in a novel family of Î±,Î±â€²-bisphenyl end-capped oligothiophenes by means of Raman spectroscopy. Journal of Chemical Physics, 2002, 116, 10419-10427.	1.2	63
823	Synthesis, Spectroscopic and Voltammetric Studies of a Novel Dioxovanadate(V) 8-Hydroxyquinoline Complex. Journal of Coordination Chemistry, 2002, 55, 1461-1471.	0.8	4
824	Ab initio study of the reaction mechanism of CO2 with Ti atom in the ground and excited electronic states. Journal of Chemical Physics, 2002, 116, 5633-5642.	1.2	25
825	Practical failures from the inclusion of exact exchange: how much exact exchange is appropriate?. Molecular Physics, 2002, 100, 483-497.	0.8	22
826	Time-resolved resonance Raman spectroscopy and density functional theory investigation of the CH2Iâ€“I isomer and CH2I2â‹¯I molecular complex products produced from ultraviolet photolysis of CH2I2 in the solution phase: Comparison of the structure and chemical reactivity of polyhalomethane isomers and polyhalomethaneâ€“halogen atom molecular complexes. Journal of Chemical Physics, 2002, 117, 7931-7941.	1.2	19
827	Thermochemistry of Species Produced from Monomethylhydrazine in Propulsion and Space-Related Applications. Journal of Propulsion and Power, 2002, 18, 1242-1253.	1.3	16
828	Ab initio quantum mechanical modeling of infrared vibrational frequencies of the OH group in dioctahedral phyllosilicates. Part I: Methods, results and comparison to experimental data. American Mineralogist, 2002, 87, 1215-1223.	0.9	29
829	Transition State Analysis Using Multiple Kinetic Isotope Effects: Mechanisms of Enzymatic and Non-enzymatic Glycoside Hydrolysis and Transfer. Advances in Physical Organic Chemistry, 2002, 37, 239-314.	0.5	56
830	The reactivity of ground-state carbon atoms with unsaturated hydrocarbons in combustion flames and in the interstellar medium. International Reviews in Physical Chemistry, 2002, 21, 307-356.	0.9	81
831	Resonance Raman Spectrum ofall-trans-Spheroidene. DFT Analysis and Isotope Labeling. Journal of Physical Chemistry A, 2002, 106, 9463-9469.	1.1	22
832	Synthesis and Properties of the First 1-Silanaphthalene. Organometallics, 2002, 21, 4024-4026.	1.1	54
833	Computation of pKafrom Dielectric Continuum Theory. Journal of Physical Chemistry A, 2002, 106, 7413-7422.	1.1	204
834	Dynamics of Molecules and Clusters Studied by Low-Temperature Matrix-Isolation Infrared Spectroscopy and Density-Functional-Theory Calculations. Bulletin of the Chemical Society of Japan, 2002, 75, 1173-1189.	2.0	4
835	Femtosecond Mid-Infrared Pumpâ€“Probe Study of Wave Packet Motion in a Medium-Strong Intramolecular Hydrogen Bond. Bulletin of the Chemical Society of Japan, 2002, 75, 909-917.	2.0	29
836	Density Functional Studies on the Solvation Free Energy of the Proton in Methanol. Chemistry Letters, 2002, 31, 1220-1221.	0.7	2
837	Kinetics of Hydroxyl Radical Reaction with CF2ClOCHO: A Theoretical Investigation. Chemistry Letters, 2002, 31, 132-133.	0.7	3
838	Vibrational Spectra of Dipyrido[3,2-a:2â€²,3â€²-c]phenazine and Its Radical Anion Analyzed by Ab Initio Calculations and Deuteration Studies. Bulletin of the Chemical Society of Japan, 2002, 75, 933-942.	2.0	33

#	Article	IF	Citations
839	Interstellar and Circumstellar Reaction Kinetics of Na+, Mg+, and Al+with Cyanopolyynes and Polyynes. Astrophysical Journal, 2002, 564, 792-802.	1.6	52
840	Remote Substituent Effects on Bond Dissociation Energies of Para-Substituted Aromatic Silanes. Journal of Organic Chemistry, 2002, 67, 6638-6645.	1.7	69
841	Ab Initio Quantum Chemical Study of the Coordination Preferences and Catalytic Role of Cu+ Ions in the Dehydration Reactions of Hydroxyformaldoxime Conformers and the Oxidation of HCN to Hydroxyformaldoxime by Hydrogen Peroxide. Journal of Physical Chemistry A, 2002, 106, 1425-1440.	1.1	9
842	Estimation of Câˆ'C Bond Dissociation Enthalpies of Large Aromatic Hydrocarbon Compounds Using DFT Methods. Journal of Physical Chemistry A, 2002, 106, 7184-7189.	1.1	76
843	Computational and Experimental Studies of the Effect of Substituents on the Singletâˆ'Triplet Energy Gap in Phenyl(carbomethoxy)carbene. Journal of Organic Chemistry, 2002, 67, 3079-3088.	1.7	39
844	Ab Initio Calculations and Mass Spectrometric Determination of the Gas-Phase Proton Affinities of 4,4â€˜-Disubstituted 2,2â€˜-Bipyridines. Journal of Organic Chemistry, 2002, 67, 8216-8219.	1.7	25
845	Calculated OH-Stretching Vibrational Transitions in the Waterâˆ'Nitrogen and Waterâˆ'Oxygen Complexes. Journal of Physical Chemistry A, 2002, 106, 8955-8962.	1.1	73
846	Transferable Scaling Factors for Vibrational Force Fields of Halogenated Molecules Based on Energy-Consistent Pseudopotentials. Journal of Physical Chemistry A, 2002, 106, 6810-6816.	1.1	8
847	Pyrrole-2-carboxylic Acid and Its Dimers:Â Molecular Structures and Vibrational Spectrum. Journal of Physical Chemistry A, 2002, 106, 10613-10621.	1.1	98
848	Density Functional Theory Vibrational Frequencies of Amides and Amide Dimers. Journal of Physical Chemistry A, 2002, 106, 7858-7867.	1.1	74
849	Ab Initio Study of the Mechanism and Thermochemistry of the Atmospheric Reaction NO + O3 â†' NO2 + O2. Journal of Physical Chemistry A, 2002, 106, 10302-10310.	1.1	22
850	Transition State Structure and Energetics of the N2O + X (X = Cl,Br) Reactions. Journal of Chemical Information and Computer Sciences, 2002, 42, 706-711.	2.8	11
851	Thermochemistry of Chlorine Fluorides ClFn,n= 1âˆ'7, and Their Singly Charged Cations and Anions:Â A Gaussian-3 and Gaussian-3X Study. Journal of Physical Chemistry A, 2002, 106, 11271-11276.	1.1	23
852	New Empirical Procedures for Improving ab Initio Energeticsâ€. Journal of Physical Chemistry A, 2002, 106, 9910-9917.	1.1	8
853	Phototautomerism in Uracil:Â A Quantum Chemical Investigation. Journal of Physical Chemistry A, 2002, 106, 8642-8650.	1.1	49
854	Carbanion Stabilization by Distal Silyloxy Groups. Origin of the High Diastereoselectivity in the Formation of Quaternary Centers with Aryllead(IV) Triacetate Reagents. Organic Letters, 2002, 4, 4121-4124.	2.4	11
855	Infrared Spectra and Density Functional Theory Calculations of Iminoxy Radicals Produced by Visible-Light-Induced Reaction between 1-Phenyl-1-Propyne and NO2 in Low-Temperature Argon Matrixes. Journal of Physical Chemistry A, 2002, 106, 3365-3370.	1.1	5
856	Solid-State and Theoretical Model Structures of Monolithiated (Organosulfonyl)acetonitriles and the Characterization and Reactivity of Their Geminated Dilithio Derivatives. Organometallics, 2002, 21, 606-616.	1.1	28

#	Article	IF	Citations
857	Study of Thermally Treated Lithium Montmorillonite by Ab Initio Methods. Journal of Physical Chemistry B, 2002, 106, 12470-12477.	1.2	35
858	Evidence for Pyridinium Cation Formation during Coadsorption of Pyridine and Hydrogen on (2 Ã—) Tj ETQq1 1 0.784314 rgBT /Overlo	1.2	19
859	Reinvestigation of the Gas-Phase Structure of RDX Using Density Functional Theory Predictions of Electron-Scattering Intensities. Journal of Physical Chemistry A, 2002, 106, 10437-10443.	1.1	48
860	Raman Evidence for Meisenheimer Complex Formation in the Hydrolysis Reactions of 4-Fluorobenzoyl- and 4-Nitrobenzoyl-Coenzyme A Catalyzed by 4-Chlorobenzoyl-Coenzyme A Dehalogenaseâ€. Biochemistry, 2002, 41, 7453-7463.	1.2	26
861	Highly Unsaturated Hydrogenated Silicon Clusters, SinHx(n= 3â^'10,x= 0â^'3), in Flash Pyrolysis of Silane and Disilane. Journal of Physical Chemistry A, 2002, 106, 5081-5087.	1.1	23
862	Ab Initio Studies of Thermal Syn-Elimination Reactions in Carbonates:Â Effect of Structure on Reactivity. Journal of Physical Chemistry A, 2002, 106, 12370-12375.	1.1	5
863	Catalytic Asymmetric Synthesis of Protected Tryptophan Regioisomers. Journal of Organic Chemistry, 2002, 67, 6256-6259.	1.7	27
864	An Experimental and Computational Evaluation of the Energetics of the Isomeric Methoxyphenylcarbenes Generated in Carbon Atom Reactions. Journal of the American Chemical Society, 2002, 124, 355-364.	6.6	21
865	Isolated Building Blocks of Photonic Materials:Â High-Resolution Excited-State Photoelectron Spectroscopy of Jet-Cooled Tetramethylethylene and 1,1â€˜-Bicyclohexylidene. Journal of Physical Chemistry A, 2002, 106, 5249-5262.	1.1	13
866	Theoretical investigation of the transition states leading to HCl elimination in 2-chloropropene. Molecular Physics, 2002, 100, 865-874.	0.8	10
867	Halogen Derivatives ofm-Phenylene(carbeno)nitrene:Â A Switch in Ground-State Multiplicity. Journal of Organic Chemistry, 2002, 67, 5578-5587.	1.7	15
868	Lewis Donor and Acceptor Interactions of Silylenes:Â A Theoretical Study. Organometallics, 2002, 21, 3683-3690.	1.1	37
869	Direct Infrared Detection of the Covalently Ring Linked Hisâ^'Tyr Structure in the Active Site of the Hemeâ^'Copper Oxidasesâ€. Biochemistry, 2002, 41, 14383-14390.	1.2	50
870	Blue-Shifting Câ^'HÂ·Â·Â·X (X = O, Halogen) Hydrogen Bonds in the Dimers of Formaldehyde Derivatives. Journal of Physical Chemistry A, 2002, 106, 5671-5678.	1.1	53
871	Inverse Isotope Effects of a Late Transition Metal Olefin Polymerization Catalyst:â€‰ A DFT Study. Organometallics, 2002, 21, 4950-4954.	1.1	15
872	Theoretical Study of the Reaction of Boron with Methanol and the Decomposition Paths of the Reaction Products. Journal of Physical Chemistry A, 2002, 106, 3181-3184.	1.1	6
873	Helicoid Shiftamers. Journal of the American Chemical Society, 2002, 124, 6836-6837.	6.6	11
874	An ab Initio Study of Linear XHâ^'HX Hydrogen Halide Anions. Journal of Physical Chemistry A, 2002, 106, 400-403.	1.1	8

#	Article	IF	Citations
875	Binding Energies of Proton-Bound Ether/Alcohol Mixed Dimers Determined by FTICR Radiative Association Kinetics Measurements. Journal of Physical Chemistry A, 2002, 106, 1576-1583.	1.1	13
876	Spectroelectrochemical Raman Study of Two End-Capped Sexithiophenes with Applications as Electroactive Molecular Materials. Journal of Physical Chemistry B, 2002, 106, 2488-2496.	1.2	37
877	Density Functional Study on the Adsorption of Pyrazole onto Silver Colloidal Particles. Journal of Physical Chemistry B, 2002, 106, 6875-6880.	1.2	81
878	Theoretical and Experimental Study of the Vibrational Spectra of the Î±, Î², and Î´ Phases of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Journal of Physical Chemistry B, 2002, 106, 10594-10604.	1.2	71
879	Structures, Rotational Barriers, and Thermochemical Properties of Chlorinated Aldehydes and the Corresponding Acetyl (CCâ€¢O) and Formyl Methyl Radicals (Câ€¢CO) and Additivity Groups. Journal of Physical Chemistry A, 2002, 106, 345-355.	1.1	16
880	Density Functional Theory Used in Structure Determinations and Raman Band Assignments for Pseudoisocyanine and Its Aggregate. Journal of Physical Chemistry B, 2002, 106, 5447-5454.	1.2	39
881	Rearrangement Pathways of 2-Hydroxy-2-methylpropylidene:Â An Experimental and Computational Study. Journal of Organic Chemistry, 2002, 67, 3257-3265.	1.7	14
882	Theoretical Study of the Thermolysis Reaction of Ethyl Î²-Hydroxycarboxylates in the Gas Phase. Journal of Physical Chemistry A, 2002, 106, 4377-4383.	1.1	12
883	Polarized Infrared Absorption Spectrum of Matrix-Isolated Methylperoxyl Radicals, CH3OO XÌƒ 2Aâ€˜â€‰â€˜. Journal of Physical Chemistry A, 2002, 106, 7547-7556.	1.1	44
884	Gas-Phase Identity Nucleophilic Substitution Reactions of Cyclopropenyl Halides. Journal of Organic Chemistry, 2002, 67, 1953-1960.	1.7	10
885	Density Functional Theory Investigation of Cobalt Siting in Ferrierite. Journal of Physical Chemistry B, 2002, 106, 10864-10872.	1.2	17
886	Bystander Effects on Carbene Rearrangements:â€‰ A Computational Study. Journal of Physical Chemistry A, 2002, 106, 4970-4979.	1.1	14
887	Structures, Rotational Barriers, Thermochemical Properties, and Additivity Groups for 2-Propanol, 2-Chloro-2-propanol and the Corresponding Alkoxy and Hydroxyalkyl Radicals. Journal of Physical Chemistry A, 2002, 106, 3947-3956.	1.1	25
888	Internal Methyl Rotation in the CH Stretching Overtone Spectra of 2-, 3-, and 4-Methylpyridine. Journal of Physical Chemistry A, 2002, 106, 4368-4376.	1.1	5
889	Experimental and Theoretical Study of the Infrared and Raman Spectra of a Substituted Sexithiophene in Five Oxidation States. Journal of Physical Chemistry B, 2002, 106, 3597-3605.	1.2	63
890	Vibrational Spectroscopic Features of a Novel Family of Amorphous Molecular Materials Containing an Oligothiophene Moiety as Color-Tunable Emitting Materials. Journal of Physical Chemistry B, 2002, 106, 7163-7170.	1.2	41
891	Kinetics and Mechanism of the OH + C6H6Reaction:Â A Detailed Analysis with First-Principles Calculations. Journal of Physical Chemistry A, 2002, 106, 11309-11326.	1.1	89
892	Conformational and Infrared Spectral Studies of l-Methionine and Its N-Deuterated Isotopomer as Isolated Zwitterions. Journal of Physical Chemistry A, 2002, 106, 41-50.	1.1	54

#	Article	IF	Citations
893	Thermodynamic Properties of Ketenes:Â Group Additivity Values from Quantum Chemical Calculations. Journal of Physical Chemistry A, 2002, 106, 7937-7949.	1.1	41
894	Structures and Enthalpies of Formation in the Gas Phase of the Most Toxic Polychlorinated Dibenzo-p-dioxins. A DFT Study. Journal of Physical Chemistry A, 2002, 106, 6618-6627.	1.1	23
895	A High-Level Theoretical Study on the Gas-Phase Identity Methyl Transfer Reactions. Journal of Physical Chemistry A, 2002, 106, 1081-1087.	1.1	32
896	Direct Investigation of the Validity of Vertical Approximation in the Calculation of Transition Moment Matrix Elements:â€‰n â†' Ï€* Transition in Methyl Formate. Journal of Physical Chemistry A, 2002, 106, 181-183.	1.1	18
897	Gas-Phase Basicity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives. Journal of Physical Chemistry A, 2002, 106, 7383-7389.	1.1	18
898	Surface Enhanced Raman Spectroscopy and Theoretical Studies on 1,4-Dihydrazinophthalazine Sulfate. Journal of Physical Chemistry A, 2002, 106, 3337-3344.	1.1	12
899	Vibration Spectroscopy Reveals Light-Induced Chromophore and Protein Structural Changes in the LOV2 Domain of the Plant Blue-Light Receptor Phototropin 1â€. Biochemistry, 2002, 41, 7183-7189.	1.2	109
900	Benzdiynes (1,2,4,5-Tetradehydrobenzenes):Â Direct Observation by Wavelength-Selective Photolyses of Benzenetetracarboxylic Dianhydrides in Low-Temperature Nitrogen Matrixes. Journal of the American Chemical Society, 2002, 124, 4512-4521.	6.6	26
901	Methyl Radical Addition to CS Double Bonds:â€‰ Kinetic versus Thermodynamic Preferences. Journal of Physical Chemistry A, 2002, 106, 12124-12138.	1.1	82
902	Substituent Effects in the Interconversion of Phenylcarbene, Bicyclo[4.1.0]hepta-2,4,6-triene, and 1,2,4,6-Cycloheptatetraene. Journal of Organic Chemistry, 2002, 67, 2532-2540.	1.7	32
903	Experimental and Theoretical Studies of the Products of Laser-Ablated Thorium Atom Reactions with H2O in Excess Argon. Journal of the American Chemical Society, 2002, 124, 6723-6733.	6.6	42
904	Excited and ionic states of formamide: An excited-state photoelectron spectroscopy and ab initio study. Journal of Chemical Physics, 2002, 117, 8270-8280.	1.2	20
905	An investigation of the prototype germylene addition reaction, GeH2â€‰+â€‰C2H4: Time-resolved gas-phase kinetic studies and quantum chemical calculations of the reaction energy surface. Physical Chemistry Chemical Physics, 2002, 4, 5079-5087.	1.3	46
906	Dissociative Photodetachment Dynamics of S2O2-. Journal of Physical Chemistry A, 2002, 106, 279-284.	1.1	10
907	Experimental and Computational Thermochemistry of 2- and 3-Thiophenecarboxylic Acids. Journal of Physical Chemistry A, 2002, 106, 11173-11180.	1.1	32
908	Ab initio Quantum Chemical Study on Charge Distribution and Molecular Structure of Uranyl (VI) Species with Raman Frequency. Journal of Nuclear Science and Technology, 2002, 39, 647-654.	0.7	34
909	Solvent Dependence of the 2-Naphthyl(carbomethoxy)carbene Singletâ^'Triplet Energy Gap. Journal of the American Chemical Society, 2002, 124, 1761-1767.	6.6	35
910	DFT Calculation Analysis of the Infrared Spectra of Ethylene Adsorbed on Cu(110), Pd(110), and Ag(110). Journal of Physical Chemistry B, 2002, 106, 10714-10721.	1.2	32

#	Article	IF	Citations
911	A Density Functional Theory Study of the Oxidation of Methanol to Formaldehyde over Vanadia Supported on Silica, Titania, and Zirconia. Journal of Physical Chemistry B, 2002, 106, 7832-7838.	1.2	98
912	Ketoâ^'Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. Journal of Physical Chemistry B, 2002, 106, 10220-10226.	1.2	46
913	Anchoring the Gas-Phase Acidity Scaleâ€. Journal of Physical Chemistry A, 2002, 106, 9947-9956.	1.1	190
914	Reaction Modes of Carbonyl Oxide, Dioxirane, and Methylenebis(oxy) with Ethylene:â€‰ A New Reaction Mechanism. Journal of Physical Chemistry A, 2002, 106, 3917-3929.	1.1	57
915	Arylpentazoles Revisited:Â Experimental and Theoretical Studies of 4-Hydroxyphenylpentazole and 4-Oxophenylpentazole Anion. Journal of Organic Chemistry, 2002, 67, 1354-1358.	1.7	74
916	Isotope Effects and the Mechanism of an Electron-Transfer-Catalyzed Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 2002, 124, 11552-11559.	6.6	52
917	The First Singlet (n,Ï€*) and (Ï€,Ï€*) Excited States of the Hydrogen-Bonded Complex between Water and Pyridine. Journal of Physical Chemistry A, 2002, 106, 8769-8778.	1.1	63
918	Double-Proton Transfer in the Formamidineâ^'Formamide Dimer. Post-Hartreeâ^'Fock Gas-Phase and Aqueous Solution Study. Journal of Physical Chemistry A, 2002, 106, 12103-12109.	1.1	45
919	Combined Spectroelectrochemical and Theoretical Study of a Vinylene-Bridged Sexithiophene Cooligomer:Â Analysis of the Ï€-Electron Delocalization and of the Electronic Defects Generated upon Doping. Journal of Physical Chemistry B, 2002, 106, 3872-3881.	1.2	63
920	The Infrared and Raman Spectra of Fullerene C70. DFT Calculations and Correlation with C60. Journal of Physical Chemistry A, 2002, 106, 1815-1823.	1.1	91
921	A kinetic EPR study of the dissociation of 1-carbamoyl-1-methylcyclohexa-2,5-dienyl radicals: release of aminoacyl radicals and their cyclisationElectronic supplementary information (ESI) available: Selected EPR spectra, measured radical concentrations and the corresponding rate constants at each temperature for each cyclohexadienyl. AM1 computed heats of formation and selected geometric parameters for a series of cyclohexadienyl radicals and dissociation products. UB3LYP computed energies for model aminoac. Perkin Transactions II RSC, 2002, , 1839-1843.	1.1	22
922	Temperature-Independent Rate of Electron-Transfer between a Cobalt(II) and a Ruthenium(III) of Doublet Electronic Configuration. Journal of Physical Chemistry A, 2002, 106, 11034-11044.	1.1	29
923	Density Functional Theory Study for the Cycloaddition of 1,3-Butadienes with Dimethyl Acetylenedicarboxylate. Polar Stepwise vs Concerted Mechanisms. Journal of Physical Chemistry A, 2002, 106, 952-961.	1.1	77
924	The dynamics of formation of HCl products from the reaction of Cl atoms with methanol, ethanol, and dimethyl ether. Journal of Chemical Physics, 2002, 117, 5692-5706.	1.2	69
925	Surface enhanced Raman scattering from a single molecule adsorbed on a metal particle aggregate: A theoretical study. Journal of Chemical Physics, 2002, 116, 1156-1164.	1.2	116
926	Detailed Kinetics and Thermochemistry of C2H5+ O2:Â Reaction Kinetics of the Chemically-Activated and Stabilized CH3CH2OOâ€¢Adduct. Journal of Physical Chemistry A, 2002, 106, 7276-7293.	1.1	140
927	Nitro derivatives of pyrrole, furan and 1H-tetrazole: ring or nitro bases?. New Journal of Chemistry, 2002, 26, 1567-1574.	1.4	14
928	Two Isomeric Phosphacarboranes 2,1- and 6,1-PCB8H9, the First Representatives of the 10-VertexclosoPhosphacarborane Series. Inorganic Chemistry, 2002, 41, 2817-2819.	1.9	16

#	Article	IF	Citations
929	Substituent Effects on the Bond Dissociation Enthalpies of Aromatic Amines. Journal of the American Chemical Society, 2002, 124, 11085-11092.	6.6	116
930	Oxime rearrangements: ab initio calculations and reactions in the solid state. Perkin Transactions II RSC, 2002, , 2154-2158.	1.1	2
931	Computational studies on the infrared vibrational spectra, thermodynamic properties, detonation properties, and pyrolysis mechanism of octanitrocubane. Journal of Chemical Physics, 2002, 116, 10674-10683.	1.2	127
932	A New Approach to Vibrational Analysis of Large Molecules by Density Functional Theory:â€‰ Wavenumber-Linear Scaling Method. Journal of Physical Chemistry A, 2002, 106, 3580-3586.	1.1	273
933	Global Optimization of H-Passivated Si Clusters with a Genetic Algorithm. Journal of Physical Chemistry B, 2002, 106, 6997-7004.	1.2	17
934	Structures, thermochemical properties (enthalpy, entropy and heat capacity), rotation barriers, and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxidesElectronic supplementary information (ESI) available. Structures, geometry parameters, thermochemical properties, rotation barriers and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b1/b111303h/Presented at the Bunsen Discussion on Formation and Degradation of Hydrocarbons I. Physical Chemistry Chemical Physics, 2002, 4, 3691-3703.	1.3	60
935	Quest for the Origin of Basicity:Â Initial vs Final State Effect in Neutral Nitrogen Bases. Journal of Physical Chemistry A, 2002, 106, 419-430.	1.1	73
936	Ab Initio and Improved Empirical Potentials for the Calculation of the Anharmonic Vibrational States and Intramolecular Mode Coupling ofN-Methylacetamide. Journal of Physical Chemistry A, 2002, 106, 8696-8707.	1.1	103
937	Nuclear Quantum Effects and Enzyme Dynamics in Dihydrofolate Reductase Catalysis. Journal of Physical Chemistry B, 2002, 106, 3283-3293.	1.2	178
938	Lithiumâ^'Benzene Sandwich Compounds:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 2002, 106, 9533-9537.	1.1	41
939	An Assessment of the Performance of High-Level Theoretical Procedures in the Computation of the Heats of Formation of Small Open-Shell Molecules. Journal of Physical Chemistry A, 2002, 106, 7927-7936.	1.1	109
940	Investigations of Electronic Interactions Between closo-Boranes and Triple-Bonded Substituents. Collection of Czechoslovak Chemical Communications, 2002, 67, 1061-1083.	1.0	53
941	Prototropic tautomerism of 3,5-(oxo/thioxo) derivatives of 2,7-dimethyl-1,2,4-triazepinesElectronic supplementary information (ESI) available: the B3LYP/6-31G* optimized geometries of all the structures included in Fig. 1 and the corresponding TS. See http://www.rsc.org/suppdata/nj/b1/b109397e/. New Journal of Chemistry, 2002, 26, 711-719.	1.4	13
942	High Overtones of the Câ^'H Stretching Vibrations in Anisole and Thioanisole. Journal of Physical Chemistry A, 2002, 106, 10999-11007.	1.1	26
943	Gas-Phase Chemistry of Ethyl and Vinyl Amines, Phosphines, and Arsines:â€‰ A DFT Study of the Structure and Stability of Their Cu+ Complexes. Journal of Physical Chemistry A, 2002, 106, 9306-9312.	1.1	10
944	Computational Discovery of a Novel Automerization Process for 1-Fluorocyclopropene. Organic Letters, 2002, 4, 233-235.	2.4	4
945	Computational Exploration of Rearrangements Related to the Vitamin B12-Dependent Ethanolamine Ammonia Lyase Catalyzed Transformation. Journal of the American Chemical Society, 2002, 124, 8974-8983.	6.6	37
946	Density Functional Theory Investigation of the Reaction of Isodiiodomethane with Acetylene:â€‰ Potential Utility of Isodiiodomethane for Cyclopropenation Reactions. Journal of Organic Chemistry, 2002, 67, 4619-4622.	1.7	2

#	Article	IF	Citations
947	Rate-Equilibrium Relationships in Hydride Transfer Reactions:Â The Role of Intrinsic Barriers. Journal of the American Chemical Society, 2002, 124, 4084-4092.	6.6	53
948	Quinonoid Oligothiophenes as Electron-Donor and Electron-Acceptor Materials. A Spectroelectrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 12380-12388.	6.6	109
949	1,8-Chalcogen-bridged naphthalenes. Strong carbon bases in the gas phase. New Journal of Chemistry, 2002, 26, 1747-1752.	1.4	33
950	Protonation of fluorophenols and fluoroanisoles in the gas phase: experiment and theory. Physical Chemistry Chemical Physics, 2002, 4, 2904-2910.	1.3	14
951	H-atom abstraction from thiols by C-centered radicals. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2002, 4, 2965-2974.	1.3	32
952	Density functional theory investigation of the reactions of CH2Brâ€“I, CH2Iâ€“Br, CH2Clâ€“I, and CH2Iâ€“Cl isopolyhalomethanes with ethylene. Physical Chemistry Chemical Physics, 2002, 4, 5059-5065.	1.3	6
953	An ab initio direct classical trajectory study of s-tetrazine photodissociation. Physical Chemistry Chemical Physics, 2002, 4, 2554-2559.	1.3	8
954	Intermolecular interactions of the CX3OCHO dimers, and complexes CX3OCHOâ€“n(H2O), CX3OCHOâ€“n(HO2) (Xâ€‰=â€‰H,F; nâ€‰=â€‰1,2). Physical Chemistry Chemical Physics, 2002, 4, 4902-4909.	1.3	3
955	syn-Sesquinorbornenyl carbocations and their boron analogues: an ab initio and DFT study. Perkin Transactions II RSC, 2002, , 2057-2063.	1.1	5
956	A theoretical study of hydrogen and chlorine transfer reactions from fluorine- and chlorine-substituted methanes by F3CË™ radicalsElectronic supplementary information (ESI) available: Vibrational frequencies, partition functions, hindered rotational barriers, imaginary frequencies, electronic charge distributions, polarity variation and reaction enthalpies for reactants, transition structures and products. See http://www.rsc.org/suppdata/cp/b1/b110897b/. Physical Chemistry	1.3	8
957	An electron paramagnetic resonance study of intermediates generated from aromatic aldiminesElectronic supplementary information (ESI) available: Gaussian98 or Jaguar optimised structures for precursor imines and imidoyl radicals together with their energies at all levels of theory. See http://www.rsc.org/suppdata/p2/b2/b201682f/. Perkin Transactions II RSC, 2002, , 1098-1104.	1.1	5
958	H-bridged A3H3+ (A = Si and Ge): A Ï€-ligand in organometallic chemistry. Dalton Transactions RSC, 2002, , 1857.	2.3	2
959	The dynamics of the internal phonons tris(quinolin-8-olato) aluminum(III) in crystalline Î²-phase. Journal of Chemical Physics, 2002, 116, 798-813.	1.2	30
960	Quantum-Chemical Methods for Accurate Theoretical Thermochemistry. , 2001, , 67-98.		1
961	Theoretical investigation of the effect of the rare gas matrices on the vibrational spectra of solvated molecular ions: Cu+CO. Journal of Chemical Physics, 2002, 117, 9298-9305.	1.2	22
962	FT-IR spectroscopic, AM1 and PM3 computational studies of conformation of natural products: cytisine. Talanta, 2002, 57, 609-616.	2.9	16
963	On the structure, carbonyl-stretching frequencies and relative stability of trans- and cis-[W(CO)4(Î·2-alkene)2]0/+: a theoretical and IR spectroelectrochemical study. New Journal of Chemistry, 2002, 26, 145-152.	1.4	12
964	The Effect of Substitutents on the Strain Energies of Small Ring Compounds. Journal of Organic Chemistry, 2002, 67, 2588-2599.	1.7	67

#	Article	IF	Citations
965	Prediction of Vibrational Spectra by Computational Chemistry. Ab initio Molecular Orbital Calculation of Vibrational Frequencies and infrared Intensities of Gas Phase Dichloromethane Molecules CH2Cl2, CHDCl2 and CD2Cl2.. Journal of Computer Chemistry Japan, 2002, 1, 47-58.	0.0	0
966	Origin of side bands in the FTIR spectrum of acetone oxime vinyl ether. Computational and Theoretical Chemistry, 2002, 577, 137-141.	1.5	11
967	Basic thermochemical properties of NH 2 NHOH and NH 2 ONH 2 : new potential fuels?. Computational and Theoretical Chemistry, 2002, 577, 213-218.	1.5	4
968	Thermochemistry of phosphorus fluorides: a Gaussian-3 and Gaussian-3X study. Computational and Theoretical Chemistry, 2002, 578, 221-228.	1.5	6
969	Formation and vibrational spectrum of trifluoromethyl sulfur pentafluoride, CF3SF5, a new greenhouse gas. Gaussian-2 and Gaussian-3 calculations. Computational and Theoretical Chemistry, 2002, 578, 29-34.	1.5	16
970	The C2F2O potential energy surface: a computational study. Computational and Theoretical Chemistry, 2002, 579, 155-167.	1.5	6
971	Syntheses, crystal structures and vibrational properties of Rb4Si4S10 and Rb4Si4Se10. Solid State Sciences, 2002, 4, 641-650.	1.5	9
972	Strain and Reactivity: Electrophilic Addition of Bromine and Tribromide Salts to Cyclic Allenes. Chemistry - A European Journal, 2002, 8, 967-978.	1.7	20
973	Sigmatropic Shiftamers: Fluxionality in Broken Ladderane Polymers. Angewandte Chemie - International Edition, 2002, 41, 1033-1036.	7.2	35
974	Computation of Spectroscopic Parameters in vacuo and in Condensed Phases by Methods based on the Density Functional Theory. QSAR and Combinatorial Science, 2002, 21, 105-118.	1.4	23
975	Probing the Nature of the Redox Products and Lowest Excited State of [(bpy)2Ru(Î¼-bptz)Ru(bpy)2]4+: A Resonance Raman Study. European Journal of Inorganic Chemistry, 2002, 2002, 554-563.	1.0	41
976	X-ray Crystal Structure of Triaquacopper(II) Dihydrogen 1,2,4,5- Benzenetetracarboxylate Trihydrate and Raman Spectra of Cu2+, Co2+, and Fe2+ Salts of 1,2,4,5-Benzenetetracarboxylic (Pyromellitic) Acid. European Journal of Inorganic Chemistry, 2002, 2002, 1115-1123.	1.0	47
977	Femtochemistry of Norrish Type-I Reactions: IV. Highly Excited Ketonesâ€"Experimental. ChemPhysChem, 2002, 3, 79-97.	1.0	72
978	Structure, energetics and reactivity of ternary complexes of amino acids with Cu(II) and 2,2?-bipyridine by density functional theory. A combination of radical-induced and spin-remote fragmentations. Journal of Mass Spectrometry, 2002, 37, 533-540.	0.7	41
979	C?H bond dissociation enthalpies of fluorinated formates and estimation of their rate constants for the reactions with OH radicals: A DFT study. International Journal of Chemical Kinetics, 2002, 34, 524-530.	1.0	5
980	Kinetics of hydrogen abstraction reaction between trifluoromethyl formate and OH radical: A theoretical investigation. International Journal of Chemical Kinetics, 2002, 34, 500-507.	1.0	9
981	Formation mechanism of acetaldehyde lithium enolate by reaction ofn-butyllithium with tetrahydrofuran: infrared and Raman spectroscopy and density functional theory calculations. Journal of Raman Spectroscopy, 2002, 33, 652-668.	1.2	20
982	Study of carvedilol by combined Raman spectroscopy andab initio MO calculations. Journal of Raman Spectroscopy, 2002, 33, 778-783.	1.2	25

#	Article	IF	Citations
983	Ab initio prediction of optical rotation: Comparison of density functional theory and Hartree-Fock methods for three 2,7,8-trioxabicyclo[3.2.1]octanes. Chirality, 2002, 14, 288-296.	1.3	44
984	Electronic state of small and large cavities for methane hydrate. Journal of Computational Chemistry, 2002, 23, 1071-1075.	1.5	23
985	Theoretical studies on electron delocalisation in selenourea. Journal of Chemical Sciences, 2002, 114, 223-230.	0.7	19
986	Scaling of ab initio force fields by MOLVIB. Vibrational Spectroscopy, 2002, 29, 89-95.	1.2	747
987	Infrared spectra of two sexithiophenes in neutral and doped states: a theoretical and spectroscopic study. Vibrational Spectroscopy, 2002, 30, 175-189.	1.2	7
988	Theoretical studies on the properties of acid site in isomorphously substituted ZSM-5. Journal of Molecular Catalysis A, 2002, 178, 267-274.	4.8	39
989	Quantum chemical predictions of the vibrational spectra of polyatomic molecules.. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 411-440.	2.0	168
990	3,5-Difluorobenzonitrile: ab initio calculations, FTIR and Raman spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1987-2004.	2.0	170
991	Ab initio calculations of anharmonic vibrational spectroscopy for hydrogen fluoride (HF)n (n=3, 4) and mixed hydrogen fluoride/water (HF)n(H2O)n (n=1, 2, 4) clusters. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 887-898.	2.0	42
992	Vibrational spectra and structure of benzil and its 18O- and d10-labelled derivatives: a quantum chemical and experimental study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 3127-3137.	2.0	35
993	Structural and vibrational study of the Ci(1) conformation of 18-crown-6. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 2877-2884.	2.0	8
994	The anomalous solvent effect in the vibrational spectrum of 2,3-diphenyl-cycloprop-2-enone: an experimental and theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 3139-3148.	2.0	12
995	Synthesis, structure, electronic and vibrational spectra of 9-(Diethylamino)-benzo(a)phenoxazin-7-ium-5-N-methacrylamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 3103-3111.	2.0	15
996	Dissociation behavior of ionized valeramide. International Journal of Mass Spectrometry, 2002, 214, 129-154.	0.7	16
997	Methane elimination from ionized 1-butene. International Journal of Mass Spectrometry, 2002, 214, 315-326.	0.7	5
998	Why are smaller fragments preferentially lost from radical cations at low energies and larger ones at high energies?. International Journal of Mass Spectrometry, 2002, 217, 23-44.	0.7	25
999	A theoretical study of the interaction between Ni+ and small oxygen- and nitrogen-containing bases. International Journal of Mass Spectrometry, 2002, 217, 119-129.	0.7	16
1000	The ions CH6O+ and CH7O+. International Journal of Mass Spectrometry, 2002, 217, 179-184.	0.7	6

#	Article	IF	Citations
1001	Thermochemistry and unimolecular reactivity of protonated Î±,Ï‰-aminoalcohols in the gas phase. International Journal of Mass Spectrometry, 2002, 217, 195-230.	0.7	33
1002	Adducts of NF2+ with diatomic and simple polyatomic ligands: a computational investigation on the structure, stability, and thermochemistry. International Journal of Mass Spectrometry, 2002, 216, 285-299.	0.7	24
1003	Ion rearrangement at the beginning of cluster formation: isomerization pathways and dissociation kinetics for the ionized dimethylamine dimer. International Journal of Mass Spectrometry, 2002, 218, 1-10.	0.7	19
1004	1,3-H-shift pathways in C2H4O+ and C2H4O. International Journal of Mass Spectrometry, 2002, 219, 295-303.	0.7	15
1005	Structures, thermochemistry, and infrared spectra of chloride ionâ€“fluorinated acetone complexes and neutral fluorinated acetones in the gas phase: experiment and theory. International Journal of Mass Spectrometry, 2002, 219, 593-613.	0.7	11
1006	The proton affinity of proline analogs using the kinetic method with full entropy analysis. Journal of the American Society for Mass Spectrometry, 2002, 13, 72-81.	1.2	67
1007	Differentiation of stereoisomeric steroids by reactions with phosphenium ions. Journal of the American Society for Mass Spectrometry, 2002, 13, 362-370.	1.2	15
1008	Microcanonical analysis of the kinetic method. The meaning of the â€œapparent entropyâ€• Journal of the American Society for Mass Spectrometry, 2002, 13, 435-452.	1.2	75
1009	CH3CH3+. formation from some C3H6O+. isomers according to theory. Journal of the American Society for Mass Spectrometry, 2002, 13, 1235-1241.	1.2	7
1010	Alkali chloride cluster ion dissociation examined by the kinetic method: Heterolytic bond dissociation energies, effective temperatures, and entropic effects. Journal of the American Society for Mass Spectrometry, 2002, 13, 1388-1395.	1.2	21
1011	Heats of formation for AlH, AlOH, OAlH and OAlOH and their monocations. Computational and Theoretical Chemistry, 2002, 581, 17-29.	1.5	39
1012	Density functional study of the binding of the cyclen-coordinated M(II) (M=Zn, Cu, Ni) complexes to the DNA base. Why is Zn better to bind?. Computational and Theoretical Chemistry, 2002, 581, 203-213.	1.5	27
1013	The adsorption of ethylene on the (110) surfaces of copper, silver and platinum: a DFT study. Computational and Theoretical Chemistry, 2002, 582, 159-169.	1.5	24
1014	The bonding of nitrosonium ion to sulfur in models of cytochrome c -type biomolecules: an ab initio computational study. Computational and Theoretical Chemistry, 2002, 582, 27-38.	1.5	2
1015	The hydration effect on the uracil frequencies: an experimental and quantum chemical study. Computational and Theoretical Chemistry, 2002, 585, 69-92.	1.5	66
1016	Conformations, vibrational frequencies and Raman intensities of short-chain fatty acid methyl esters using DFT with 6-31G(d) and Sadlej pVTZ basis sets. Computational and Theoretical Chemistry, 2002, 586, 91-110.	1.5	33
1017	Vibrational modes of diacetylenic monomers and the effect of the substituents: a density functional study. Computational and Theoretical Chemistry, 2002, 586, 57-70.	1.5	1
1018	Density functional theory characterization of the structure and gas-phase, mid-infrared absorption spectrum of 2-azido-N,N-dimethylethanamine (DMAZ). Computational and Theoretical Chemistry, 2002, 587, 199-218.	1.5	20

#	Article	IF	Citations
1019	Reactions of oxiranylidene and dimethyloxiranylidene, and their generation by retro Dielsâ€“Alder-type reactions: a computational study. Computational and Theoretical Chemistry, 2002, 593, 79-91.	1.5	6
1020	Structures and vibrational frequencies of ethylphosphine: post-Hartreeâ€“Fock and density functional theory study. Computational and Theoretical Chemistry, 2002, 594, 9-17.	1.5	1
1021	Anharmonicity effects on zero point energies of weakly bound molecular clusters. Computational and Theoretical Chemistry, 2002, 591, 11-18.	1.5	18
1022	Accurate scaling of the vibrational spectra of aniline and several derivatives. Computational and Theoretical Chemistry, 2002, 593, 101-131.	1.5	100
1023	A density functional theory analysis of Raman and IR spectra of 2-adamantanone. Computational and Theoretical Chemistry, 2002, 594, 79-88.	1.5	25
1024	Further studies on the rotational barriers of Carbamates. An NMR and DFT analysis of the solvent effect for Cyclohexyl N,N-dimethylcarbamate. Computational and Theoretical Chemistry, 2002, 594, 199-206.	1.5	24
1025	How different is azulene from tropylium cation and cyclopentadienyl anion? A force field and vibrational study. Computational and Theoretical Chemistry, 2002, 618, 59-64.	1.5	5
1026	A Gaussian-3 study of N7+ and N7â^' isomers. Computational and Theoretical Chemistry, 2002, 617, 121-131.	1.5	15
1027	Comparison of calculated structural parameters and infrared spectra with experimental data for dimeric dibenzyl carbamic acid. Computational and Theoretical Chemistry, 2002, 618, 101-108.	1.5	14
1028	Computational chemistry study of the environmentally important acid-catalyzed hydrolysis of atrazine and related 2-chloro-s-triazines. Pest Management Science, 2002, 58, 759-768.	1.7	12
1029	Preparation of the tricyclo[5.3.1.13,9]dodeca-1,5-diyl dication: attempts to prepare a novel Âµ-H cation. Journal of Physical Organic Chemistry, 2002, 15, 36-47.	0.9	7
1030	Theoretical studies on the S?N interaction in sulfinamides. Journal of Physical Organic Chemistry, 2002, 15, 197-203.	0.9	27
1031	Theoretical study of the gas-phase decomposition of neutral Î±-amino acid ethyl esters. Part 1-The elimination ofN,N-dimethylglycine ethyl ester and ethyl 1-piperidineacetate. Journal of Physical Organic Chemistry, 2002, 15, 413-419.	0.9	12
1032	An ab initio/Rice-Ramsperger-Kassel-Marcus study of photodissociation of carbonyl cyanide. International Journal of Quantum Chemistry, 2002, 90, 566-574.	1.0	6
1033	Interaction of acetonitrile with alkaline metal cations: A density functional, coupled-cluster, and quadratic configuration interaction study. International Journal of Quantum Chemistry, 2002, 86, 356-367.	1.0	21
1034	Theoretical quantum chemical study of benzoic acid: Geometrical parameters and vibrational wavenumbers. International Journal of Quantum Chemistry, 2002, 89, 1-24.	1.0	37
1035	Investigation of the frequency-dispersion effects on the Raman spectra of small polyenes. International Journal of Quantum Chemistry, 2002, 89, 341-348.	1.0	14
1036	Study of phenothiazine andN-methyl phenothiazine by infrared, raman,1H-, and13C-NMR spectroscopies. International Journal of Quantum Chemistry, 2002, 89, 147-171.	1.0	27

#	Article	IF	Citations
1037	Explicitly correlated SCF study of anharmonic vibrations in (H2O)2. International Journal of Quantum Chemistry, 2002, 90, 1414-1420.	1.0	3
1038	Structure and relative energies of the conformers ofn-butyl cyanide and 5-hexynenitrile. International Journal of Quantum Chemistry, 2002, 90, 1440-1447.	1.0	16
1039	Theoretical studies on Sâ€“N interactions in sulfonamides. Tetrahedron, 2002, 58, 1759-1764.	1.0	58
1040	N-Chloro-N,Nâ€²,Nâ€²-tris(ethoxycarbonyl)hydrazine and N,N-dichloro-Nâ€²,Nâ€²-bis(ethoxycarbonyl)hydrazine: synthesis, stability and reactions with nucleophiles. Tetrahedron, 2002, 58, 2085-2090.	1.0	5
1041	Electronic structure of N -sulfonylimines. Tetrahedron, 2002, 58, 10335-10339.	1.0	8
1042	Regio- and stereoisomeric composition of the product mixture in the Dielsâ€“Alder reaction of dicyclopentadiene with bicyclononadiene: a NMR and DFT quantum chemical investigation. Tetrahedron, 2002, 58, 10447-10453.	1.0	6
1043	Torsion potentials and electronic structure of trifluoromethoxy- and trifluoromethylthiobenzene: an ab initio study. Journal of Fluorine Chemistry, 2002, 113, 227-237.	0.9	28
1044	Ab initio and density functional theory study of the enthalpies of formation of F2SOx and FClSOx (x=1, 2). Journal of Fluorine Chemistry, 2002, 116, 135-141.	0.9	15
1045	Artificial neural network study for the estimation of the Câ€“H bond dissociation enthalpies. Journal of Fluorine Chemistry, 2002, 116, 163-171.	0.9	27
1046	Large-amplitude motion in 1,4-cyclohexadiene and 1,4-dioxin: theoretical background for joint treatment of spectroscopic, electron diffraction and ab initio data. Journal of Molecular Structure, 2002, 607, 163-174.	1.8	34
1047	Conformational stabilization of phthalan: physical origin of tiny ring-puckering barrier. Journal of Molecular Structure, 2002, 609, 159-167.	1.8	9
1048	Infrared absorption spectra and structures of zwitterions of glycyl-l-alanine and its N-deuterated isotopomer in a KBr matrix. Journal of Molecular Structure, 2002, 613, 175-188.	1.8	28
1049	Remarkable aromatic substitution by a 1,5-diradical. Tetrahedron Letters, 2002, 43, 1927-1929.	0.7	5
1050	Density functional study of the adsorption of 1,4-cyclohexadiene on Pt(111): origin of the Câ€“H stretch red shift. Surface Science, 2002, 513, 315-327.	0.8	27
1051	Solvent dependence of structure and electronic properties in the ground and first excited singlet state of 4-dimethylamino-4â€²-nitrostilbene (DANS) â€“ semiempirical calculations. Chemical Physics, 2002, 277, 257-270.	0.9	24
1052	In situ FTIR study of 2-chloropyridine adsorbed on Au(111) and Au(110) electrodes. Electrochimica Acta, 2002, 47, 2921-2925.	2.6	6
1053	An ab initio study of potential energy surfaces of CH3COCN dissociation on the low-lying states. Chemical Physics Letters, 2002, 351, 9-17.	1.2	12
1054	On the evaluation of quasi-thermodynamic magnitudes from rate constant values. Influence of the variational and tunnelling contributions. Chemical Physics Letters, 2002, 353, 154-162.	1.2	8

#	Article	IF	Citations
1055	Câ€“Hâ‹¯O bonded dimers in 2-methoxy-benzaldehyde studied by X-ray crystallography, vibrational spectroscopy, and ab initio calculations. Chemical Physics Letters, 2002, 356, 318-324.	1.2	58
1056	Ab initio study of reaction of dimethyl sulfoxide (DMSO) with OH radical. Chemical Physics Letters, 2002, 356, 490-496.	1.2	38
1057	Density functional theory study on the geometric, electronic and vibrational structures of alkali metal porphyrin complexes. Chemical Physics Letters, 2002, 361, 106-114.	1.2	28
1058	Thermodynamic properties of chloroacetylene, dichloroacetylene, ethynyl radical, and chloroethynyl radical. Chemical Physics Letters, 2002, 362, 445-452.	1.2	11
1059	An efficient implementation of second analytical derivatives for density functional methods. Chemical Physics Letters, 2002, 362, 511-518.	1.2	561
1060	An experimental study of the mechanism and branching ratio for the reaction between methyl formate and chlorine atoms. Chemical Physics Letters, 2002, 365, 267-278.	1.2	5
1061	Thermochemical functions for gas-phase, 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX), its condensed phases, and its larger reaction products. Combustion and Flame, 2002, 130, 185-203.	2.8	54
1062	Substituent effects on the Sâ€“H bond dissociation energies of thiophenolsElectronic supplementary information (ESI) available: detailed results of the bond lengths, charge and spin distributions, and vibration frequencies. See http://www.rsc.org/suppdata/p2/b2/b201003h/. Perkin Transactions II RSC, 2002, , 1223-1230.	1.1	41
1063	Isomerization of 2,3-Dihydrofuran and 5-Methyl-2,3-dihydrofuran:Â Quantum Chemical and Kinetics Calculations. Journal of Physical Chemistry A, 2002, 106, 1026-1034.	1.1	14
1064	IR and Theoretical Studies of Monocarbonyl Ni Complexes Formed by Adsorption of CO at Low Pressure on Silica-Supported NiIIIons. Journal of the American Chemical Society, 2002, 124, 7210-7217.	6.6	32
1065	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 564-572.	0.3	12
1066	Measurement of the Metal Surface Acidity/Electronegativity of Pt(110). Catalysis Letters, 2002, 83, 43-48.	1.4	4
1067	Synthesis, IR Spectra, and Steric Structure of Macrocycles Derived from Pyrimidine Compounds. Russian Journal of General Chemistry, 2002, 72, 1625-1632.	0.3	5
1068	Title is missing!. Russian Journal of General Chemistry, 2002, 72, 1894-1900.	0.3	2
1069	Phosphaborane chemistry. Syntheses and calculated molecular structures of mono- and di-chloro derivatives of 1,2-diphospha-closo-dodecaborane(10). Dalton Transactions RSC, 2002, , 2954-2959.	2.3	15
1070	Molecular, Thermodynamic, and Kinetic Parameters of the Free Radical C2H5 Â· in the Gas Phase. Russian Journal of General Chemistry, 2003, 73, 75-84.	0.3	1
1071	Density Functional Theory Calculations of Normal Modes and Infrared Intensities for Tetraazaporphin. Journal of Applied Spectroscopy, 2003, 70, 201-207.	0.3	5
1072	Title is missing!. Structural Chemistry, 2003, 14, 337-348.	1.0	23

#	Article	IF	Citations
1073	Steric and Electronic Structure of C6H5XCF3 Molecules (X = O or S): A Quantum-Chemical Study. Russian Journal of General Chemistry, 2003, 73, 229-239.	0.3	4
1074	Title is missing!. Russian Chemical Bulletin, 2003, 52, 1312-1325.	0.4	11
1075	Title is missing!. Russian Journal of General Chemistry, 2003, 73, 731-742.	0.3	4
1076	Calculation of Chlorin IR Spectrum by Density Functional Theory. Chemistry of Natural Compounds, 2003, 39, 540-548.	0.2	5
1077	Geometry Optimization and Quantum-Chemical Calculations of Normal Vibrations for Methyl-N-methylurethane and Methyl-N-(a)Naphthylurethane. Journal of Structural Chemistry, 2003, 44, 388-396.	0.3	5
1078	Calculation of Second- and Higher-Order Force Constants Including Electron Correlation Effects and Hartree-Fock Force Constant Scaling. Journal of Structural Chemistry, 2003, 44, 538-545.	0.3	0
1079	Force Constant Transportability Problem. Journal of Structural Chemistry, 2003, 44, 970-974.	0.3	1
1080	Molecular structure, conformational mobility, vibrational spectra, and thermochemistry of peroxyacetic acid: an ab initio and density functional study. Russian Chemical Bulletin, 2003, 52, 1908-1919.	0.4	5
1081	Thermal isomerization of acetylnitrene: a quantum-chemical study. Russian Chemical Bulletin, 2003, 52, 2328-2333.	0.4	18
1082	Thermochemical Study of the Methoxy- and Dimethoxyphenol Isomers. Journal of Chemical & Engineering Data, 2003, 48, 669-679.	1.0	50
1083	What Is the Origin of the Contrathermodynamic Behavior in Methyl Radical Addition to Alkynes versus Alkenes?. Journal of Physical Chemistry A, 2003, 107, 6082-6090.	1.1	43
1084	Bis(pyrazol-1-yl)acetates as Tripodal Heteroscorpionate Ligands in Iron Chemistry:Â Syntheses and Structures of Iron(II) and Iron(III) Complexes with bpza, bdmpza, and bdtbpza Ligands. Inorganic Chemistry, 2003, 42, 7182-7188.	1.9	85
1085	Ab Initio Calculations for Hydrocarbons:Â Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. Journal of Physical Chemistry A, 2003, 107, 9147-9159.	1.1	170
1086	Structure and reactivity of hydrocarbon radical cations. Advances in Physical Organic Chemistry, 2003, 38, 87-109.	0.5	5
1087	The vibrational spectra of furoxan and dichlorofuroxan: A comparative theoretical study using density functional theory and local electron correlation methods. Physical Chemistry Chemical Physics, 2003, 5, 2001.	1.3	32
1088	Computational studies of Cu(II)[peptide] binding motifs: Cu[HGGG] and Cu[HG] as models for Cu(II) binding to the prion protein octarepeat region. Journal of Biological Inorganic Chemistry, 2003, 8, 53-65.	1.1	65
1089	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. Tetrahedron, 2003, 59, 9167-9171.	1.0	32
1090	A theoretical investigation on DPPH radical-Scavenging mechanism of edaravone. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3789-3792.	1.0	63

#	Article	IF	Citations
1091	DFT study on the electrophilic aromatic substitution catalyzed byÂLewisÂacids. Journal of Catalysis, 2003, 220, 333-346.	3.1	13
1092	Cyclization Triggered by Deprotonation: The Gas-Phase Acidity of 1,8-Chalcogen-Bridged Naphthalenes. ChemPhysChem, 2003, 4, 830-837.	1.0	4
1093	New Insights into the Jahn-Teller Effect through ab initio Quantum-Mechanical/Molecular-Mechanical Molecular Dynamics Simulations of CuII in Water. ChemPhysChem, 2003, 4, 931-943.	1.0	91
1094	Gas-Phase Reactivity of Uracil, 2-Thiouracil, 4-Thiouracil, and 2,4-Dithiouracil towards the Cu+ Cation: A DFT Study. ChemPhysChem, 2003, 4, 1011-1016.	1.0	45
1095	Gas-Phase Chemistry of Ethynylamine, -Phosphine and -Arsine. Structure and Stability of their Cu+ and Ni+ Complexes. ChemPhysChem, 2003, 4, 72-78.	1.0	5
1096	Quasiharmonic Vibrations of Water, Water Dimer, and Liquid Water from Principal Component Analysis of Quantum or QM/MM Trajectories. ChemPhysChem, 2003, 4, 382-384.	1.0	37
1097	Helicoid Shiftamers for the Transport ofÏ€-Clumps and Charges. Helvetica Chimica Acta, 2003, 86, 3525-3532.	1.0	9
1098	Fast approximate methods for calculating nucleic acid base pair interaction energies. Journal of Computational Chemistry, 2003, 24, 57-67.	1.5	30
1099	Ab initiostudy on the structures of fluorinated formates and hydrogen abstraction reaction with OH radical. Journal of Computational Chemistry, 2003, 24, 396-407.	1.5	2
1100	Concerning the reaction between singlet nitrenium ions and water: A computational investigation on competitive reaction paths. Journal of Computational Chemistry, 2003, 24, 547-564.	1.5	5
1101	A computational study of conformational interconversions in 1,4-dithiacyclohexane (1,4-dithiane). Journal of Computational Chemistry, 2003, 24, 909-919.	1.5	17
1102	Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. Journal of Computational Chemistry, 2003, 24, 1120-1131.	1.5	79
1103	Ab initio studies for the photodissociation mechanism of hydroxyacetone. Journal of Computational Chemistry, 2003, 24, 931-938.	1.5	10
1104	Direct hydroxide attack is a plausible mechanism for amidase antibody 43C9. Journal of Computational Chemistry, 2003, 24, 1371-1377.	1.5	14
1105	Ab initiostudy of the mechanism of the atmospheric reaction: NO2+ O3â†' NO3+ O2. Journal of Computational Chemistry, 2003, 24, 1657-1663.	1.5	53
1106	Acidity of Substituted Benzenesâ^' An Ab Initio Study of the Influence of Methoxy, Trifluoromethyl and Trifluoromethoxy Groups by a Novel Trichotomy Formula. European Journal of Organic Chemistry, 2003, 2003, 3777-3783.	1.2	14
1107	On the Mechanism of the Oxygen Transfer to Sulfoxides by (Peroxo)[tris(hydroxyalkyl)amine]TiIV Complexesâ^' Evidence for a Metal-Template-Assisted Process. European Journal of Organic Chemistry, 2003, 2003, 507-511.	1.2	18
1108	Raman spectra of putrescine, spermidine and spermine polyamines and theirN-deuterated andN-ionized derivatives. Journal of Raman Spectroscopy, 2003, 34, 357-366.	1.2	22

#	Article	IF	Citations
1109	Density functional and vibrational spectroscopic analysis of Î²-carotene. Journal of Raman Spectroscopy, 2003, 34, 413-419.	1.2	89
1110	Density functional andab initio studies of the molecular structure and vibrational spectra of novelO,O?-diethyl-N-(?-aryloxyacetyl)thiophosphorylhydrazine herbicides. Journal of Raman Spectroscopy, 2003, 34, 892-901.	1.2	2
1111	Anharmonic thermochemistry of cyclopentadiene derivatives. International Journal of Chemical Kinetics, 2003, 35, 453-463.	1.0	16
1112	Kinetics and mechanism for the thermal chlorination of chloroform in the gas phase: Inclusion of HCl elimination from CHCl3. International Journal of Chemical Kinetics, 2003, 35, 647-660.	1.0	14
1116	Configurational stability of chiral lithiated cyclopropylnitriles: A density functional study. Chirality, 2003, 15, 340-347.	1.3	31
1117	Vibrational and Quantum-Chemical Study of Pushâ€“Pull Chromophores for Second-Order Nonlinear Optics from Rigidified Thiophene-Based Ï€-Conjugating Spacers. Chemistry - A European Journal, 2003, 9, 3670-3682.	1.7	57
1118	Gas-Phase Activation and Reaction Dynamics of Chiral Ionâ€“Dipole Complexes. Chemistry - A European Journal, 2003, 9, 5274-5282.	1.7	7
1119	Facial Selectivity of the (R)-1,3-Dimethyl-1-Cyclohexyl Cation in the Gas Phase. Chemistry - A European Journal, 2003, 9, 5396-5403.	1.7	3
1120	The Effect of Ring Nitrogen Atoms on the Homolytic Reactivity of Phenolic Compounds: Understanding the Radical-Scavenging Ability of 5-Pyrimidinols. Chemistry - A European Journal, 2003, 9, 4997-5010.	1.7	94
1121	Electron Density Investigation of a Pushâ€“Pull Ethylene (C14H24N2O2â‹…H2O) by X-ray Diffraction atT= 21 K. Chemistry - A European Journal, 2003, 9, 5528-5537.	1.7	38
1122	The Final Steps of the Oppolzer Cyclization: Mechanism of the Insertion of Alkenes into Allylpalladium(II) Complexes. Chemistry - A European Journal, 2003, 9, 96-105.	1.7	19
1123	Substituent Effects on Oï£¿H Bond Dissociation Enthalpies and Ionization Potentials of Catechols: A DFT Study and Its Implications in the Rational Design of Phenolic Antioxidants and Elucidation of Structureâ€“Activity Relationships for Flavonoid Antioxidants. Chemistry - A European Journal, 2003, 9, 502-508.	1.7	204
1124	Criteria for the Elucidation of the Pseudopericyclic Character of the Cyclization of (Z)-1,2,4,6-Heptatetraene and Its Heterosubstituted Analogues: Magnetic Properties and Natural Bond Orbital Analysis. Chemistry - A European Journal, 2003, 9, 1837-1843.	1.7	66
1125	Equilibrium and Kinetic Deuterium Isotope Effects on the Hetero-Dielsâ€“Alder Addition of Sulfur Dioxide. Angewandte Chemie - International Edition, 2003, 42, 3924-3927.	7.2	13
1126	Dicyanocarbodiimide and Trinitreno-s-triazine Generated by Consecutive Photolysis of Triazido-s-triazine in a Low-Temperature Nitrogen Matrix. Angewandte Chemie - International Edition, 2003, 42, 5206-5209.	7.2	30
1127	Breaking Down Barriers: The Liaison Between Sigmatropic Shifts, Electrocyclic Reactions, and Three-Center Cations. Angewandte Chemie - International Edition, 2003, 42, 5877-5882.	7.2	20
1128	Theoretical and pH dependent surface enhanced Raman spectroscopy study on caffeine. Biopolymers, 2003, 72, 25-37.	1.2	68
1129	Numerical simulations of Raman spectra of guanine-cytosine Watson-Crick and protonated Hoogsteen base pairs. Biopolymers, 2003, 72, 339-344.	1.2	15

#	Article	IF	Citations
1130	Classical and QM/MM molecular dynamics simulations of Co2+ in water. Chemical Physics, 2003, 295, 63-70.	0.9	22
1131	Vibrational spectrum and molecular structure of [Cu(NH3)5](ClO4)2. Chemical Physics Letters, 2003, 381, 329-334.	1.2	8
1132	Multiphoton ionization and zero kinetic energy photoelectron spectroscopy of the 1-naphthol(H2O) cluster. Chemical Physics Letters, 2003, 381, 346-353.	1.2	7
1133	CO2 adsorption on carbonaceous surfaces: a combined experimental and theoretical study. Carbon, 2003, 41, 29-39.	5.4	111
1134	Theoretical studies on structures and reactivity of 8-hydroxyquinoline and its one-water complex in the ground and excited states. Chemical Physics Letters, 2003, 367, 637-644.	1.2	28
1135	A combined CASSCF and TDDFT study on the structures and properties of formyl cyanide in low-lying electronic states. Chemical Physics Letters, 2003, 369, 570-578.	1.2	9
1136	Conformations of nitro-substituted spiropyran and merocyanine studied by low-temperature matrix-isolation infrared spectroscopy and density-functional-theory calculation. Chemical Physics Letters, 2003, 370, 460-468.	1.2	75
1137	Gas-phase energy differences between the Z and E rotamers and the rotational barrier heights of methyl formate and trifluromethyl formate: an ab initio study. Chemical Physics Letters, 2003, 373, 182-190.	1.2	6
1138	Scaled quantum mechanical computations of vibrational spectra of organoelement molecules, containing the atoms P, S, and Cl. Chemical Physics Letters, 2003, 377, 658-662.	1.2	53
1139	Double perturbation theory: a powerful tool in computational coordination chemistry. Coordination Chemistry Reviews, 2003, 238-239, 83-126.	9.5	101
1140	Quantum chemical calculations and vibrational analysis of compounds containing carbonâ€“phosphorus multiple and single bonds. Computational and Theoretical Chemistry, 2003, 639, 53-67.	1.5	9
1141	l-2-Hydroxypropionic acid in aqueous solutionâ€”a vibrational spectroscopic and computational study. Computational and Theoretical Chemistry, 2003, 666-667, 159-162.	1.5	7
1142	Sâ€“H proton dissociation enthalpies of thiophenolic cation radicals: a DFT study. Computational and Theoretical Chemistry, 2003, 663, 167-174.	1.5	42
1143	Adsorption states of heptyl viologen on an Au(111) electrode surface studied by infrared reflection absorption spectroscopy. Journal of Electroanalytical Chemistry, 2003, 550-551, 149-159.	1.9	17
1144	The kinetic method reveals secondary deuterium isotope effects on the proton affinity and gas-phase basicity of glycine and alanine methyl esters. International Journal of Mass Spectrometry, 2003, 230, 175-183.	0.7	14
1145	Modeling the framework stability and catalytic activity of pure and transition metal-doped zeotypes. Journal of Solid State Chemistry, 2003, 176, 496-529.	1.4	50
1146	Experimental and theoretical investigations for the tandem alkylationâ€“isomerization reactions between unsaturated carboxylic acids and allyl halides. Tetrahedron, 2003, 59, 6233-6239.	1.0	20
1147	Amino acids as selective sulfonamide acylating agents. Tetrahedron, 2003, 59, 7473-7480.	1.0	11

#	Article	IF	Citations
1148	Vibrational study of pushâ€“pull chromophores for second-order non-linear optics derived from rigidified thiophene Ì€-conjugating spacers. Journal of Molecular Structure, 2003, 651-653, 151-158.	1.8	34
1149	Structure and vibrational spectra of benzidine. Journal of Molecular Structure, 2003, 651-653, 571-577.	1.8	13
1150	Structure and molecular vibrations of dimethylglyoxime. Journal of Molecular Structure, 2003, 651-653, 615-619.	1.8	8
1151	Theoretical description of the Raman spectrum of a vinylene-bridged quaterthiophene oligomer. Journal of Molecular Structure, 2003, 651-653, 657-664.	1.8	9
1152	UVâ€“Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. Journal of Molecular Structure, 2003, 651-653, 665-673.	1.8	10
1153	Structural characterization of two novel potential anticholinesterasic agents. Journal of Molecular Structure, 2003, 657, 191-198.	1.8	10
1154	Vibrational and structural analysis of (hydroxypyridin-3-yl-methyl)phosphonic acid. Journal of Molecular Structure, 2003, 658, 229-239.	1.8	1
1155	Theoretical determination of Î´ in 18+Î´ organometallic complexes. Journal of Organometallic Chemistry, 2003, 677, 96-100.	0.8	4
1156	Two-ring vibrational modes on silica surfaces investigated via fully coordinated nanoclusters. Surface Science, 2003, 539, L554-L559.	0.8	18
1157	Enhancement of 1,2-dehydration of alcohols by alkali cations and protons: a model for dehydration of carbohydrates. Journal of Analytical and Applied Pyrolysis, 2003, 66, 3-27.	2.6	55
1158	Theoretical study of cation substitution in trioctahedral sheet of phyllosilicates. An effect on inner OH group. Computational and Theoretical Chemistry, 2003, 620, 1-8.	1.5	23
1159	Theoretical studies on the conformational preferences of 1,3-diazabuta-1,3-dienes. Computational and Theoretical Chemistry, 2003, 640, 1-12.	1.5	11
1160	Ab initio MO study on the S1â†S0 transitions of polychlorinated dibenzo-p-dioxins. Computational and Theoretical Chemistry, 2003, 622, 229-237.	1.5	12
1161	An ab initio study of the electrostatics of protonated amines: application to the molecular mechanics (MM3) force field. Computational and Theoretical Chemistry, 2003, 623, 145-158.	1.5	6
1162	Changes in the vibrational characteristics arising from the hydrogen bonding between N2 and HNO3. Ab initio and DFT studies. Computational and Theoretical Chemistry, 2003, 623, 179-184.	1.5	5
1163	Study of the influence of the non-pyridyl nitrogen hybridisation on the stability of axially chiral analogues of 4-(dimethylamino)pyridine (DMAP). Computational and Theoretical Chemistry, 2003, 623, 263-276.	1.5	26
1164	Ab initio, DFT and experimental studies on the IR spectra and structure of propanedinitrile (malononitrile) and its carbanion. Computational and Theoretical Chemistry, 2003, 625, 207-214.	1.5	18
1165	Scale factors for Cî€†O vibrational frequencies in organometallic complexes. Computational and Theoretical Chemistry, 2003, 625, 215-220.	1.5	33

#	Article	IF	Citations
1166	Ab initio conformational study of caffeic acid. Computational and Theoretical Chemistry, 2003, 625, 265-275.	1.5	44
1167	A Gaussian-3 study of the C3H6S isomers and the dissociation channels of diradical CH2CH2SCH2 and its radical cation CH2CH2SCH2+. Computational and Theoretical Chemistry, 2003, 629, 237-250.	1.5	7
1168	Computational estimates of the gas-phase acidities of dihydroxybenzoic acid radical cations and their corresponding neutral species. Computational and Theoretical Chemistry, 2003, 629, 223-235.	1.5	30
1169	On the link atom distance in the ONIOM scheme. An harmonic approximation analysis. Computational and Theoretical Chemistry, 2003, 632, 61-69.	1.5	20
1170	Theoretical investigation of the conformational behaviour of 3-monosubstituted 2-methylpropenes. Computational and Theoretical Chemistry, 2003, 637, 43-54.	1.5	11
1171	A proposal of the source and the evolution of the bubble in the glass melts. Molecular orbital and molecular dynamics studies. Computational and Theoretical Chemistry, 2003, 635, 91-103.	1.5	0
1172	Density functional investigation on copper carbonyl complexes. Computational and Theoretical Chemistry, 2003, 637, 101-107.	1.5	12
1173	A computational investigation on the Lewis acidity of fluoro- and chloronitrenium ions. Computational and Theoretical Chemistry, 2003, 635, 221-227.	1.5	5
1174	The formation and isomerization of 3-amino-2-butenenitrile (diacetonitrile) and its anion, followed by IR spectra, ab initio and DFT force field calculations. Computational and Theoretical Chemistry, 2003, 636, 167-183.	1.5	8
1175	Structure and vibrational spectra of p-methylaniline: Hartree-Fock, MP2 and density functional theory studies. Computational and Theoretical Chemistry, 2003, 637, 155-169.	1.5	216
1176	Molecular conformation, vibrational spectra and solvent effect studies on glycyl-L-alanine zwitterion by ab initio method. Computational and Theoretical Chemistry, 2003, 638, 79-90.	1.5	5
1177	Studies on the isomerization of acetone CH3COCH3. Computational and Theoretical Chemistry, 2003, 638, 215-228.	1.5	9
1178	Spectroscopic and theoretical study of the 1,2,3-Triazole-4,5-dicarbonitrile anion and its lithium ion pairs. Solid State Ionics, 2003, 156, 129-139.	1.3	40
1179	X-ray, MP2 and DFT studies of the structure and vibrational spectra of trigonellinium chloride. Chemical Physics, 2003, 289, 201-219.	0.9	21
1180	Development of a detailed high-pressure reaction model for methane/methanol mixtures under pyrolytic and oxidative conditions and comparison with experimental data. Fuel Processing Technology, 2003, 83, 111-145.	3.7	40
1181	Why CH3CH3+Â· formation competes with hÂ· loss from CCCO C3H6O+Â· isomers. Journal of the American Society for Mass Spectrometry, 2003, 14, 136-142.	1.2	6
1182	Strategic use of amino acid N-substituents to limit Î±-carbon-centered radical formation and consequent loss of stereochemical integrity. Tetrahedron: Asymmetry, 2003, 14, 2919-2926.	1.8	21
1183	Why B-ring is the active center for genistein to scavenge peroxyl radical: A DFT study. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 909-911.	1.0	31

#	Article	IF	Citations
1184	FT-IR and FT-Raman study of selected pyridinephosphonocarboxylic acids. Vibrational Spectroscopy, 2003, 31, 295-311.	1.2	43
1185	Vibrational and quantum-chemical study of pH dependent molecular structures of (hydroxypyridin-4-yl-methyl)phosphonic acid. Vibrational Spectroscopy, 2003, 33, 83-92.	1.2	4
1186	Density functional theory study of vibrational spectra of acridine and phenazine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 245-253.	2.0	65
1187	Ab initio prediction of the vibrational spectrum of the hydrogen bonded complex O 2 Nâ‹¯HONO 2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1919-1927.	2.0	2
1188	IR spectral and structural changes caused by the conversion of 3-hydroxybenzaldehyde into the oxyanion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1541-1548.	2.0	10
1189	Vibrational frequencies and structure of 2-thiouracil by Hartreeâ€“Fock, post-Hartreeâ€“Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2473-2486.	2.0	56
1190	Experimental and computational studies of the structure and vibrational spectra of pyridinium-betaine of squaric acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1805-1813.	2.0	11
1191	Calculated gas-phase infrared spectra of imidazo[1,2-a]pyrazinediones derived from alanine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 1867-1879.	2.0	4
1192	A coupled-cluster study of the structure and vibrational spectra of pyrazole and imidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2009-2025.	2.0	19
1193	Structure and vibrational frequencies of 2-butanimine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2593-2601.	2.0	1
1194	The conversion of phenylpropanedinitrile (phenylmalononitrile) into the carbanion, followed by IR spectra, ab initio and DFT force field calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 3041-3052.	2.0	26
1195	Experimental and computational studies of the structure and vibrational spectra of 2-[5,5-dimethyl-3-(2-phenyl-vinil)-cyclohex-2-enylidene]-malononitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 3325-3335.	2.0	16
1196	The water-solvated methanol ion and its isomers: experiment and theory. International Journal of Mass Spectrometry, 2003, 222, 41-48.	0.7	3
1197	On the acidity of cyclopropanaphthalenes. International Journal of Mass Spectrometry, 2003, 222, 11-26.	0.7	9
1198	Involvement of salt bridges in a novel gas phase rearrangement of protonated arginine-containing dipeptides which precedes fragmentation. International Journal of Mass Spectrometry, 2003, 222, 229-242.	0.7	67
1199	Loss of HF from C2H4FO+ produced from 2-hydroxy-2-trifluoromethylpropanoic acid upon electron ionization. International Journal of Mass Spectrometry, 2003, 222, 1-9.	0.7	8
1200	Theoretical calculation of isotope effects, kinetic energy release and effective temperatures for alkylamines. International Journal of Mass Spectrometry, 2003, 225, 233-248.	0.7	12
1201	Sequential bond energies of Pt+(NH3)x (x=1â€“4) determined by collision-induced dissociation and theory. International Journal of Mass Spectrometry, 2003, 227, 47-62.	0.7	12

#	Article	IF	Citations
1202	Binding energies of Cu+ to saturated and Î±,Î²-unsaturated alkanes, silanes and germanes. International Journal of Mass Spectrometry, 2003, 227, 401-412.	0.7	26
1203	How does chlorine substitution on acetonitrile affect the internal SN2 isomerization of proton-bound pairs (ClCH2CN)(ROH)H+ (R=CH3, C2H5, C3H7)?. International Journal of Mass Spectrometry, 2003, 227, 471-478.	0.7	4
1204	Gas-phase basicity and enantiodiscrimination of some phosphorous-containing Î±-amino acid mimics. International Journal of Mass Spectrometry, 2003, 228, 349-358.	0.7	16
1205	How ergodic is the fragmentation of the pyridine cation?. International Journal of Mass Spectrometry, 2003, 228, 389-402.	0.7	15
1206	Berylliumâ€“helium cations: computational evidence for a large class of thermodynamically stable species. International Journal of Mass Spectrometry, 2003, 228, 415-427.	0.7	19
1207	Ion/ion reactions of multiply charged nucleic acid anions: electron transfer, proton transfer, and ion attachment. International Journal of Mass Spectrometry, 2003, 228, 577-597.	0.7	27
1208	Theoretical studies of methane elimination from C4H9+ and H2 elimination from C3H7+. International Journal of Mass Spectrometry, 2003, 228, 955-967.	0.7	10
1209	Adsorption of alcohols on Î³-alumina (1 1 0 C). Journal of Molecular Catalysis A, 2003, 193, 157-164.	4.8	62
1210	Theoretical study of the gas-phase decomposition of neutral Î±-amino acid ethyl esters. Part 2-Elimination of ethyl picolinate and ethyl 1-methylpipecolinate. Journal of Physical Organic Chemistry, 2003, 16, 166-174.	0.9	13
1211	Electronic structure ofN-sulfenylimines. Journal of Physical Organic Chemistry, 2003, 16, 183-188.	0.9	11
1212	A theoretical approach to the regioselectivity in 1,3-dipolar cycloadditions of diazoalkanes, hydrazoic acid and nitrous oxide to acetylenes, phosphaalkynes and cyanides. Journal of Physical Organic Chemistry, 2003, 16, 615-625.	0.9	29
1213	Benzonitriles: Survey of their importance and scaling of their vibrational frequencies. International Journal of Quantum Chemistry, 2003, 94, 189-204.	1.0	51
1214	Investigation of nucleoside analogs with anti-HIV activity. International Journal of Quantum Chemistry, 2003, 93, 422-432.	1.0	20
1215	C3H4: Density functional study of interconversion of isomers. International Journal of Quantum Chemistry, 2003, 94, 93-104.	1.0	14
1216	Potential energy barriers for dissociative attachment to HF.HF and HCl.HCl: Ab initio study. International Journal of Quantum Chemistry, 2003, 95, 683-696.	1.0	6
1217	Global optimization of SixHy at the ab initio level via an iteratively parametrized semiempirical method. International Journal of Quantum Chemistry, 2003, 95, 617-626.	1.0	12
1218	Proton affinity of proline and modified prolines using the kinetic method: role of the conformation investigated byab initio calculations. Rapid Communications in Mass Spectrometry, 2003, 17, 1626-1632.	0.7	26
1219	Thermometer ions for matrix-enhanced laser desorption/ionization internal energy calibration. Rapid Communications in Mass Spectrometry, 2003, 17, 1847-1854.	0.7	50

#	Article	IF	Citations
1220	Mixed Solvent and Polymer Coordination in PAN and PMMA Gel Polymer Electrolytes Studied byAb InitioCalculations and Raman Spectroscopy. Journal of Physical Chemistry B, 2003, 107, 12622-12627.	1.2	42
1221	Coherent Three-Pulse Spectroscopy of Coupled Vibrations in a Rigid Dipeptide:Â Density Functional Theory Simulations. Journal of Physical Chemistry B, 2003, 107, 5967-5985.	1.2	22
1222	Lithium-Cation/Ï€ Complexes of Aromatic Systems. The Effect of Increasing the Number of Fused Rings. Journal of the American Chemical Society, 2003, 125, 10394-10401.	6.6	82
1223	Azacarbaborane chemistry. Butyl nitrite synthesis of the new eight-, nine- and ten-vertex azacarbaboranes exo- and endo-7-CH3-hypho-7,8-NCB6H11, nido-6,8,9-NC2B7H10, arachno-6,5,9-NC2B7H12 and arachno-6,5,10-C2NB7H12. Dalton Transactions, 2003, , 1326.	1.6	10
1224	Primary photoreactions of phylloquinone (vitamin K1) and plastoquinone-1 in solution. Photochemical and Photobiological Sciences, 2003, 2, 524-535.	1.6	43
1225	Conformational behavior of some hydroxamic acids. Organic and Biomolecular Chemistry, 2003, 1, 2200.	1.5	50
1226	Determination of the Stereochemistry of 3-Hydroxymethyl-2,3-dihydro-[1,4]dioxino[2,3-b]- pyridine by Vibrational Circular Dichroism and the Effect of DFT Integration Grids. Journal of Physical Chemistry A, 2003, 107, 542-553.	1.1	60
1227	Decomposition Mechanism of 1,1-Diamino Dinitroethylene (Fox-7): An Overview of the Quantum Chemical Calculation. Theoretical and Computational Chemistry, 2003, , 91-109.	0.2	4
1228	Surface Characterization of PBO Fibers. Macromolecules, 2003, 36, 8662-8672.	2.2	26
1229	Fundamental vibrational frequencies of small polyatomic molecules from density-functional calculations and vibrational perturbation theory. Journal of Chemical Physics, 2003, 118, 7215.	1.2	259
1230	A Theoretical Study of C4B Isomers. The Interconversion of CCBCC and CCCCB via Cyclic C4B. Journal of Physical Chemistry A, 2003, 107, 10149-10153.	1.1	23
1231	Linear Free Energy Relationship and Kinetic Isotope Effects as Measures for the Transition State Variation. A Computational Study. Journal of Organic Chemistry, 2003, 68, 7772-7778.	1.7	11
1232	A Computational Study of Conformations and Conformers of 1,3-Dithiane (1,3-Dithiacyclohexane). Journal of Physical Chemistry A, 2003, 107, 2908-2918.	1.1	40
1233	Electron Delocalization in Isocyanates, Formamides, and Ureas: Importance of Orbital Interactions. Journal of Physical Chemistry A, 2003, 107, 1627-1634.	1.1	43
1234	Theoretical Calculation of Accurate Absolute and Relative Gas- and Liquid-Phase Oâ˜H Bond Dissociation Enthalpies of 2-Mono- and 2,6-Disubstituted Phenols, Using DFT/B3LYP. Journal of Physical Chemistry A, 2003, 107, 8594-8606.	1.1	74
1235	Origins of Opposite Absolute Stereoselectivities in Proline-Catalyzed Direct Mannich and Aldol Reactions. Organic Letters, 2003, 5, 1249-1251.	2.4	154
1236	Hydrogen-Bonding Effects on the Properties of Phenoxyl Radicals. An EPR, Kinetic, and Computational Study. Journal of the American Chemical Society, 2003, 125, 8318-8329.	6.6	117
1237	Formation and photodepletion of cluster ionâ€“messenger atom complexes in a cold ion trap: Infrared spectroscopy of VO+, VO2+, and VO3+. Journal of Chemical Physics, 2003, 119, 12700-12703.	1.2	142

#	Article	IF	Citations
1238	Infrared Spectroscopy of Carbon Materials:Â A Quantum Chemical Study of Model Compounds. Journal of Physical Chemistry B, 2003, 107, 6350-6359.	1.2	328
1239	Mechanisms of Hydrogen-, Oxygen-, and Electron-Transfer Reactions of Cumylperoxyl Radical. Journal of the American Chemical Society, 2003, 125, 9074-9082.	6.6	93
1240	DFT Study on Nitration Mechanism of Benzene with Nitronium Ion. Journal of Physical Chemistry A, 2003, 107, 11440-11444.	1.1	39
1241	Aromaticity and antiaromaticity in fulvenes, ketocyclopolyenes, fulvenones, and diazocyclopolyenes. Organic and Biomolecular Chemistry, 2003, 1, 3410-3417.	1.5	52
1242	Computer simulation of the mechanisms and energetics of circumambulatory rearrangements of Dewar furan, thiophene and selenophene. Mendeleev Communications, 2003, 13, 205-207.	0.6	3
1243	Stability and Three-Dimensional Aromaticity of closo-NBn-1Hn Azaboranes, n = 5â^'12. Inorganic Chemistry, 2003, 42, 4190-4203.	1.9	21
1244	Raman, Infrared, and Surface-Enhanced Raman Spectroscopy in Combination with ab Initio and Density Functional Theory Calculations on 10-Isopropyl-10H-phenothiazine-5-oxide. Journal of Physical Chemistry A, 2003, 107, 1811-1818.	1.1	40
1245	Accurate Calculations of Bond Dissociation Enthalpies with Density Functional Methods. Journal of Physical Chemistry A, 2003, 107, 9991-9996.	1.1	107
1246	Redox-Triggered FTIR Difference Spectra of FAD in Aqueous Solution and Bound to Flavoproteins. Biochemistry, 2003, 42, 14814-14821.	1.2	56
1247	Properties of the phosphorus oxide radical, PO, its cation and anion in their ground electronic states: comparison of theoretical and experimental data. International Reviews in Physical Chemistry, 2003, 22, 641-675.	0.9	22
1248	Prediction of Solvent Effects on Vibrational Absorption Intensities and Raman Activities in Solution within the Polarizable Continuum Model:â€‰ A Study on Pushâ^'Pull Molecules. Journal of Physical Chemistry A, 2003, 107, 10261-10271.	1.1	13
1249	Structures and Energetics of Clusters (n = 5â^'11). Journal of Physical Chemistry A, 2003, 107, 4768-4772.	1.1	42
1250	Reactivity Descriptors and Rate Constants for Acid Zeolite Catalyzed Ethylation and Isopropylation of Benzene. Journal of Physical Chemistry B, 2003, 107, 2001-2008.	1.2	29
1251	Electronic Spectrum of Dicyanoacetylene. 1. Calculations of the Geometries and Vibrations of Ground and Excited States of Diacetylene, Cyanoacetylene, Cyanogen, Triacetylene, Cyanodiacetylene, and Dicyanoacetyleneâ€. Journal of Physical Chemistry A, 2003, 107, 10631-10636.	1.1	21
1252	Ab Initio/RRKM Study of the Potential Energy Surface of Triplet Ethylene and Product Branching Ratios of the C(3P) + CH4 Reaction. Journal of Physical Chemistry A, 2003, 107, 1788-1796.	1.1	35
1253	Probing Biotransformation Relationships among Pyridoacridines by Focusing on Oxygenated Analogues. Journal of Natural Products, 2003, 66, 873-875.	1.5	4
1254	Analytic and Variational XÎ± in the Slaterâ^'Roothaan Method. Journal of Physical Chemistry A, 2003, 107, 10082-10089.	1.1	18
1255	Self-Assembled Oligo(phenylene-ethynylene) Molecular Electronic Switch Monolayers on Gold:Â Structures and Chemical Stability. Langmuir, 2003, 19, 8245-8255.	1.6	144

#	Article	IF	Citations
1256	DFT Calculation on the Thermodynamic Properties of Polychlorinated Dibenzo-p-dioxins:â€‰Intramolecular Clâ‹¯Cl Repulsion Effects and Their Thermochemical Implications. Journal of Physical Chemistry A, 2003, 107, 2693-2699.	1.1	55
1257	Combining Theory and Experiment to Study the Photooxidation of Polyethylene and Polypropylene. Journal of Physical Chemistry B, 2003, 107, 11880-11888.	1.2	40
1258	Agostic vs Ï€-Interactions in Complexes of Ethynylsilanes and Ethynylgermanes with Cu+in the Gas Phase. Journal of Physical Chemistry A, 2003, 107, 1370-1376.	1.1	37
1259	Anionâ‹¯Water Clusters A-(H2O)1-6, A = OH, F, SH, Cl, and Br. An Effective Fragment Potential Test Case. Journal of Physical Chemistry A, 2003, 107, 7852-7860.	1.1	37
1260	A Theoretical Rationalization of the Asymmetric Induction in Sulfinyl-Directed [5C + 2C] Intramolecular Cycloadditions. Journal of Organic Chemistry, 2003, 68, 9780-9786.	1.7	18
1261	Vibrational Band Assignments for the Chiral Modifier Cinchonidine:Â Implications for Surface Studies. Journal of Physical Chemistry B, 2003, 107, 14365-14373.	1.2	112
1262	Infrared Spectra of Aluminum Hydrides in Solid Hydrogen:â€‰Al2H4 and Al2H6. Journal of the American Chemical Society, 2003, 125, 9218-9228.	6.6	117
1263	Free-Energy Calculations of Proteinâ‹¯Ligand Cationâ‹¯Ï€ and Aminoâ‹¯Ï€ Interactions: From Vacuum to Proteinlike Environments. Journal of the American Chemical Society, 2003, 125, 13988-13994.	6.6	79
1264	Experimental and Theoretical Study of the Secondary Equilibrium Isotope Effect (SEIE) in the Proton Transfer between the Pyridinium-d5 Cation and Pyridine. Journal of Physical Chemistry A, 2003, 107, 6160-6167.	1.1	8
1265	Theoretical and Spectroscopic Study of a Series of Styryl-Substituted Terthiophenes. Journal of Physical Chemistry A, 2003, 107, 11505-11516.	1.1	56
1266	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for â€¢NHX Radicals. Journal of Physical Chemistry A, 2003, 107, 7985-7990.	1.1	37
1267	The Excited-State Symmetry Characteristics of Platinum Phenylacetylene Compounds. Journal of Physical Chemistry A, 2003, 107, 11340-11346.	1.1	64
1268	Theoretical Calculations of Carbonâ‹¯Oxygen Bond Dissociation Enthalpies of Peroxyl Radicals Formed in the Autoxidation of Lipids. Journal of the American Chemical Society, 2003, 125, 5801-5810.	6.6	148
1269	Structure and Dynamics of Hydrated Ag (I): Ab Initio Quantum Mechanical-Molecular Mechanical Molecular Dynamics Simulation. Journal of Physical Chemistry A, 2003, 107, 3132-3138.	1.1	52
1270	Tautomeric Equilibria of Pyridoxal-5â€˜-phosphate (Vitamin B6) and 3-Hydroxypyridine Derivatives:Â A Theoretical Study of Solvation Effects. Journal of Organic Chemistry, 2003, 68, 2874-2881.	1.7	30
1271	Dynamics of Molecules near Ionization. Journal of Physical Chemistry A, 2003, 107, 10872-10887.	1.1	24
1272	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides:â€‰Surprisingly Demanding Targets for High-Level ab Initio Procedures. Journal of Physical Chemistry A, 2003, 107, 5617-5630.	1.1	76
1273	Ketene Formation in Benzdiyne Chemistry:â€‰Ring Cleavage versus Wolff Rearrangement. Journal of the American Chemical Society, 2003, 125, 11936-11941.	6.6	15

#	Article	IF	Citations
1274	Theoretical Conformational Analysis for Neurotransmitters in the Gas Phase and in Aqueous Solution. Norepinephrine. Journal of the American Chemical Society, 2003, 125, 2770-2785.	6.6	58
1275	Modeling of a Rotaxane-Based Molecular Device. Journal of Physical Chemistry A, 2003, 107, 1207-1215.	1.1	26
1276	Structure, Intramolecular Rotation Barrier, and Thermochemical Properties of Hydroxycyclohexadienyl Radical. Journal of Physical Chemistry A, 2003, 107, 6451-6456.	1.1	7
1277	Electron Transfer and Singlet Oxygen Mechanisms in the Photooxygenation of Dibutyl Sulfide and Thioanisole in MeCN Sensitized byN-Methylquinolinium Tetrafluoborate and 9,10-Dicyanoanthracene. The Probable Involvement of a Thiadioxirane Intermediate in Electron Transfer Photooxygenations. Journal of the American Chemical Society, 2003, 125, 16444-16454.	6.6	156
1278	Rate Constants for D + C2H2â† ' C2HD + H at High Temperature:Â Implications to the High Pressure Rate Constant for H + C2H2â† ' C2H3â€. Journal of Physical Chemistry A, 2003, 107, 10533-10543.	1.1	22
1279	Conformation of Secondary Amides. A Predictive Algorithm That Correlates DFT-Calculated Structures and Experimental Proton Chemical Shiftsâ€. Journal of Organic Chemistry, 2003, 68, 1834-1842.	1.7	18
1280	Proton Transfers from Carbon Acids Activated by Ï€-Acceptors. Changes in Intrinsic Barriers and Transition State Imbalances Induced by a Cyano Group. An ab Initio Study. Journal of Organic Chemistry, 2003, 68, 6870-6879.	1.7	9
1281	Calorimetric and Computational Study of Thiacyclohexane 1-Oxide and Thiacyclohexane 1,1-Dioxide (Thiane Sulfoxide and Thiane Sulfone). Enthalpies of Formation and the Energy of the SO Bond. Journal of Organic Chemistry, 2003, 68, 1762-1770.	1.7	28
1282	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Methyl Ethyl, Methyl Isopropyl, and Methyl tert-Butyl Ethers and the Corresponding Radicals. Journal of Physical Chemistry A, 2003, 107, 4531-4546.	1.1	40
1283	Kinetics of Elementary Reactions in the Chain Chlorination of Cyclopropane. Journal of Physical Chemistry A, 2003, 107, 2003-2010.	1.1	13
1284	A Detailed Investigation of Subsitituent Effects on Nâ^'H Bond Enthalpies in Aniline Derivatives and on the Stability of Corresponding N-Centered Radicals. Journal of Organic Chemistry, 2003, 68, 7350-7360.	1.7	37
1285	Thermochemistry of Furancarboxylic Acids. Journal of Physical Chemistry A, 2003, 107, 11460-11467.	1.1	20
1286	Structures, Rotational Barriers, and Thermochemical Properties of Î²-Chlorinated Ethyl Hydroperoxides. Journal of Physical Chemistry A, 2003, 107, 1018-1024.	1.1	11
1287	Thermodynamic Properties and Kinetic Parameters for Cyclic Ether Formation from Hydroperoxyalkyl Radicals. Journal of Physical Chemistry A, 2003, 107, 4908-4920.	1.1	110
1288	Crystal structures and properties of mutagenic N-acyloxy-N-alkoxyamides â€" â€œmost pyramidalâ€•acyclic amides. Organic and Biomolecular Chemistry, 2003, 1, 3430-3437.	1.5	35
1289	Building Blocks of Eumelanin:Â Relative Stability and Excitation Energies of Tautomers of 5,6-Dihydroxyindole and 5,6-Indolequinone. Journal of Physical Chemistry B, 2003, 107, 7162-7171.	1.2	75
1290	Resonance Raman and DFT Studies of Tetra-tert-butyl Porphine:â€‰ Assignment of Strongly Enhanced Distortion Modes in a Ruffled Porphyrin. Journal of Physical Chemistry A, 2003, 107, 2964-2973.	1.1	21
1291	Protonation Thermochemistry of Î±,Ï‰-Alkane Diols in the Gas Phase:Â A Theoretical Study. Journal of Physical Chemistry A, 2003, 107, 7931-7937.	1.1	18

#	Article	IF	Citations
1292	S1 1A2(nÏ€*) and S2 1A1(Ï€Ï€*) States of Jet-Cooled Xanthone. Journal of Physical Chemistry A, 2003, 107, 8851-8855.	1.1	18
1293	Vibrational Assignments for High Molecular Weight Linear Polyethylenimine (LPEI) Based on Monomeric and Tetrameric Model Compounds. Macromolecules, 2003, 36, 7348-7351.	2.2	40
1294	Reaction of Phenyl Radicals with Acetylene:Â Quantum Chemical Investigation of the Mechanism and Master Equation Analysis of the Kinetics. Journal of the American Chemical Society, 2003, 125, 11397-11408.	6.6	73
1295	In-Situ Investigation of Binary-Component Self-Assembled Monolayers:Â A SERS-Based Spectroelectrochemical Study of the Effects of Monolayer Composition on Interfacial Structure. Langmuir, 2003, 19, 5794-5801.	1.6	21
1296	Calculations of Site-Specific CO Stretching Frequencies for Copper Carbonyls with the â€œNear Spectroscopic Accuracyâ€•â€‰ CO Interaction with Cu+/MFI. Journal of Physical Chemistry A, 2003, 107, 10381-10388.	1.1	71
1297	Computational Studies of the Origin of Regiospecificity in the [4+2] Dielsâ^'Alder Reaction between R2BNR2â€˜ Compounds and Substitutedcis-Butadienes. Organometallics, 2003, 22, 3748-3752.	1.1	4
1298	Spectroscopic and Theoretical Study of Pushâ^'Pull Chromophores Containing Thiophene-Based Quinonoid Structures as Electron Spacers. Journal of Physical Chemistry B, 2003, 107, 12175-12183.	1.2	40
1299	Sodium hydroxide formation in water clusters: The role of hydrated electrons and the influence of electric field. Journal of Chemical Physics, 2003, 118, 10461-10469.	1.2	30
1300	Why Do Losses of Polyatomic Fragments Strongly Dominate Losses of Atoms at High Internal Energies? Methyl versus Clâ€¢ Loss from the 2-Chloropropane Cation. Journal of Physical Chemistry A, 2003, 107, 512-517.	1.1	3
1301	Study of the Interaction of Pollutant Nitro Polycyclic Aromatic Hydrocarbons with Different Metallic Surfaces by Surface-Enhanced Vibrational Spectroscopy (SERS and SEIR). Journal of Physical Chemistry A, 2003, 107, 9611-9619.	1.1	52
1302	Ab Initio Studies of Solvent Effects on Molecular Conformation and Vibrational Spectra of Diglycine Zwitterion. Journal of Physical Chemistry A, 2003, 107, 11391-11400.	1.1	13
1303	Catalytic Model Reactions for the HCN Isomerization. I. Theoretical Characterization of Some Water-Catalyzed Mechanisms. Journal of Physical Chemistry A, 2003, 107, 3925-3934.	1.1	17
1304	Thermal Rate Coefficients via Variational Transition State Theory for the Unimolecular Decomposition/Isomerization of 1-Pentyl Radical:Â Ab Initio and Direct Dynamics Calculations. Journal of Physical Chemistry A, 2003, 107, 8607-8617.	1.1	34
1305	Infrared Spectra and Structures of the Valyl-Alanine and Alanyl-Valine Zwitterions Isolated in a KBr Matrix. Journal of Physical Chemistry A, 2003, 107, 6136-6143.	1.1	8
1306	Guided Ion Beam and Ab Initio Studies of Platinum Chloride Cations. Journal of Physical Chemistry A, 2003, 107, 10303-10310.	1.1	9
1307	Reaction Mechanism of N2/H2 Conversion to NH3:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2003, 107, 2865-2874.	1.1	69
1308	Assessment of Experimental Bond Dissociation Energies Using Composite ab Initio Methods and Evaluation of the Performances of Density Functional Methods in the Calculation of Bond Dissociation Energies. Journal of Chemical Information and Computer Sciences, 2003, 43, 2005-2013.	2.8	144
1309	The Transoid, Ortho, and Gauche Conformers of Decamethyl-n-tetrasilane, n-Si4Me10:â€‰ Electronic Transitions in the Multistate Complete Active Space Second-Order Perturbation Theory Description. Journal of Physical Chemistry A, 2003, 107, 4661-4668.	1.1	20

#	Article	IF	Citations
1310	Evaluating the Potential of Fluorinated Tyrosines as Spectroscopic Probes of Local Protein Environments:â€‰ A UV Resonance Raman Study. Biochemistry, 2003, 42, 2441-2448.	1.2	11
1311	Experimental and Theoretical Investigation of Reversible Interconversion, Thermal Reactions, and Wavelength-Dependent Photochemistry of Diazo Meldrum's Acid and Its Diazirine Isomer, 6,6-Dimethyl-5,7-dioxa-1,2-diaza-spiro[2,5]oct-1-ene-4,8-dione1. Journal of the American Chemical Society, 2003, 125, 14153-14162.	6.6	46
1312	Acid Strength of Low-Valence Dopant Ions in Microporous Zeolites and AlPOs. Journal of Physical Chemistry B, 2003, 107, 11866-11870.	1.2	9
1313	Catalytic Model Reactions for the HCN Isomerization. II. Theoretical Investigation of an Anionic Pathway. Journal of Physical Chemistry A, 2003, 107, 3935-3941.	1.1	8
1314	Study of Complexation in Methanol/Water Mixtures by Infrared and Raman Spectroscopy and Multivariate Curve Resolutionâ€”Alternating Least-Squares Analysis. Applied Spectroscopy, 2003, 57, 483-490.	1.2	46
1315	Enhancing Reactivity of Carbonyl Compounds via Hydrogen-Bond Formation. A DFT Study of the Hetero-Dielsâ^'Alder Reaction between Butadiene Derivative and Acetone in Chloroform. Journal of Organic Chemistry, 2003, 68, 8662-8668.	1.7	91
1316	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. 3. A Single Approach for Xâ^'H, Xâ^'X, and Xâ^'Y (X, Y = C, N, O, S, Halogen) Bonds. Journal of Physical Chemistry A, 2003, 107, 9953-9963.	1.1	109
1317	Conceptual Density Functional Theory. Chemical Reviews, 2003, 103, 1793-1874.	23.0	4,111
1318	A theoretical study on nitration mechanism of benzene and solvent effects. Science in China Series B: Chemistry, 2003, 46, 453.	0.8	8
1319	Hydrogen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2003, 67, 1259-1276.	1.6	20
1320	Theoretical estimates of equilibrium chlorine-isotope fractionations. Geochimica Et Cosmochimica Acta, 2003, 67, 3267-3281.	1.6	143
1321	Electrochemical and Photon Polarization Modulation Infrared Reflection Absorption Spectroscopy Study of the Electric Field Driven Transformations of a Phospholipid Bilayer Supported at a Gold Electrode Surface. Biophysical Journal, 2003, 85, 4055-4075.	0.2	92
1322	Nitro-Functionalized Oligothiophenes as a Novel Type of Electroactive Molecular Material:Â Spectroscopic, Electrochemical, and Computational Study. Journal of the American Chemical Society, 2003, 125, 2524-2534.	6.6	106
1323	Experimental Thermodynamics of Cluster Ions Composed of H2SO4 and H2O. 2. Measurements and ab Initio Structures of Negative Ions. Journal of Physical Chemistry A, 2003, 107, 9812-9824.	1.1	97
1324	Formation of Alkali Metal/Alkaline Earth Cation Water Clusters, M(H2O)1-6, M = Li+, Na+, K+, Mg2+, and Ca2+: An Effective Fragment Potential (EFP) Case Study. Journal of Physical Chemistry A, 2003, 107, 386-396.	1.1	74
1325	G3-RAD and G3X-RAD: Modified Gaussian-3 (G3) and Gaussian-3X (G3X) procedures for radical thermochemistry. Journal of Chemical Physics, 2003, 118, 4849-4860.	1.2	276
1326	The Formation of CCBO and [CCBO]+ from [CCBO]- in the Gas Phase:â€‰ A Joint Experimental and Theoretical Study. Journal of Physical Chemistry A, 2003, 107, 1181-1187.	1.1	16
1327	Infrared, Density-Functional Theory, and Atoms in Molecules Method Studies on Conformers of Some 2-Substituted 1H-Pyrroles. Journal of Physical Chemistry A, 2003, 107, 8723-8729.	1.1	26

#	Article	IF	Citations
1328	Ab Initio Evidence for Slow Fragmentation in RAFT Polymerization. Journal of the American Chemical Society, 2003, 125, 1490-1491.	6.6	148
1329	Highly Efficient Photochemical Generation of a Triple Bond:Â Synthesis, Properties, and Photodecarbonylation of Cyclopropenones. Journal of Organic Chemistry, 2003, 68, 7833-7840.	1.7	90
1330	Molecular Interactions between Glycine and H2O Affording the Zwitterion. Journal of Physical Chemistry A, 2003, 107, 7915-7922.	1.1	53
1331	Characterization of the Cu+Sites in High-Silica Zeolites Interacting with the CO Molecule:Â Combined Computational and Experimental Study. Journal of Physical Chemistry B, 2003, 107, 2327-2332.	1.2	69
1332	Enthalpies of Formation of Dibenzo-p-dioxin and Polychlorinated Dibenzo-p-dioxins Calculated by Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 2848-2854.	1.1	13
1333	Identity Proton-Transfer Reactions from Câˆ'H, Nâˆ'H, and Oâˆ'H Acids. An ab Initio, DFT, and CPCM-B3LYP Aqueous Solvent Model Study. Journal of the American Chemical Society, 2003, 125, 11730-11745.	6.6	52
1334	Kinetics and Thermochemistry for the Gas-Phase Ketoâˆ'Enol Tautomerism of Phenol â†" 2,4-Cyclohexadienone. Journal of Physical Chemistry A, 2003, 107, 3696-3703.	1.1	70
1335	Singlet and Triplet Valence Excited States of Pyrimidine. Journal of Physical Chemistry A, 2003, 107, 3093-3106.	1.1	45
1336	Reaction Mechanism of the Synthesis of Ammonia in the N2/H2/BeO and N2/H2/FeO Systems:Â A Theoretical Study. Journal of Physical Chemistry A, 2003, 107, 5092-5100.	1.1	9
1337	The Infrared Spectrum of Al2H6 in Solid Hydrogen. Science, 2003, 299, 2049-2052.	6.0	130
1338	Influence of heteroligands on structural and dynamical properties of hydrated Cu2+: QM/MM MD simulations. Physical Chemistry Chemical Physics, 2003, 5, 3418.	1.3	35
1339	Time-resolved IR studies of cyclic enone triplet excited states and their reactions with alkenes. Physical Chemistry Chemical Physics, 2003, 5, 1059-1063.	1.3	4
1340	The importance of agostic-type interactions for the binding energies of Ni+to saturated and Î±,Î²-unsaturated alkanes, silanes and germanes. New Journal of Chemistry, 2003, 27, 1657-1664.	1.4	20
1341	Electronic spectroscopy of the CaCCCH3 and SrCCCH3 free radicals. Physical Chemistry Chemical Physics, 2003, 5, 36-40.	1.3	4
1342	Infrared absorption spectra of 2-(hydroxyimino)propanohydroxamic and oxalodihydroxamic acids isolated in argon matrices. Physical Chemistry Chemical Physics, 2003, 5, 2337-2343.	1.3	11
1343	H-Atom abstraction by C-centered radicals from cyclic and acyclic dipeptides. A theoretical and experimental study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3278-3288.	1.3	14
1344	Nucleophilic identity substitution reactions. The reaction between water and protonated alcoholsPart I. For Part II, see following paper (DOI: 10.1039/b302270f).Electronic supplementary information (ESI) available: Cartesian co-ordinates for all species together with analytical imaginary frequencies for the transition structures. See http://www.rsc.org/suppdata/ob/b3/b302268d/. Organic and Biomolecular Chemistry, 2003, 1, 2935.	1.5	25
1345	Computational study on the electrocyclic reactions of [16]annuleneElectronic supplementary information (ESI) available: cartesian coordinates of all the equilibrium and transition structures optimized at the B3LYP/6-31G(d) level. See http://www.rsc.org/suppdata/ob/b3/b304654k/. Organic and Biomolecular Chemistry, 2003, 1, 2748.	1.5	8

#	Article	IF	Citations
1346	Thermodynamic properties (S298, Cp(T), internal rotations and group additivity parameters) in vinyl and phenyl hydroperoxidesElectronic supplementary information (ESI) available: Internal rotation barriers, Fourier expansion coefficients for internal rotation potentials for vinyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b2/b207030h/. Physical Chemistry Chemical Physics, 2003, 5, 300-307.	1.3	13
1347	Hydrogen bonding interactions of benzylidene type Schiff bases studied by vibrational spectroscopic and computational methods. Physical Chemistry Chemical Physics, 2003, 5, 2009-2014.	1.3	33
1348	First signals of electrochemically oxidized species of TTF and TTM-TTF: A study by in situ spectroelectrochemical FTIR and DFT calculations. Physical Chemistry Chemical Physics, 2003, 5, 4672-4679.	1.3	26
1349	H-atom abstraction by thiyl radicals from peptides and cyclic dipeptides. A theoretical study of reaction rates. Physical Chemistry Chemical Physics, 2003, 5, 3994-3999.	1.3	34
1350	The product branching and dynamics of the reaction of chlorine atoms with methylamine. Physical Chemistry Chemical Physics, 2003, 5, 1205-1212.	1.3	41
1351	Nucleophilic identity substitution reactions. The reaction between ammonia and protonated aminesPart II. For Part I, see preceding paper (DOI: 10.1039/b302268d).Electronic supplementary information (ESI) available: Cartesian co-ordinates for all species together with imaginary frequencies for the transition structures. See http://www.rsc.org/suppdata/ob/b3/b302270f/. Organic and Biomolecular Chemistry, 2003, 1, 2943.	1.5	17
1352	Dissociation reactions of CuI(hfac)L compounds relevant to the chemical vapor deposition of copper. Physical Chemistry Chemical Physics, 2003, 5, 2818.	1.3	26
1353	Matrix isolation, time-resolved IR, and computational study of the photochemistry of benzoyl azideDedicated to Professor Dr Z. R. Grabowski and Professor Dr J. Wirz on the occasions of their 75th and 60th birthdays.Electronic supplementary information (ESI) available: Cartesian coordinates and details of the CASSCF/CASPT2 calculations, details of the excited-state calculations on formylnitrene, the full IR spectra, additional results from the TRIR experiments and two tables with results from CASPT2 calculat. Physical Chemistry Chemical Physics, 2003, 5, 1010-1018.	1.3	94
1354	The Usefulness of Density Functional Theory To Describe the Tautomeric Equilibrium of 4,6-Dimethyl-2-mercaptopyrimidine in Solution. Journal of Physical Chemistry A, 2003, 107, 7490-7495.	1.1	35
1355	Improving ab initio infrared spectra of glucoseâ€“water complexes by considering explicit intermolecular hydrogen bonds. Journal of Chemical Physics, 2003, 119, 10133-10137.	1.2	21
1356	Infrared and Raman features of a series of Î±,Ï‰-bis(arylthio)oligothiophenes as molecular wires. A Ï€-electron delocalization efficiency study. Journal of Chemical Physics, 2003, 118, 1912-1920.	1.2	21
1357	The influence of isotopomers on calculated thermodynamics quantities. Molecular Physics, 2003, 101, 2315-2318.	0.8	0
1358	Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax. Molecular Physics, 2003, 101, 1329-1338.	0.8	37
1359	Trends in alkyl substituent effects on nucleophilic reactions of carbonyl compounds: Gas phase reactions between ammonia and R1R2COCH3+ oxonium ionsElectronic supplementary information (ESI) available: proton affinities, geometries and energies of optimised structures, structures of the stationary points and a plot of experimental and RRKM ln(kae/ksub) against a-stabilisation constants. See http://www.rsc.org/suppdata/ob/b2/b208955c/. Organic and Biomolecular Chemistry, 2003, 1, 705-712.	1.5	8
1360	Homolytic bond dissociation energies associated with acyl radicals and electron demands of acyl groupsElectronic supplementary information (ESI) available: Effects of method and basis on geometry optimizations, radical structures, bond orders, spins and bond lengths. See http://www.rsc.org/suppdata/cp/b2/b211078d/. Physical Chemistry Chemical Physics, 2003, 5, 685-690.	1.3	16
1361	On the electronic structure and spectroscopic properties of a pseudo-tetrahedral cationic cobalt(II) tetraamine complex ? ([35]adamanzane)cobalt(ii)Electronic supplementary information (ESI) available: Table S1: Cartesian coordinates of the DFT optimized geometry of the [Co([35]adz)]2+ ion. Table S2: Results of experimental and calculated infrared absorption spectra for the [Co([35]adz)]2+ ion. See http://www.rsc.org/suppdata/dt/b2/b205712c/. Dalton Transactions, 2003, 2100.	1.6	14
1362	DENSITY FUNCTIONAL STUDY OF SELECTED MONO-ZINC AND GEM-DIZINC RADICAL CARBENOID CYCLOPROPANATION REACTIONS: OBSERVATION OF AN EFFICIENT RADICAL ZINC CARBENOID CYCLOPROPANATION REACTION AND THE INFLUENCE OF THE LEAVING GROUP ON RING CLOSURE. Journal of Theoretical and Computational Chemistry, 2003, 02, 357-369.	1.8	6
1363	Coordination and Thermodynamics of Stable Zn(II) Complexes in the Gas Phase. Journal of Biomolecular Structure and Dynamics, 2003, 20, 759-770.	2.0	11

#	Article	IF	Citations
1364	Computational Study on Mechanistic Details of the Aminoethanol Rearrangement Catalyzed by the Vitamin B12-Dependent Ethanolamine Ammonia Lyase:Â His and Asp/Glu Acting Simultaneously as Catalytic Auxiliaries. Journal of Organic Chemistry, 2003, 68, 6967-6983.	1.7	24
1365	Observation of a HI leaving group following ultraviolet photolysis of CH2I2 in water and anab initioinvestigation of the Oâ€“H insertion/HI elimination reactions of the CH2Iâ€“I isopolyhalomethane species with H2O and 2H2O. Journal of Chemical Physics, 2003, 119, 4671-4681.	1.2	17
1366	Spectroscopy and dynamics of excited states in maleimide and N-methyl maleimide: Ionic projection and ab initio calculations. Journal of Chemical Physics, 2003, 118, 10944-10955.	1.2	17
1367	Ab initiosimulation of the two-dimensional vibrational spectrum of dicarbonylacetylacetonato rhodium(I). Journal of Chemical Physics, 2003, 118, 1347-1355.	1.2	40
1368	A path integral approach to molecular thermochemistry. Journal of Chemical Physics, 2003, 118, 1596-1603.	1.2	23
1369	The 1,5-H-shift in 1-butoxy: A case study in the rigorous implementation of transition state theory for a multirotamer system. Journal of Chemical Physics, 2003, 119, 5159-5170.	1.2	121
1370	Theoretical and experimental study of the chemisorption of 1,3 disilabutane on the Si(100) surface. Journal of Chemical Physics, 2003, 118, 6089-6097.	1.2	4
1371	Extendedab initioquantum mechanical/molecular mechanical molecular dynamics simulations of hydrated Cu2+. Journal of Chemical Physics, 2003, 119, 9523-9531.	1.2	97
1372	High pressure reactivity of solid furan probed by infrared and Raman spectroscopy. Journal of Chemical Physics, 2003, 118, 1499-1506.	1.2	46
1373	Stability of Ta-encapsulating Si clusters on Si(111)-(7Â7) surfaces. Journal Physics D: Applied Physics, 2003, 36, L43-L46.	1.3	21
1374	Computational approaches to heats of formation. Theoretical and Computational Chemistry, 2003, 12, 247-277.	0.2	4
1375	Locally Aromatic Polycyclic Hydrocarbons as Potential Carriers of Infrared Emission Features. Astrophysical Journal, 2003, 594, 869-873.	1.6	15
1376	Gas-phase reactivity of lactones: structure and stability of their Cu+complexes. Molecular Physics, 2003, 101, 1249-1258.	0.8	7
1377	Is Allylphosphine a Carbon or a Phosphorus Base in the Gas Phase?. European Journal of Mass Spectrometry, 2003, 9, 245-255.	0.5	5
1378	Reactions of CH3CHOâ€¢+ and of CH3COHâ€¢+ with Water upon Fourier Transform Ion Cyclotron Resonance Conditions. European Journal of Mass Spectrometry, 2003, 9, 319-326.	0.5	7
1379	The Gas-Phase Basicity and Proton Affinity of 1,3,5-Cycloheptatrieneâ€”Energetics, Structure and Interconversion of Dihydrotropylium Ions. European Journal of Mass Spectrometry, 2003, 9, 361-376.	0.5	24
1380	Nucleophilic Reactions of 5-tert-Butyl-2-methoxy-3H-azepine with Alkoxides and Alkyllithium Reagents. Bulletin of the Chemical Society of Japan, 2003, 76, 805-811.	2.0	10
1381	Electronic Structure of Sulfanenitriles. Bulletin of the Chemical Society of Japan, 2003, 76, 1911-1917.	2.0	7

#	Article	IF	Citations
1382	Intramolecular Substitution Reaction of Lithium Alkylidene Carbenoids. Regioselective Synthesis of Indenes. Bulletin of the Chemical Society of Japan, 2003, 76, 2009-2026.	2.0	22
1383	Ab Initio Study of the Prototropic Tautomerism of Cytosine and Guanine and Their Contribution to Spontaneous Point Mutations. International Journal of Molecular Sciences, 2003, 4, 410-421.	1.8	88
1384	CH4 Loss from (CH3)4N+ Revisited: How Does This High Energy Elimination Compete with â€¢CH3 Loss?. European Journal of Mass Spectrometry, 2004, 10, 767-773.	0.5	3
1385	3. Applying Stable Isotope Fractionation Theory to New Systems. , 2004, , 65-112.		50
1386	Quantum Chemical Study on La2@C80 : Configuration of Endohedral Metals. AIP Conference Proceedings, 2004, , .	0.3	0
1387	Combined electronic structure/molecular dynamics approach for ultrafast infrared spectroscopy of dilute HOD in liquid H2O and D2O. Journal of Chemical Physics, 2004, 120, 8107-8117.	1.2	330
1388	Equation of state and structural changes in diaminodinitroethylene under compression. Journal of Chemical Physics, 2004, 120, 8060-8066.	1.2	64
1389	Gas phase infrared spectroscopy of mono- and divanadium oxide cluster cations. Journal of Chemical Physics, 2004, 120, 6461-6470.	1.2	110
1390	The energetics of naphthalene derivatives, III: phenylacetic acid and the isomeric 1- and 2-naphthylacetic acids. Molecular Physics, 2004, 102, 1909-1917.	0.8	22
1391	Fast vibrational self-consistent field calculations through a reduced modeâ€“mode coupling scheme. Journal of Chemical Physics, 2004, 120, 562-573.	1.2	103
1392	Quantum Monte Carlo study of the reaction: Cl+CH3OHâ†'CH2OH+HCl. Journal of Chemical Physics, 2004, 121, 1357-1363.	1.2	16
1393	Accurate theoretical prediction of vibrational frequencies in an inhomogeneous dynamic environment: A case study of a glutamate molecule in water solution and in a protein-bound form. Journal of Chemical Physics, 2004, 121, 1516-1524.	1.2	23
1394	A complete nearest-neighbor force field model for C60. Journal of Chemical Physics, 2004, 120, 6912-6921.	1.2	8
1395	<title>Physical properties of anticancer drug 6-thioguanine</title>. , 2004, 5507, 346.		3
1396	The Concept of the Potential Energy Surface. , 2004, , 9-41.		0
1397	Experimental (FT-IR and Raman) and theoretical (DFT) studies on the vibrational dynamics in cytisine. Vibrational Spectroscopy, 2004, 36, 105-115.	1.2	34
1398	Experimental and theoretical study of the IR spectrum of 4-amyloxy-4â€²-cyanobiphenyl. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2004, 96, 351-358.	0.2	3
1399	Oxidation pathways of adenine and guanine in aqueous solution from first principles electrochemistry. Physical Chemistry Chemical Physics, 2004, 6, 4707.	1.3	51

#	Article	IF	Citations
1400	Antioxidant Activity of Hydroxystilbene Derivatives in Homogeneous Solution. Journal of Organic Chemistry, 2004, 69, 7101-7107.	1.7	69
1401	Oâ˜H Bond Dissociation Enthalpies in Oximes:Â Order Restored. Journal of the American Chemical Society, 2004, 126, 10667-10675.	6.6	61
1402	Comparison of Theoretical Methods and Basis Sets for ab initio and DFT Calculations of the Structure and Frequencies of Normal Vibrations of Polyatomic Molecules. Journal of Applied Spectroscopy, 2004, 71, 164-172.	0.3	8
1403	Calculation of Normal Vibrations of Chlorin by the Method of Density Functionals. Journal of Applied Spectroscopy, 2004, 71, 307-319.	0.3	3
1404	Density Functional Study of the Structure and Infrared Spectrum of Ethyl Chlorophyllide (A). Journal of Structural Chemistry, 2004, 45, 217-224.	0.3	3
1405	Pressure Effect on Conformational Equilibria of Analog Peptides in Aqueous Solution by Raman Spectroscopy. Journal of Solution Chemistry, 2004, 33, 761-775.	0.6	7
1406	Early Prediction of Pharmaceutical Oxidation Pathways by Computational Chemistry and Forced Degradation. Pharmaceutical Research, 2004, 21, 1708-1717.	1.7	34
1407	Synthesis, NMR, and Computational Study of 1,2-Diethyl-3-(trimethylsilyl)cyclopropenylium Hexachloroantimonate. Structural Chemistry, 2004, 15, 195-206.	1.0	2
1408	A Nonempirical Quantum-Chemical Study and Natural Bond Orbital Analysis of C6H5XCY3Species (X =) Tj ETQq0 0 0 rgBT /Overlock 10	1.0	10
1409	Comparison of the Kinetics and Thermodynamics for Methyl Radical Addition to CC, CO, and CS Double Bonds. Journal of the American Chemical Society, 2004, 126, 1732-1740.	6.6	70
1410	Infrared depletion spectra of 2-aminopyridineâ‹…2-pyridone, a Watsonâ€“Crick mimic of adenineâ‹…uracil. Journal of Chemical Physics, 2004, 121, 8237.	1.2	38
1411	Electron Delocalization in Aminoguanidine:Â A Computational Study. Journal of Physical Chemistry A, 2004, 108, 10509-10517.	1.1	37
1412	Kinetics, thermodynamics, and ab initio calculations of HS2O7â˜(H2SO4)x (x=1â€“3) cluster ions. International Journal of Mass Spectrometry, 2004, 232, 9-15.	0.7	6
1413	Theoretical characterizations of novel C2H5O+ reactions. International Journal of Mass Spectrometry, 2004, 232, 17-24.	0.7	13
1414	Standard molar enthalpies of formation of the methoxynitrophenol isomers: a combined experimental and theoretical investigation. Journal of Chemical Thermodynamics, 2004, 36, 431-436.	1.0	23
1415	Propagation rate coefficient of acrylic acid: theoretical investigation of the solvent effect. Polymer, 2004, 45, 6993-6999.	1.8	57
1416	Synthesis, complete NMR assignments, and NOE versus GIAO data assisted ab initio modelling the overall conformations of amide 3,4â€²-diquinolinyl sulfides in solution. Another approach to analysis of flexible systems. Tetrahedron, 2004, 60, 9213-9222.	1.0	11
1417	Effects of geminal disubstitution on Câ€“H and Nâ€“H bond dissociation energies. Tetrahedron, 2004, 60, 9909-9923.	1.0	33

#	Article	IF	Citations
1418	New solid state Ni(II)-famotidine square-planar complex: powder diffraction and spectroscopic studies. Journal of Inorganic Biochemistry, 2004, 98, 995-1001.	1.5	12
1419	The crystal and molecular structure of N2H5[M(N2H3COO)3]Â·H2O (Mâ^{Co, Zn}) isomorphic compoundsâ€"an X-ray crystallographic, vibrational spectroscopic and quantum-chemical study. Journal of Solid State Chemistry, 2004, 177, 4482-4493.	1.4	8
1420	Surface Raman characterization of cinchonidine-modified platinum in ethanol: effects of liquid-phase concentration and co-adsorbed hydrogen. Journal of Molecular Catalysis A, 2004, 212, 277-289.	4.8	49
1421	Electron Diffraction Determination of Equilibrium Structure for Rigid Molecules. Equilibrium Configuration of 1,2-Thiaarsol According to Gas-Phase Electron Diffraction and Quantum-Chemical Data. Journal of Structural Chemistry, 2004, 45, 778-785.	0.3	9
1422	Molecular, thermodynamic, and kinetic parameters of iodomethanes and iodomethyl radicals: ab initio calculations. Russian Journal of General Chemistry, 2004, 74, 1686-1696.	0.3	3
1423	The vibrational spectrum of calcite (CaCO3): an ab initio quantum-mechanical calculation. Physics and Chemistry of Minerals, 2004, 31, 559-564.	0.3	182
1424	Vibrational study of dialkylphosphonates: di-n-propyl- and di-i-propylphosphonates by semiempirical and ab initio methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 41-51.	2.0	17
1425	Vibrational properties of the free and adsorbed acridone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 337-342.	2.0	8
1426	Vibrational spectrum, ab initio calculations, conformational equilibria and torsional modes of 1,3-dichloropropane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 659-671.	2.0	5
1427	Vibrational study of the Fe(phen)2(NCS)2 spin-crossover complex by density-functional calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1013-1025.	2.0	21
1428	Molecular structure and scaled quantum mechanical force fields of bis(dimethylamino)chloroborane, [(CH3)2N]2BCl, determined by gas-phase electron diffraction and molecular orbital calculations; and supplementary computations for [(CH3)2N]3B, (CH3)2NBCl2, and BCl3. Journal of Molecular Structure, 2004, 691, 1-24.	1.8	5
1429	Computational study of the chair-chair interconversion and stereoelectronic interactions in 1,2,3-trithiacyclo-hexane (1,2,3-trithiane). Journal of Physical Organic Chemistry, 2004, 17, 32-41.	0.9	12
1430	The gas-phase reactivity of epichlorohydrin with hydroxide. Journal of Physical Organic Chemistry, 2004, 17, 241-248.	0.9	8
1431	Theoretical study of the thermolysis reaction of methylÎ²-hydroxycarboxylates in the gas phase. Journal of Physical Organic Chemistry, 2004, 17, 294-302.	0.9	5
1432	Nucleophilic attack on ketene, 6-methylene-2,4-cyclohexadienylideneketene, 6-oxo-2,4-cyclohexadienylideneketene and 4-oxo-2,5-cyclohexadienylideneketene: anab initiostudy. Journal of Physical Organic Chemistry, 2004, 17, 1075-1083.	0.9	5
1433	Time-resolved IR studies of Î±-lactones. Journal of Physical Organic Chemistry, 2004, 17, 743-748.	0.9	12
1434	Ab initio calculations of proton affinities of glycine, proline, cysteine and phenylalanine: comparison with the experimental values obtained using an electrospray ionisation ion trap mass spectrometer. Rapid Communications in Mass Spectrometry, 2004, 18, 307-312.	0.7	31
1435	A mass spectrometric and molecular orbital study of H2O loss from protonated tryptophan and oxidized tryptophan derivatives. Rapid Communications in Mass Spectrometry, 2004, 18, 978-988.	0.7	23

#	Article	IF	Citations
1436	Computational study of the conformational interconversion of 5,5-dimethyl-1,2,3-trithiacyclohexane (5,5-dimethyl-1,2,3-trithiane). International Journal of Quantum Chemistry, 2004, 96, 443-455.	1.0	8
1437	Reactivity and aromaticity of polyaromatics in radical cyclization reactions. International Journal of Quantum Chemistry, 2004, 96, 568-576.	1.0	51
1438	Potential energy surfaces of fluorinated benzene radical cations. International Journal of Quantum Chemistry, 2004, 100, 469-476.	1.0	27
1439	Theoretical investigation of the structures and properties of fluoromethyl peroxyl radicals. International Journal of Quantum Chemistry, 2004, 98, 502-514.	1.0	4
1440	Conformational studies of benzyl alcohol and benzyl fluoride. International Journal of Quantum Chemistry, 2004, 100, 964-972.	1.0	16
1441	Relative energies, stereoelectronic interactions, and conformational interconversion in silacycloalkanes. International Journal of Quantum Chemistry, 2004, 100, 720-732.	1.0	26
1442	Theoretical Explorations of Enantioselective Alkylation Reactions of Pyrroles and Indoles Organocatalyzed by Chiral Imidazolidinones. Advanced Synthesis and Catalysis, 2004, 346, 1175-1185.	2.1	91
1443	Hydrogen Migration Over Organic Tapes: [1,5] Sigmatropic Shiftamers. European Journal of Organic Chemistry, 2004, 2004, 273-280.	1.2	6
1444	Aspects of the Aromaticity of Anthranil. European Journal of Organic Chemistry, 2004, 2004, 3340-3345.	1.2	28
1445	The Gas-Phase Hydrogen Bond Complexes between Formic Acid with Hydroxyl Radical: A Theoretical Study. ChemPhysChem, 2004, 5, 183-191.	1.0	37
1446	Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. ChemPhysChem, 2004, 5, 529-539.	1.0	46
1447	Cuii in Liquid Ammonia: An Approach by Hybrid Quantum-Mechanical/Molecular-Mechanical Molecular Dynamics Simulation. ChemPhysChem, 2004, 5, 342-348.	1.0	26
1448	On the Bond-Stretch Isomerism in the Benzo[1,2:4,5]dicyclobutadiene Systemâ€"An ab initio MR-AQCC Study. ChemPhysChem, 2004, 5, 975-981.	1.0	18
1449	FN+Cl Ions from Ionized F2NCl: a Computational Investigation on the Structure and Reactivity toward H2O. Helvetica Chimica Acta, 2004, 87, 1467-1482.	1.0	3
1450	Vibrational center-ligand couplings in transition metal complexes. Journal of Computational Chemistry, 2004, 25, 587-597.	1.5	26
1451	Solvation model induced structural changes in peptides. A quantum chemical study on Ramachandran surfaces and conformers of alanine diamide using the polarizable continuum model. Journal of Computational Chemistry, 2004, 25, 1522-1531.	1.5	35
1452	Solvation effects on alanine dipeptide: A MP2/cc-pVTZ//MP2/6-31G** study of (?, ?) energy maps and conformers in the gas phase, ether, and water. Journal of Computational Chemistry, 2004, 25, 1699-1716.	1.5	114
1453	Systematic study of vibrational frequencies calculated with the self-consistent charge density functional tight-binding method. Journal of Computational Chemistry, 2004, 25, 1858-1864.	1.5	80

#	Article	IF	Citations
1454	A theoretical study of solvent effects on tautomerism and electronic absorption spectra of 3-hydroxy-2-mercaptopyridine and 2,3-dihydroxypyridine. Journal of Computational Chemistry, 2004, 25, 1833-1839.	1.5	27
1455	Internal energy build-up in matrix-assisted laser desorption/ionization. Journal of Mass Spectrometry, 2004, 39, 579-593.	0.7	115
1456	Chiral recognition in solution and the gas phase. Experimental and theoretical studies of aromaticD- andL-amino acidâ€“Cu(II)â€“chiragen complexes. Journal of Mass Spectrometry, 2004, 39, 1044-1052.	0.7	26
1457	A Critical Evaluation of the Factors Determining the Effect of Intramolecular Hydrogen Bonding on the Oï£¿H Bond Dissociation Enthalpy of Catechol and of Flavonoid Antioxidants. Chemistry - A European Journal, 2004, 10, 933-939.	1.7	85
1458	Vibrational and Quantum-Chemical Study of Nonlinear Optical Chromophores Containing Dithienothiophene as the Electron Relay. Chemistry - A European Journal, 2004, 10, 3805-3816.	1.7	44
1459	Computational Investigation of Hydrogen Abstraction from 2-Aminoethanol by the 1,5-Dideoxyribose-5-yl Radical: A Model Study of a Reaction Occurring in the Active Site of Ethanolamine Ammonia Lyase. Chemistry - A European Journal, 2004, 10, 2781-2788.	1.7	10
1460	Controlling the Conformation of Arylamides: Computational Studies of Intramolecular Hydrogen Bonds between Amides and Ethers or Thioethers. Chemistry - A European Journal, 2004, 10, 5008-5016.	1.7	36
1461	Improved Reaction and Activation Energies of [4+2] Cycloadditions, [3,3] Sigmatropic Rearrangements and Electrocyclizations with the Spin-Component-Scaled MP2 Method. Chemistry - A European Journal, 2004, 10, 6468-6475.	1.7	64
1462	Understanding the Nature of the Molecular Mechanisms Associated with the Competitive Lewis Acid Catalyzed[4+2] and[4+3] Cycloadditions between Arylidenoxazolone Systems and Cyclopentadiene: A DFT Analysis. Chemistry - A European Journal, 2004, 10, 4742-4749.	1.7	27
1463	Interaction of divalent metal cations with ferrierite: insights from density functional theory. Microporous and Mesoporous Materials, 2004, 68, 45-53.	2.2	13
1464	Ab initio and density functional force field studies on the IR spectra and structure of diazonium dicyanomethylide (diazodicyanomethane). Journal of Molecular Structure, 2004, 691, 71-77.	1.8	7
1465	Experimental and computational studies of the structure and vibrational spectra of 4-dimethylamino pyridinium-betaine of squaric acid. Journal of Molecular Structure, 2004, 691, 241-248.	1.8	23
1466	Î²-Nitrostyrene derivativesâ€”a conformational study by combined Raman spectroscopy and ab initio MO calculations. Journal of Molecular Structure, 2004, 692, 91-106.	1.8	13
1467	A theoretical study of tetrabutylammonium [bis(1,3-dithiole-2-thione-4,5-dithiolato)bismuthate], [NBu4][Bi(dmit)2]: infrared spectrum in the solid state and solvation effects on the molecular geometry. Inorganica Chimica Acta, 2004, 357, 1047-1053.	1.2	12
1468	3-Silaoxetane and 3-silathietane: structure and reactivity studies on the basis of spectroscopic data and theoretical calculations. Inorganica Chimica Acta, 2004, 357, 1920-1930.	1.2	8
1469	Sulfurous acid (H2SO3) on Io?. Icarus, 2004, 169, 242-249.	1.1	20
1470	Climbing the internal energy ladder: the unimolecular decomposition of ionized poly(vinyl acetate). International Journal of Mass Spectrometry, 2004, 231, 59-68.	0.7	13
1471	Catalyzed isomerization and decarbonylation of ionized formic acid and dihydroxycarbene. International Journal of Mass Spectrometry, 2004, 231, 83-95.	0.7	7

#	Article	IF	Citations
1472	Isomerization and dissociation of the acetonitrile molecular cation. International Journal of Mass Spectrometry, 2004, 235, 15-23.	0.7	22
1473	Formation of C6HnSi+ (n = 5â€“8) from phenylsilane: an experimental and theoretical study. International Journal of Mass Spectrometry, 2004, 237, 1-12.	0.7	14
1474	Cyclic diphenic hydrazide: crystal structure, resolution, absolute configuration, and enantiomerization pathway investigation. Tetrahedron: Asymmetry, 2004, 15, 537-543.	1.8	9
1475	Structures, harmonic vibrational frequencies and interconversion potential energy profile of Ni+(C2H2)2 complexes. Computational and Theoretical Chemistry, 2004, 709, 167-170.	1.5	6
1476	Quantum chemical DFT and spectroscopic study of a pushâ€“pull chromophore for second-order nonlinear optics containing bithiophene as the electron relay. Computational and Theoretical Chemistry, 2004, 709, 187-193.	1.5	27
1477	On the atomic additivity of the zero point vibrational energy in molecules. Computational and Theoretical Chemistry, 2004, 672, 201-207.	1.5	10
1478	Theoretical elucidation of structureâ€“activity relationship for coumarins to scavenge peroxyl radical. Computational and Theoretical Chemistry, 2004, 673, 199-202.	1.5	36
1479	A Hartreeâ€“Fock, MP2 and DFT computational study of the structures and energies of â€³b2 ions derived from deprotonated peptides. A comparison of method and basis set used on relative product stabilities. Computational and Theoretical Chemistry, 2004, 675, 149-162.	1.5	18
1480	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. Computational and Theoretical Chemistry, 2004, 674, 213-225.	1.5	15
1481	A DFT study on the intramolecular dissociation pathways of ethyl fluoroformate radical cation in the gas phase; I. Enol path. Computational and Theoretical Chemistry, 2004, 677, 97-104.	1.5	1
1482	On simple, accurate calculations of atomic charges, bond properties and molecular energies. IV. Butane gauche interactions and vibrational energies of alkylcyclohexanes and related polycyclic hydrocarbons. Computational and Theoretical Chemistry, 2004, 682, 153-158.	1.5	6
1483	Theoretical group 14 chemistry. Part 2. Si4R6: a theoretical approach. Computational and Theoretical Chemistry, 2004, 680, 91-97.	1.5	38
1484	Silylisocyanates and silylisothiocyanates: a comparative theoretical study. Computational and Theoretical Chemistry, 2004, 682, 17-27.	1.5	5
1485	Theoretical studies on unimolecular reactions of thioacetaldehyde. Computational and Theoretical Chemistry, 2004, 682, 29-35.	1.5	3
1486	Substituent effect on the stability of TS of Type-I ene cyclization: a theoretical study. Computational and Theoretical Chemistry, 2004, 684, 187-195.	1.5	4
1487	Additivity of electron correlation energy and the ab initio MO calculation of (0â€“0) S1â†S0 transition energies: polychlorinated dibenzofurans. Computational and Theoretical Chemistry, 2004, 710, 19-23.	1.5	4
1488	A theoretical study of the ion pair SN2 reaction between lithium isocyanates with methyl fluoride with inversion and retention mechanism. Computational and Theoretical Chemistry, 2004, 686, 65-70.	1.5	7
1489	A G3(MP2) study on the electrocyclic reactions of [12]annulene. Computational and Theoretical Chemistry, 2004, 711, 133-139.	1.5	0

#	Article	IF	Citations
1490	Ab initio study of the cycloaddition reaction between hexatriene and ethylene. Computational and Theoretical Chemistry, 2004, 712, 49-66.	1.5	3
1491	A theoretical study on bond dissociation energies and oxidation potentials of monolignols. Computational and Theoretical Chemistry, 2004, 712, 197-205.	1.5	28
1492	aCLIMAX 4.0.1, The new version of the software for analyzing and interpreting INS spectra. Computer Physics Communications, 2004, 157, 226-238.	3.0	295
1493	The adsorption site of methoxy and ethoxy on Cu(100) as determined by vibrational spectroscopy and first principle calculations. Surface Science, 2004, 549, 87-96.	0.8	4
1494	Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces. Surface Science, 2004, 549, 121-133.	0.8	90
1495	Fermi resonance coupling in the Câ€“H stretching region of methoxide adsorbed on clean Ru(001): a combined RAIRS and theoretical study. Surface Science, 2004, 566-568, 965-970.	0.8	13
1496	Unusual reversal of regioselectivity in antibody-mediated aldol additions with unsymmetrical methyl ketones. Tetrahedron, 2004, 60, 619-632.	1.0	25
1497	Computational studies of vinyl-stabilized halonium ions. Tetrahedron, 2004, 60, 1191-1196.	1.0	7
1498	Kinetics and mechanism of thermal gas-phase elimination of Î±- and Î²- (N-arylamino)propanoic acid: experimental and theoretical analysis. Tetrahedron, 2004, 60, 3045-3049.	1.0	14
1499	A DFT study of the Huisgen 1,3-dipolar cycloaddition between hindered thiocarbonyl ylides and tetracyanoethylene. Tetrahedron, 2004, 60, 5053-5058.	1.0	63
1500	Gas phase UV and IR absorption spectra of CxF2x+1CHO (x = 1â€“4). Journal of Fluorine Chemistry, 2004, 125, 1925-1932.	0.9	20
1501	Ab initio studies of solvent effect on molecular conformation and vibrational spectra of diacetamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1115-1126.	2.0	5
1502	IR spectral and structural changes caused by the conversion of 3-methoxy-4-hydroxybenzaldehyde (vanillin) into the oxyanion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2013-2019.	2.0	25
1503	Raman, SERS and theoretical studies of papaverine hydrochloride and its neutral species. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2021-2028.	2.0	14
1504	Density functional theory and ab initio studies of geometry, electronic structure and vibrational spectra of novel benzothiazole and benzotriazole herbicides. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2343-2354.	2.0	44
1505	Spectrochemical, ab initio and density functional studies on the conversion of 2-hydroxybenzonitrile (o-cyanophenol) into the oxyanion. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2601-2610.	2.0	50
1506	Ab initio and DFT studies of the vibrational spectra of hydrogen-bonded PhOHâ€¦(H2O)4 complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 3049-3057.	2.0	15
1507	Relationship between force constants and bond lengths for CX (X = C, Si, Ge, N, P, As, O, S, Se, F, Cl and) Tj ETQq1 1 0.784314 rgBT /Ov Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 3013-3023.	2.0	37

#	Article	IF	Citations
1508	Experimental and computational studies of the structure and vibrational spectra of aminomethyl-dimethyl-phosphine oxide and its labeled isomer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 2993-3000.	2.0	3
1509	Gas-phase reactions of protonated tryptophan. Journal of the American Society for Mass Spectrometry, 2004, 15, 65-76.	1.2	106
1510	Circumvention of orbital symmetry restraints by 1,3-H-shifts of enolic radical cations. Journal of the American Society for Mass Spectrometry, 2004, 15, 972-981.	1.2	7
1511	Decomposition of protonated formic acid: One transition stateâ€"Two product channels. Journal of the American Society for Mass Spectrometry, 2004, 15, 982-988.	1.2	14
1512	Experimental and theoretical study of the dissociation enthalpy of the Nâ€"O bond on 2-hydroxypyridine N-oxide: theoretical analysis of the energetics of the Nâ€"O bond for hydroxypyrydine N-oxide isomers. Journal of Chemical Thermodynamics, 2004, 36, 107-113.	1.0	14
1513	Thermochemical study of chloropyrazines and chloroquinoxalines. Journal of Chemical Thermodynamics, 2004, 36, 377-383.	1.0	13
1514	Vapour pressure of diethyl phthalate. Journal of Chemical Thermodynamics, 2004, 36, 929-937.	1.0	23
1515	Structure and dynamics of hydrated ionsâ€"new insights through quantum mechanical simulations. Journal of Molecular Liquids, 2004, 110, 105-122.	2.3	94
1516	The conversion of 3- and 4-hydroxybenzonitriles (m- and p-cyanophenols) into oxyanions, followed by IR spectra, ab initio and density functional calculations. Journal of Molecular Structure, 2004, 692, 23-35.	1.8	18
1517	X-Ray, MP2 and DFT studies of the structure and vibrational spectra of homarinium chloride. Journal of Molecular Structure, 2004, 700, 109-125.	1.8	15
1518	Vibrational spectra of aluminosilicate structural clusters. Journal of Molecular Structure, 2004, 704, 247-257.	1.8	37
1519	Conformational analysis of a trihydroxylated derivative of cinnamic acidâ€"a combined Raman spectroscopy and Ab initio study. Journal of Molecular Structure, 2004, 693, 103-118.	1.8	37
1520	Vibrational spectroscopy of the ring structures in silicates and siloxanes. Journal of Molecular Structure, 2004, 704, 63-69.	1.8	27
1521	Simulation of IR and Raman spectra based on scaled DFT force fields: a case study of 2-(methylthio)benzonitrile, with emphasis on band assignment. Journal of Molecular Structure, 2004, 702, 9-21.	1.8	202
1522	Infrared absorption, Raman, and SERS investigations in conjunction with theoretical simulations on a phenothiazine derivative. Chemical Physics, 2004, 298, 87-95.	0.9	27
1523	FT-Raman, surface-enhanced Raman spectroscopy and theoretical investigations of diclofenac sodium. Chemical Physics, 2004, 298, 167-174.	0.9	37
1524	Molecular and vibrational structure of 2,4-dinitrophenol: FT-IR, FT-Raman and quantum chemical calculations. Chemical Physics, 2004, 300, 1-11.	0.9	96
1525	Acetylenic/cyanoacetylenic complexes: simulation of the Titanâ€™s atmosphere chemistry. Chemical Physics, 2004, 300, 143-151.	0.9	13

#	Article	IF	Citations
1526	Reaction of the C3 carbon cluster with benzene. Chemical Physics, 2004, 303, 165-177.	0.9	10
1527	Theoretical study on the reaction path and rate constants of the hydrogen atom abstraction reaction of CH2O with CH3/OH. Chemical Physics, 2004, 307, 35-43.	0.9	17
1528	Semiempirical calculations of the collective optical excitations in substituted oligodiacetylenes. Applied Surface Science, 2004, 226, 99-107.	3.1	3
1529	Ab initio study of the hydrolysis of carbonyl difluoride (CF2O): importance of an additional water molecule. Chemical Physics Letters, 2004, 396, 110-116.	1.2	24
1530	A new model for the molecular structure of supported vanadium oxide catalysts. Chemical Physics Letters, 2004, 397, 277-281.	1.2	48
1531	Hydrogen bonding in complex of serine with histidine: computational and spectroscopic study of model compounds. Chemical Physics Letters, 2004, 400, 117-121.	1.2	20
1532	On the microscopic mechanism of carbon gasification: A theoretical study. Carbon, 2004, 42, 2921-2928.	5.4	58
1533	Molecule orientation in self-assembled monolayers determined by infrared-visible sum-frequency generation spectroscopy. Applied Surface Science, 2004, 237, 445-450.	3.1	12
1534	The infrared spectrum of matrix isolated aminoacetonitrile, a precursor to the amino acid glycine. Advances in Space Research, 2004, 33, 40-43.	1.2	27
1535	Optimising the EVA descriptor for prediction of biological activity. Organic and Biomolecular Chemistry, 2004, 2, 3301.	1.5	9
1536	Methane activation by silica-supported Zr(iv) hydrides: the dihydride [(î€,SiO)2ZrH2] is much faster than the monohydride [(î€,SiO)3ZrH]. Chemical Communications, 2004, , 1729-1731.	2.2	35
1537	An investigation of the germylene addition reaction, GeH2â€‰+â€‰C2H2: Time-resolved gas-phase kinetic studies and quantum chemical calculations of the reaction energy surface. Physical Chemistry Chemical Physics, 2004, 6, 3370-3382.	1.3	27
1538	Proton Affinity of Lysine Homologues from the Extended Kinetic Method. Journal of Physical Chemistry A, 2004, 108, 326-332.	1.1	60
1539	A DFT Study on Isomorphously Substituted MCM-22 Zeolite. Journal of Physical Chemistry A, 2004, 108, 6730-6734.	1.1	47
1540	Solid state study of the copper(ii) complex of 2-hydroxyiminopropanoic acid. New Journal of Chemistry, 2004, 28, 477-483.	1.4	22
1541	Thermochemistry of 2-amino-3-quinoxalinecarbonitrile-1,4-dioxide. Evaluation of the mean dissociation enthalpy of the (Nâ€“O) bond. Organic and Biomolecular Chemistry, 2004, 2, 2507-2512.	1.5	21
1542	Neutral and ionic dissociation patterns in hexacoordinate silicon chelates: a model nucleophilic substitution at pentacoordinate silicon. Chemical Communications, 2004, , 1644.	2.2	27
1543	Calculating vibrational frequencies of amides: From formamide to concanavalin A. Physical Chemistry Chemical Physics, 2004, 6, 998-1005.	1.3	25

#	Article	IF	Citations
1544	Characterization by time-resolved UV-Vis and infrared absorption spectroscopy of an intramolecular charge-transfer state in an organic electron-donorâ€“bridgeâ€“acceptor system. Photochemical and Photobiological Sciences, 2004, 3, 246-251.	1.6	17
1545	Vibrationally resolved electronic spectroscopy and theoretical studies of deuterated 2-(2â€²-pyridyl)indole. Physical Chemistry Chemical Physics, 2004, 6, 363-367.	1.3	16
1546	Reaction of tetramethylpiperidine N-oxides with persistent triplet diphenylcarbenes. Organic and Biomolecular Chemistry, 2004, 2, 1500.	1.5	4
1547	Ab initio MO and DFT study of syn-sesquinorbornatrienyl dication and its isoelectronic boron analogueElectronic supplementary information (ESI) available: bond distances and bond angles of structures 6a, 6c, 7a and 7c calculated at the MP2/6-31+G* and B3LYP/6-31G* levels of theory (Table S1). See http://www.rsc.org/suppdata/nj/b4/b403802a/. New Journal of Chemistry, 2004, 28, 880.	1.4	7
1548	Infrared and resonance Raman studies of metal cation sensors in which an azacrown ether is linked to (bpy)Re(CO)3 via an alkenyl or alkynyl spacerElectronic supplementary information available (ESI): synthesis and characterisation of L1b, L2b, 1b and 2b; colour figure of displacement vectors calculated for selected equivalent modes of L1b and L2b. See http://www.rsc.org/suppdata/cp/b4/b408338e/. Physical Chemistry Chemical Physics, 2004, 6, 4595.	1.3	13
1549	Formation of the heterocumulene anion SCCCN? by a cyano migration from the radical anion of 1,2-dicyanoethylenedithiolateDedicated to Professor John H. Bowie on the occasion of his 65th Birthday and in recognition to his pioneering work on the gas phase chemistry of anions.. Organic and Biomolecular Chemistry, 2004, 2, 190.	1.5	2
1550	Dissociative recombination cross section and branching ratios of protonated dimethyl disulfide and N-methylacetamide. Journal of Chemical Physics, 2004, 121, 5700-5708.	1.2	21
1551	Density Functional Calculations. , 2004, , 385-445.		0
1552	Accurate prediction of heat of formation by combining Hartreeâ€“Fock/density functional theory calculation with linear regression correction approach. Journal of Chemical Physics, 2004, 121, 7086-7095.	1.2	52
1553	Photodissociation spectroscopy and dynamics of the CH2CFO radical. Journal of Chemical Physics, 2004, 120, 8494-8504.	1.2	10
1554	Confirmation of the â€œlong-livedâ€•tetra-nitrogen (N4) molecule using neutralization-reionization mass spectrometry and ab initio calculations. Journal of Chemical Physics, 2004, 120, 10561-10578.	1.2	46
1555	Assignment of photoelectron spectra of Au[sub n]O[sub 2][sup â^’] (n=2,4,6) clusters. Journal of Chemical Physics, 2004, 121, 621.	1.2	19
1556	The energetics of the isomeric anthrols. Molecular Physics, 2004, 102, 623-625.	0.8	11
1557	Entropy Changes in the Dissociation of Proton-Bound Complexes:Â A Variational RRKM Studyâ€. Journal of Physical Chemistry A, 2004, 108, 9726-9732.	1.1	9
1558	Structure and Dynamics of Au+Ion in Aqueous Solution: Ab Initio QM/MM MD Simulations. Journal of the American Chemical Society, 2004, 126, 2582-2587.	6.6	37
1559	Theoretical Survey of the Potential Energy Surfaces Associated with the N+(3P,1D) + C2H4Reactions in the Gas Phaseâ€. Journal of Physical Chemistry A, 2004, 108, 9762-9767.	1.1	2
1560	Photolysis of 3-(2-Formylphenyl)-3-chlorodiazirine in an Ar Matrix at Low Temperature. Journal of Organic Chemistry, 2004, 69, 3538-3545.	1.7	7
1561	Computational Study of the Oxygen Initiated Decomposition of 2-Oxepinoxy Radical:Â A Key Intermediate in the Oxidation of Benzene. Journal of Physical Chemistry A, 2004, 108, 8419-8433.	1.1	20

#	Article	IF	Citations
1562	A Study of the Thermal Decomposition of 2-Azidoacetamide by Ultraviolet Photoelectron Spectroscopy and Matrix-Isolation Infrared Spectroscopy:Â Identification of the Imine Intermediate H2NCOCHNH. Journal of Physical Chemistry A, 2004, 108, 5299-5307.	1.1	25
1563	Mechanism of Addition of Organocuprates to Alkynyl Carbonyl Compounds. A Mechanistic Bridge between Carbocupration and Conjugate Addition. Organometallics, 2004, 23, 1081-1088.	1.1	26
1564	Ab Initio MR-CISD Study of Gas-Phase Basicity of Formamide in the First Excited Singlet State. Journal of Physical Chemistry A, 2004, 108, 10317-10325.	1.1	24
1565	Structures and Properties of Polyphosphinoborane:Â an Oligomeric Theoretical Study. Macromolecules, 2004, 37, 1009-1015.	2.2	31
1566	Kinetic and Thermodynamic Acidities of Pentacarbonyl(cyclobutenylidene)chromium Complexes. Effect of Antiaromaticity in the Conjugate Anion. An Experimental and Computational Studyâ€. Journal of Organic Chemistry, 2004, 69, 5232-5239.	1.7	8
1567	Theoretical study of nitric oxide adsorption on Au clusters. Journal of Chemical Physics, 2004, 121, 2558.	1.2	78
1568	Generation of Neutral CCCCBO in the Gas Phase from [CCCCBO]-and Rearrangement of Energized CCCCBO to OCCCCB:Â A Joint Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2004, 108, 2426-2430.	1.1	13
1569	Polycyclic Aromatic Hydrocarbons with Five-Membered Rings:Â Distributions within Isomer Families in Experiments and Computed Equilibria. Journal of Physical Chemistry A, 2004, 108, 5399-5407.	1.1	8
1570	Theoretical Study of the Straight-Chain C4H7Radical Isomers and Their Dissociation and Isomerization Transition States. Journal of Physical Chemistry A, 2004, 108, 2268-2277.	1.1	28
1571	The Woodwardâ^'Hoffmannâ^'De Puy Rule Revisitedâ€. Organic Letters, 2004, 6, 905-908.	2.4	31
1572	On the Origin of Cis Selectivity in the Cyclization of N-Protected 2-Substituted 3-Aza-5-hexenyl Radicals:Â A Density Functional Study. Journal of Organic Chemistry, 2004, 69, 1487-1491.	1.7	13
1573	A Theoretical Study of the Reaction of GeH2with CO2and the Dissociation Paths of the Reaction Products. Journal of Physical Chemistry A, 2004, 108, 4002-4007.	1.1	7
1574	â€œStructure Breakingâ€•Effect of Hydrated Cs+. Journal of Physical Chemistry A, 2004, 108, 1509-1514.	1.1	93
1575	A Practical Spectroscopic and Theoretical Approach To Study the Electrochromism in Molecular-Based Materials:â€‰ The Case of a Family of Dendrimerlike Poly(6-azulenylethenyl)benzenes. Journal of Physical Chemistry B, 2004, 108, 18463-18471.	1.2	6
1576	The Formic Acidâ^'Trifluoroacetic Acid Bimolecule. Gas-Phase Infrared Spectrum and Computational Studies. Journal of Physical Chemistry A, 2004, 108, 4610-4618.	1.1	16
1577	Complexation of the Lowest Generation Poly(amidoamine)-NH2Dendrimers with Metal Ions, Metal Atoms, and Cu(II) Hydrates:Â An ab Initio Study. Journal of Physical Chemistry B, 2004, 108, 15992-16001.	1.2	61
1578	A Raman and Computational Study of Two Dithienyl Naphthodithiophenes:Â Synthesis and Characterization of New Polymers Showing Low Band Gap Optical and Electroactive Features. Journal of Physical Chemistry B, 2004, 108, 7611-7619.	1.2	4
1579	Harmonic Model Description of the Franckâ^'Condon Density for a Betaine Dye Molecule. Journal of Physical Chemistry A, 2004, 108, 2607-2616.	1.1	21

#	Article	IF	Citations
1580	Rate Constants for the Hydrogen Abstractions in the OH-Initiated Oxidation of Glycolaldehyde. A Variational Transition-state Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 5117-5125.	1.1	12
1581	Application of a Lumped-Inertia Technique to Vibrational Analysis of the Torsional-Twisting Modes of Low Molecular Weight Polyphenylenes and Polyethynylphenylenes. Journal of Physical Chemistry A, 2004, 108, 2499-2507.	1.1	5
1582	Ab Initio Study of the Formation of Glycine via Amino Acetonitrile and Amino-Cyano-Acetic Acid. Journal of Physical Chemistry A, 2004, 108, 3798-3805.	1.1	21
1583	Evidence for Specific Solvation of Two Halocarbene Amides. Journal of the American Chemical Society, 2004, 126, 5750-5762.	6.6	31
1584	Substituent Effects in Xanthate-Mediated Polymerization of Vinyl Acetate:â€‰Ab Initio Evidence for an Alternative Fragmentation Pathway. Macromolecules, 2004, 37, 590-596.	2.2	124
1585	Experimental and Theoretical Analysis of the Photochemistry and Thermal Reactivity of Ethyl Diazomalonate and Its Diazirino Isomer. The Role of Molecular Geometry in the Decomposition of Diazocarbonyl Compounds. Journal of the American Chemical Society, 2004, 126, 11293-11302.	6.6	24
1586	Spin Trapping by 5-Carbamoyl-5-methyl-1-pyrrolineN-Oxide (AMPO):Â Theoretical and Experimental Studies. Journal of Organic Chemistry, 2004, 69, 7994-8004.	1.7	56
1587	Time-Resolved in Situ ATR Spectroscopy of 2-Propanol Oxidation over Pd/Al2O3:Â Evidence for 2-Propoxide Intermediate. Journal of Physical Chemistry B, 2004, 108, 13364-13369.	1.2	46
1588	Ab Initio Study of the Additionâ^'Fragmentation Equilibrium in RAFT Polymerization:Â When Is Polymerization Retarded?. Macromolecules, 2004, 37, 5023-5031.	2.2	115
1589	Activation of the Sulfhydryl Group by Mo Centers:Â Kinetics of Reaction of Benzyl Radical with a Binuclear Mo(Î¼-SH)Mo Complex and with Arene and Alkane Thiols. Journal of the American Chemical Society, 2004, 126, 6680-6691.	6.6	9
1590	Density Functional Theory Studies on Structure, Spectra, and Electronic Properties of 3,7-Dinitrodibenzobromolium Cation and Chloride. Journal of Physical Chemistry A, 2004, 108, 7596-7602.	1.1	1
1591	Entropies in Solution from Entropies in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 2720-2725.	1.1	98
1592	Characterization of 5-Hydroxy-8-oxo-7,8-dihydroguanosine in the Photosensitized Oxidation of 8-Oxo-7,8-dihydroguanosine and Its Rearrangement to Spiroiminodihydantoin. Journal of the American Chemical Society, 2004, 126, 16777-16782.	6.6	80
1593	Electronic Decoherence Induced by Intramolecular Vibrational Motions in a Betaine Dye Molecule. Journal of Physical Chemistry B, 2004, 108, 6723-6732.	1.2	55
1594	Raman Spectra of Electrosynthesized Polyfuran:â€‰A Combined Experimental and Theoretical Study. Journal of Physical Chemistry B, 2004, 108, 2195-2199.	1.2	33
1595	Theoretical Study of the Thermal Dissociation Mechanism of AH4(A = Si, Ge, Sn, Pb). Journal of Physical Chemistry A, 2004, 108, 4909-4915.	1.1	6
1596	Chiroptical Properties of Organic Radical Cations. The Electronic and Vibrational Circular Dichroism Spectra of Î±-Tocopherol Derivatives and Sterically Hindered Chiral Hydroquinone Ethers. Journal of Physical Chemistry A, 2004, 108, 9540-9549.	1.1	14
1597	Theoretical Analysis of the Smallest Carbon Cluster Containing a Planar Tetracoordinate Carbon. Journal of the American Chemical Society, 2004, 126, 16160-16169.	6.6	126

#	Article	IF	Citations
1598	Solvent and Structural Effects in the Nâˆ’H Bond Homolytic Dissociation Energy. Journal of Physical Chemistry A, 2004, 108, 2119-2130.	1.1	54
1599	Atmospheric Chemistry ofn-CxF2x+1CHO (x= 1, 3, 4):Â Reaction with Cl Atoms, OH Radicals and IR Spectra of CxF2x+1C(O)O2NO2. Journal of Physical Chemistry A, 2004, 108, 5189-5196.	1.1	46
1600	Reactions of One-Electron-Oxidized Methionine with Oxygen:Â An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 6222-6230.	1.1	32
1601	The Role of Odd-Electron Intermediates and In-Cage Electron Transfer in Ultrafast Photochemical Disproportionation Reactions in Lewis Bases. Journal of the American Chemical Society, 2004, 126, 11414-11415.	6.6	19
1602	DFT and HF Studies of the Geometry, Electronic Structure, and Vibrational Spectra of 2-Nitrotetraphenylporphyrin and Zinc 2-Nitrotetraphenylporphyrin. Journal of Physical Chemistry A, 2004, 108, 6052-6058.	1.1	7
1603	Structural, Electronic, and Vibrational Properties of the Tiâˆ’Oâˆ’Ti Quantum Wires in the Titanosilicate ETS-10. Journal of Physical Chemistry B, 2004, 108, 1328-1336.	1.2	79
1604	Surface-Enhanced Raman Scattering and Density Functional Theoretical Study of Anthranil Adsorbed on Colloidal Silver Particles. Journal of Physical Chemistry B, 2004, 108, 17491-17496.	1.2	36
1605	A Density Functional Theory Study on the Adsorption of Chlorobenzene on the Si(111)-7 Ã— 7 Surface. Journal of Physical Chemistry B, 2004, 108, 14049-14055.	1.2	16
1606	Pericyclic Reactions between Aminoboranes R2BNR2â€˜ and Alkenes:â€‰ [4+2] vs [2+2] Transition States. Organometallics, 2004, 23, 850-854.	1.1	12
1607	Reduction Mechanisms of Ethylene, Propylene, and Vinylethylene Carbonates. Journal of the Electrochemical Society, 2004, 151, A178.	1.3	181
1608	Gas-Phase Reactivity of Charged Ï€-Type Biradicals. Journal of the American Chemical Society, 2004, 126, 12957-12967.	6.6	16
1609	DFT Study of Pericyclic Reaction Cascades in the Synthesis of Antibiotic TAN-1085. Organic Letters, 2004, 6, 4273-4275.	2.4	17
1610	Surprises with strain energy and sulpholane (tetrahydrothiophene 1,1-dioxide): a combined experimental and theoretical investigation. Molecular Physics, 2004, 102, 525-530.	0.8	9
1611	Silylene and Germylene Additions to 1,3-Diynes:Â Bis(silacyclopropenes) versus Germaethenes Formation, a DFT Study. Organometallics, 2004, 23, 1570-1575.	1.1	8
1612	The Application of the Effective Fragment Potential Method to Molecular Anion Solvation:Â A Study of Ten Oxyanionâˆ’Water Clusters, A-(H2O)1-4. Journal of Physical Chemistry A, 2004, 108, 833-839.	1.1	23
1613	Computational Study of Î³-Butyrolactone and Li+/Î³-butyrolactone in Gas and Liquid Phases. Journal of Physical Chemistry B, 2004, 108, 17992-18002.	1.2	38
1614	Transient Mixed-Valence Character of ReI4(CO)12(4,4â€˜-bpy)4Cl4. Inorganic Chemistry, 2004, 43, 132-141.	1.9	14
1615	Intramolecular and Low-Frequency Intermolecular Vibrations of Pentacene Polymorphs as a Function of Temperature. Journal of Physical Chemistry B, 2004, 108, 1822-1826.	1.2	53

#	Article	IF	Citations
1616	Thermochemical Properties, Rotation Barriers, Bond Energies, and Group Additivity for Vinyl, Phenyl, Ethynyl, and Allyl Peroxides. Journal of Physical Chemistry A, 2004, 108, 8353-8366.	1.1	60
1617	Reliable Theoretical Procedures for the Calculation of Electronic-Structure Information in Hydrogen Abstraction Reactions. Journal of Physical Chemistry A, 2004, 108, 3865-3872.	1.1	148
1618	Infrared Cavity Ringdown Spectroscopy of Jet-Cooled Nucleotide Base Clusters and Water Complexes. Journal of Physical Chemistry A, 2004, 108, 10989-10996.	1.1	44
1619	Experimental and Computational Studies of the Metalâ^'Metal Stretching Vibration in X3Mâ‹®MX3Compounds (X = Alkoxide, Alkyl, Amide). Inorganic Chemistry, 2004, 43, 1762-1769.	1.9	5
1620	Photochemistry of Butyrophenone:Â Combined Complete-Active-Space Self-Consistent Field and Density Functional Theory Study of Norrish Type I and II Reactions. Journal of Physical Chemistry A, 2004, 108, 5386-5392.	1.1	34
1621	Semiempirical and Ab Initio Studies of the Structure and Spectroscopy of the Azo Dye Direct Blue 1:Â Comparison with Experiment. Journal of Physical Chemistry A, 2004, 108, 10208-10218.	1.1	17
1622	Molecular Modeling of Environmentally Important Processes: Reduction Potentials. Journal of Chemical Education, 2004, 81, 596.	1.1	150
1623	Kinetic Energy Release Distributions for Tropylium and Benzylium Ion Formation from the Toluene Cationâ€. Journal of Physical Chemistry A, 2004, 108, 9777-9786.	1.1	24
1624	Adhesion of Bacterial Exopolymers to Î±-FeOOH:Â Inner-Sphere Complexation of Phosphodiester Groups. Langmuir, 2004, 20, 11108-11114.	1.6	122
1625	Pericyclic Reactions between Iminoboranes RBâ‹®NRâ€˜ and Alkynes:Â [4 + 2] vs [2 + 2] Transition Statesâ€. Organometallics, 2004, 23, 5048-5053.	1.1	6
1626	Water Molecule Adsorption on Protonated Dipeptides. Journal of the American Chemical Society, 2004, 126, 1206-1213.	6.6	32
1627	Gas-Phase Synthesis and Reactivity of the Organomagnesates [CH3MgL2]-(L = Cl and O2CCH3):Â From Ligand Effects to Catalysis. Journal of the American Chemical Society, 2004, 126, 12173-12183.	6.6	109
1628	Combined Raman and Computational Study of a Novel Series of Macrocyclic Ï€-Conjugated Diacetylene-Bridged Î±-Linked Oligothiophenes. Journal of Physical Chemistry B, 2004, 108, 3158-3167.	1.2	24
1629	Poly(ethylene oxide):Â Electronic Structure, Energetics, and Vibrational Spectrum. Journal of Physical Chemistry B, 2004, 108, 12677-12684.	1.2	19
1630	The hydrogenation of 1,3-pentadiene over an alumina-supported palladium catalyst: an FTIR study. Physical Chemistry Chemical Physics, 2004, 6, 5588.	1.3	11
1631	Structure and Dynamics of Neutral Î²-H Agostic Nickel Alkyls:Â A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2004, 126, 11984-11994.	6.6	76
1632	Phonons and structures of tetracene polymorphs at low temperature and high pressure. Physical Review B, 2004, 70, .	1.1	75
1633	Generation and Trapping of the 4-Biphenylyloxenium Ion by Water and Azide:â€‰ Comparisons with the 4-Biphenylylnitrenium Ion. Journal of the American Chemical Society, 2004, 126, 7748-7749.	6.6	35

#	Article	IF	Citations
1634	Harmonic Vibrational Frequencies:â€‰ Scaling Factors for HF, B3LYP, and MP2 Methods in Combination with Correlation Consistent Basis Sets. Journal of Physical Chemistry A, 2004, 108, 9213-9217.	1.1	405
1635	Nanostructured Oxides in Chemistry:â€‰ Characterization and Properties. Chemical Reviews, 2004, 104, 4063-4104.	23.0	909
1636	A DFT Study of the Ground State Multiplicities of Linear vs Angular Polyheteroacenes. Journal of the American Chemical Society, 2004, 126, 16232-16241.	6.6	74
1637	Isotope effect on the Jâ€“T distortion of partially deuteriated benzene cation radicals: an experimental EPR and theoretical DFT study. Physical Chemistry Chemical Physics, 2004, 6, 1658-1665.	1.3	6
1638	STUDY OF INTRAMOLECULAR HYDROGEN BONDING IN ORTHO-SUBSTITUTED ACETANILIDE COMPOUNDS USING COMPUTATIONAL METHODS. Journal of Theoretical and Computational Chemistry, 2004, 03, 527-542.	1.8	5
1639	Efficient calculation of potential energy surfaces for the generation of vibrational wave functions. Journal of Chemical Physics, 2004, 121, 9313-9322.	1.2	267
1640	On the Mechanisms of Oxidation of Organic Sulfides by H2O2in Aqueous Solutions. Journal of the American Chemical Society, 2004, 126, 900-908.	6.6	98
1641	Nature of the Cu+â^'NO Bond in the Gas Phase and at Different Types of Cu+Sites in Zeolite Catalysts. Journal of Physical Chemistry B, 2004, 108, 13674-13682.	1.2	86
1642	Electronic Modulation of Dithienothiophene (DTT) as Ï€-Center of D-Ï€-D Chromophores on Optical and Redox Properties:Â Analysis by UVâ^'Visâ^'NIR and Raman Spectroscopies Combined with Electrochemistry and Quantum Chemical DFT Calculations. Journal of the American Chemical Society, 2004, 126, 13363-13376.	6.6	52
1643	Identification of synthetic precursors of amphetamine-like drugs using Raman spectroscopy and ab initio calculations: Î²-Methyl-Î²-nitrostyrene derivatives. Analyst, The, 2004, 129, 1106-1117.	1.7	18
1644	Ab Initio Investigation of the Structures and Properties of Polyaminoborane. Journal of Physical Chemistry A, 2004, 108, 9616-9624.	1.1	19
1645	DENSITY FUNCTIONAL THEORETICAL STUDY OF NITRATED POLYCYCLIC AROMATIC HYDROCARBONS. Polycyclic Aromatic Compounds, 2004, 24, 37-64.	1.4	33
1646	A Comparison of Acetyl- and Methoxycarbonylnitrenes by Computational Methods and a Laser Flash Photolysis Study of Benzoylnitrene. Journal of Organic Chemistry, 2004, 69, 8583-8593.	1.7	84
1647	Gas phase ion chemistry of charged silver(I) adenine ions via multistage mass spectrometry experiments and DFT calculationsGas phase ion chemistry of biomolecules, Part 38. For part 37, see ref. 1.Electronic supplementary information available: Tables (energies and bond lengths) and figures (MS) Tj ETQq1 1 0.784314 rgBT /Overl Transactions, 2004, , 197.	1.7	39
1648	Ab Initio Study of the Lowest Energy Conformers and IR Spectra of Poly(amidoamine)-G0 Dendrimers. Journal of Physical Chemistry B, 2004, 108, 15982-15991.	1.2	39
1649	Experimental and Theoretical Studies of Fused-Ring Persistent [1,2,4]Thiadiazinyl Radicalsâ€. Journal of Organic Chemistry, 2004, 69, 7525-7536.	1.7	35
1650	Ab initio Calculations. , 2004, , 159-337.		1
1651	Double hydrogen tunneling revisited: The breakdown of experimental tunneling criteria. Journal of Chemical Physics, 2004, 120, 11650-11657.	1.2	54

#	Article	IF	Citations
1652	Firstâ€“principles quantum chemistry in the life sciences. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 2653-2670.	1.6	11
1653	Triplet Diphenylcarbenes Protected byo-Aryl Groups. Journal of the American Chemical Society, 2004, 126, 11900-11913.	6.6	20
1654	Global Optimization of H-Passivated Si Clusters at the Ab Initio Level via the GAM1 Semiempirical Method. Journal of Physical Chemistry B, 2004, 108, 6025-6034.	1.2	12
1655	Thermochemistry of Siliconâ^'Hydrogen Compounds Generalized from Quantum Chemical Calculations. Journal of Physical Chemistry A, 2004, 108, 874-897.	1.1	51
1656	Ab Initio Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution. Journal of Physical Chemistry A, 2004, 108, 6373-6377.	1.1	119
1657	First principles electrochemical study of redox events in DNA bases and chemical repair in aqueous solution. Physical Chemistry Chemical Physics, 2004, 6, 2426.	1.3	20
1658	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. Journal of Physical Chemistry A, 2004, 108, 2475-2486.	1.1	70
1659	Importance of Entropy in the Diastereoselectivity of 5-Substituted 2-Methyladamant-2-yl Cations. Journal of Organic Chemistry, 2004, 69, 5537-5546.	1.7	9
1660	Experimental and Numerical Studies of Ethanol Decomposition Reactions. Journal of Physical Chemistry A, 2004, 108, 7671-7680.	1.1	155
1661	Thermochemical Properties, Pathway, and Kinetic Analysis on the Reactions of Benzene with OH:â€‰ An Elementary Reaction Mechanism. Journal of Physical Chemistry A, 2004, 108, 4632-4652.	1.1	49
1662	Ab initiodirect dynamics trajectory simulation of C2H5Fâ†'C2H4+HF product energy partitioning. Journal of Chemical Physics, 2004, 121, 8831-8845.	1.2	43
1663	Amide I vibrational circular dichroism of dipeptide:â€‚Conformation dependence and fragment analysis. Journal of Chemical Physics, 2004, 120, 4383-4392.	1.2	66
1664	Vibrational Signature of Charge Solvation vs Salt Bridge Isomers of Sodiated Amino Acids in the Gas Phase. Journal of the American Chemical Society, 2004, 126, 1836-1842.	6.6	260
1665	Structural Changes upon Reduction of Dipyrido[2,3-a:3â€˜,2â€˜-c]phenazine Probed by Vibrational Spectroscopy, ab Initio Calculations, and Deuteration Studies. Inorganic Chemistry, 2004, 43, 2876-2887.	1.9	29
1666	1H-1,3-Diazepines, 5H-1,3-diazepines, 1,3-diazepinones, and 2,4-diazabicyclo[3.2.0]heptenes,. Organic and Biomolecular Chemistry, 2004, 2, 1227-1238.	1.5	29
1668	2,3,5,6-Tetrasilyl- and 2,3,5,6-Tetragermyl-1,4-benzoquinones:Â X-ray Crystallographic Analysis, Cyclic Voltammetry, and DFT Calculations. Organometallics, 2004, 23, 1554-1561.	1.1	5
1669	Combined Quantum Chemical/RRKM-ME Computational Study of the Phenyl + Ethylene, Vinyl + Benzene, and H + Styrene Reactionsâ€‚. Journal of Physical Chemistry A, 2004, 108, 9697-9714.	1.1	50
1670	Matrix infrared spectra and density functional calculations of transition metal hydrides and dihydrogen complexes. Chemical Society Reviews, 2004, 33, 123.	18.7	312

#	Article	IF	Citations
1671	Theoretical estimates of equilibrium chromium-isotope fractionations. Chemical Geology, 2004, 205, 99-114.	1.4	165
1672	Oxygen isotope exchange kinetics between H2O and H4SiO4 from ab initio calculations. Geochimica Et Cosmochimica Acta, 2004, 68, 949-958.	1.6	13
1673	The Performance of Hybrid Density Functionals in Solid State Chemistry. Structure and Bonding, 2004, , 171-232.	1.0	171
1674	Vibrational Spectra and Surface-Enhanced Vibrational Spectra of 1-Nitropyrene. Applied Spectroscopy, 2004, 58, 555-561.	1.2	26
1675	Studies of Liquid-Phase Complexes in Acetonitrile/Water Solutions by Attenuated Total Reflection Infrared Spectroscopy with Acetaldehyde as a Model Solute. Applied Spectroscopy, 2004, 58, 1187-1194.	1.2	10
1676	Surface-Enhanced Infrared Spectroscopy. Applied Spectroscopy, 2004, 58, 324A-338A.	1.2	273
1677	Applying Stable Isotope Fractionation Theory to New Systems. Reviews in Mineralogy and Geochemistry, 2004, 55, 65-111.	2.2	501
1678	Combined Spectroscopic and Theoretical Study of Narrow Band Gap Heterocyclic Co-oligomers Containing Alternating Aromatic Donor ando-Quinoid Acceptor Units. Journal of Physical Chemistry B, 2004, 108, 2516-2526.	1.2	66
1679	Raman and Infrared Spectra and ab Initio Calculations of C2-4MIM Imidazolium Hexafluorophosphate Ionic Liquids. Journal of Physical Chemistry B, 2004, 108, 13177-13184.	1.2	419
1680	The Vibronic Structure of Electronic Absorption Spectra of Large Molecules:Â A Time-Dependent Density Functional Study on the Influence of â€œExactâ€•Hartreeâ^'Fock Exchange. Journal of Physical Chemistry A, 2004, 108, 10225-10237.	1.1	319
1681	Introduction to Active Thermochemical Tables:Â Several â€œKeyâ€•Enthalpies of Formation Revisitedâ€. Journal of Physical Chemistry A, 2004, 108, 9979-9997.	1.1	582
1682	Theoretical Study on the Reaction of OH Radicals with Polychlorinated Dibenzo-p-dioxins. Journal of Physical Chemistry A, 2004, 108, 607-614.	1.1	43
1683	Applications of Group Theory: Infrared and Raman Spectra of the Isomers of 1,2-Dichloroethylene. A Physical Chemistry Experiment. Journal of Chemical Education, 2004, 81, 1199.	1.1	14
1684	ADVENTURES OF QUANTUM CHEMISTRY IN THE REALM OF INORGANIC CHEMISTRY. Comments on Inorganic Chemistry, 2004, 25, 19-74.	3.0	11
1685	The energetics of isomeric benzoxazine diones: isatoic anhydride revisited. Organic and Biomolecular Chemistry, 2004, 2, 1647.	1.5	16
1686	Mechanism of the catalytic oxidation of hydrocarbons by N-hydroxyphthalimide: a theoretical studyElectronic supplementary information (ESI) available: all discussed TS and important intermediates (geometries, energies, ZPE, rotational constants and frequencies). See http://www.rsc.org/suppdata/cc/b4/b401050g/. Chemical Communications, 2004, , 1140.	2.2	71
1688	Extended Barbaralanes:Â Sigmatropic Shiftamers or Ïƒ-Polyacenes?. Journal of the American Chemical Society, 2004, 126, 4256-4263.	6.6	26
1689	A Quantum-Chemical Approach to Understanding Reversible Addition Fragmentation Chain-Transfer Polymerization. Australian Journal of Chemistry, 2004, 57, 1125.	0.5	21

#	Article	IF	Citations
1690	A Vibrational Analysis on Possible Peroxo Forms of Soluble Methane Monooxygenase. Bulletin of the Chemical Society of Japan, 2004, 77, 1305-1311.	2.0	12
1691	The Gas-Phase Rearrangement of HCCBCCH to a Trans Pentacyclic Isomer. A Joint Experimental and Theoretical Study. European Journal of Mass Spectrometry, 2004, 10, 829-835.	0.5	3
1692	Evidence for the Participation of Excited Electronic States in the Unimolecular Dissociation Reactions of Ionic Complexes between NO and Aromatic Compounds. European Journal of Mass Spectrometry, 2004, 10, 899-907.	0.5	4
1693	Li+ vs Cu+ Association to Toluene, Phenylsilane and Phenylgermane. Conventional vs Non-Conventional Ï€-Complexes. European Journal of Mass Spectrometry, 2004, 10, 921-929.	0.5	8
1694	Trends in Alkyl Substituent Effects on Nucleophilic Reactions of Carbonyl Compounds: Gas-Phase Reactions between Amines and the Methoxy Methyl Cation. European Journal of Mass Spectrometry, 2004, 10, 233-238.	0.5	2
1695	Semiempirical Calculations. , 2004, , 339-379.		0
1696	End-Cap Effects on Vibrational Structures of Finite-Length Carbon Nanotubes. Journal of the American Chemical Society, 2005, 127, 11769-11776.	6.6	59
1697	Theoretical Study on Acylacetanilide Azomethine Dyes: A Relationship between Electronic Absorption Properties and Molecular Structures. Bulletin of the Chemical Society of Japan, 2005, 78, 1929-1938.	2.0	4
1698	Reaction of (4-Nitorophenyl)nitrene with Molecular Oxygen in Low-temperature Matrices: First IR Detection and Photochemistry of Aryl Nitroso Oxide. Chemistry Letters, 2005, 34, 478-479.	0.7	31
1699	Electronic Structure of Sulfimides: A Theoretical Study. Bulletin of the Chemical Society of Japan, 2005, 78, 1417-1424.	2.0	7
1700	Synthesis of Kinetically Stabilized 1-Silanaphthalenes and Their Properties. Bulletin of the Chemical Society of Japan, 2005, 78, 977-987.	2.0	23
1701	Isotope Effects in the Reaction of Benzo[h]quinoline N-Oxides with Methylsulfinyl Carbanion Examined by ab Initio Molecular Orbital Methods. Chemical and Pharmaceutical Bulletin, 2005, 53, 576-578.	0.6	1
1702	Thermochemical and kinetic analysis of the allyl radical with O2 reaction system. Proceedings of the Combustion Institute, 2005, 30, 1015-1022.	2.4	46
1703	Chemical kinetic modeling of dimethyl carbonate in an opposed-flow diffusion flame. Proceedings of the Combustion Institute, 2005, 30, 1111-1118.	2.4	155
1704	A theoretical and experimental kinetic study of phenyl radical addition to butadiene. Proceedings of the Combustion Institute, 2005, 30, 1049-1056.	2.4	21
1705	Threshold energies for dissociative electron attachment to HBr.HX clusters with different HX partners: an ab initio study. Radiation Physics and Chemistry, 2005, 72, 93-98.	1.4	0
1706	Vibrational and surface-enhanced vibrational spectra of 6-nitrochrysene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 509-514.	2.0	14
1707	Vibrational spectra of Na, K, Mn2+, Ni2+ and Zn2+ salts of 1,2,4,5-benzenetetracarboxylic (pyromellitic) acidâ€"a short hydrogen bond evidence. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1747-1757.	2.0	14

#	Article	IF	Citations
1708	Theoretical prediction of gas-phase infrared spectra of imidazo[1,2-a]pyrazinediones and imidazo[1,2-a]imidazo[1,2-d]pyrazinediones derived from glycine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2560-2575.	2.0	8
1709	Vibrational spectrum of glycine molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2741-2746.	2.0	124
1710	Vibrational spectra of tris(dmit) complexes of main group metals: infrared, Raman and ab initio calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2663-2676.	2.0	15
1711	Vibrational spectroscopic characterization of fluoroquinolones. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1505-1517.	2.0	94
1712	DFT study on the geometric, electronic structure and Raman spectra of 5,15-diphenylporphine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 83-91.	2.0	12
1713	Raman spectrum, conformational stability, barriers to internal rotations and DFT calculations of 1,1,1-trifluoro-propane-2-thione with double-internal-symmetric rotor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 800-807.	2.0	5
1714	Density functional theory studies on the Raman and IR spectra of meso-tetraphenylporphyrin diacid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 850-862.	2.0	33
1715	Vibrational spectroscopic encoding of polystyrene-based resin beads: Converting the encoding peaks into barcodes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 1039-1044.	2.0	2
1716	Millimeter and submillimeter wave rotational spectrum of pyridine in the ground and excited vibrational states. Journal of Molecular Spectroscopy, 2005, 232, 61-65.	0.4	21
1717	S0 and S1 spectroscopy of jet cooled 9-cyano-10-methylanthracene: The methyl group as a molecular rotor. Journal of Molecular Spectroscopy, 2005, 233, 98-109.	0.4	5
1718	Cyclic voltammetry and theoretical calculations of silyl-substituted 1,4-benzoquinones. Journal of Organometallic Chemistry, 2005, 690, 1324-1331.	0.8	8
1719	Computational study of conformations and of sulfinyl oxygen-induced pentacoordination at silicon in 4-chloro-4-silathiacyclohexane 1-oxide and 4,4-dichloro-4-silathiacyclohexane 1-oxide. Journal of Organometallic Chemistry, 2005, 690, 4103-4113.	0.8	12
1720	Synthetic, spectral, magnetic and in vitro cytotoxic activity studies of cobalt(II) complexes with cytokinin derivatives: X-ray structure of 6-(3-methoxybenzylamino)purinium chloride monohydrate. Journal of Inorganic Biochemistry, 2005, 99, 776-786.	1.5	24
1721	A computational study of alkane hydrogen-exchange reactions on zeolites. Journal of Molecular Catalysis A, 2005, 242, 18-25.	4.8	20
1722	Vibrational dynamics study of the effect of the substituents on the Ï€-conjugation of different bithiophene molecules. Journal of Molecular Structure, 2005, 744-747, 393-401.	1.8	4
1723	FT-Raman spectroscopic study, aided by quantum chemical DFT calculations, of a series of oligothiophenes end-capped by nitriles. Journal of Molecular Structure, 2005, 744-747, 403-409.	1.8	6
1724	Combined theoretical and spectroscopic Raman study of 3,4-ethylenedioxy and S,S-dioxide substituted terthiophenes and their parent polymers. Journal of Molecular Structure, 2005, 744-747, 551-556.	1.8	5
1725	Vibrational spectroscopic encoding of polystyrene resin bead: a combined FT-IR and computational study. Journal of Molecular Structure, 2005, 738, 155-159.	1.8	9

#	Article	IF	Citations
1726	Vibrational spectroscopy and theoretical studies on 2,4-dinitrophenylhydrazine. Journal of Molecular Structure, 2005, 744-747, 363-368.	1.8	22
1727	The experimental and computational study on the IR spectra and structure of pyridine-3-carboxamide (nicotinamide)-d0 and -d2. Journal of Molecular Structure, 2005, 741, 85-92.	1.8	19
1728	Determination of the optical constants of 2-amino-5-phenyl-1,3,4-thiadiazole by Hartreeâ€“Fock and density functional method (B3LYP). Journal of Molecular Structure, 2005, 779, 72-76.	1.8	2
1729	Proton affinity of Î²-oxalylaminoalanine (BOAA): Incorporation of direct entropy correction into the single-reference kinetic method. Journal of the American Society for Mass Spectrometry, 2005, 16, 1151-1161.	1.2	23
1730	Experimental and theoretical investigations of the loss of amino acid side chains in electron capture dissociation of model peptides. Journal of the American Society for Mass Spectrometry, 2005, 16, 1523-1535.	1.2	89
1731	Cyclization of the substituted N-(Ortho-cyclopropylphenyl)-Nâ€²-aryl ureas and thioureas in the gas phase and solution. Journal of the American Society for Mass Spectrometry, 2005, 16, 1739-1749.	1.2	6
1732	Manipulating the fragmentation patterns of phosphopeptides via gas-phase boron derivatization: Determining phosphorylation sites in peptides with multiple serines. Journal of the American Society for Mass Spectrometry, 2005, 16, 1905-1914.	1.2	31
1733	Î”(Î”Sâ€¡) and Î”(Î”S) for the Competing Bond Cleavage Reactions in (CH3CN)(ROH)H+ [R = CH3, C2H5, C3H7, (CH3)2CH]. Journal of the American Society for Mass Spectrometry, 2005, 16, 2039-2044.	1.2	1
1734	Hydrogen/chlorine exchange reactions of gaseous carbanions. Journal of the American Society for Mass Spectrometry, 2005, 16, 2045-2051.	1.2	12
1735	Effect of nanosizing on some properties of one-dimensional polyacetylene chains. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 25, 404-408.	1.3	18
1736	Probing ab initio MP2 approach towards the prediction of vibrational infrared spectra of DNA base pairs. Journal of Molecular Structure, 2005, 744-747, 19-34.	1.8	10
1737	Vibrational spectra and molecular structure of 4,4â€²-azobis(pyridine N-oxide). Journal of Molecular Structure, 2005, 744-747, 339-343.	1.8	7
1738	X-ray and DFT studies of the structure, vibrational and NMR spectra of 2-amino-pyridine betaine hydrochloride. Journal of Molecular Structure, 2005, 744-747, 59-73.	1.8	16
1739	Vibrational spectra of D4R and D6R structural units. Journal of Molecular Structure, 2005, 744-747, 663-670.	1.8	52
1740	Vibrational spectroscopy of the double 4-, 6-membered rings in silicates and siloxanes. Journal of Molecular Structure, 2005, 744-747, 671-675.	1.8	17
1741	Quantum-mechanical calculations of magnesium aspartateâ€“arginine structure and spectroscopic characteristics. Journal of Molecular Structure, 2005, 743, 85-92.	1.8	3
1742	Experimental and quantum chemical studies of structure and vibrational spectra of platinum(II) and palladium(II) thiourea chlorides. Journal of Molecular Structure, 2005, 740, 229-235.	1.8	27
1743	NMR and theoretical study of the (CO)â€“N rotational barrier in the isomers cis- and trans-2-N,N-dimethylaminecyclohexyl 1-Nâ€²,Nâ€²-dimethylcarbamate. Journal of Molecular Structure, 2005, 753, 139-146.	1.8	16

#	Article	IF	Citations
1744	DFT studies of the structure, vibrational and NMR spectra of 2-amino-pyridine betaine monohydrate. Journal of Molecular Structure, 2005, 754, 85-95.	1.8	7
1745	Density-functional theory and ab initio Hartreeâ€“Fork studies on the structural parameters and chemical activity of the free radicals generated by benzoquinone and hydroquinone. Bioorganic and Medicinal Chemistry, 2005, 13, 5658-5667.	1.4	18
1746	Structure and dynamics of solvated Ba(II) in dilute aqueous solution â€“ an ab initio QM/MM MD approach. Chemical Physics, 2005, 312, 81-88.	0.9	47
1747	The vacuum UV photoabsorption spectrum of methyl bromide (CH3Br) and its perdeuterated isotopomer CD3Br: a vibrational analysis. Chemical Physics, 2005, 317, 87-102.	0.9	16
1748	Theoretical study of deuterium kinetic isotope effect in peroxidation of phenol and toluene. Chemical Physics, 2005, 320, 1-8.	0.9	11
1749	SERS spectrum and DFT calculations of 6-nitrochrysene on silver islands. Vibrational Spectroscopy, 2005, 37, 153-160.	1.2	15
1750	Computational study of the infrared spectrum of acetic acid, its cyclic dimer, and its methyl ester. Vibrational Spectroscopy, 2005, 39, 15-22.	1.2	45
1751	Theoretical studies on molecular structure and vibrational spectra of copper phthalocyanine. Vibrational Spectroscopy, 2005, 39, 191-199.	1.2	73
1752	A probe method for studying dibromocarbene by time resolved infrared spectroscopy. Tetrahedron Letters, 2005, 46, 8245-8247.	0.7	2
1753	DFT study of the thermochemistry of gas-phase 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (Î²-HMX). Computational and Theoretical Chemistry, 2005, 714, 147-152.	1.5	26
1754	A DFT study on the intramolecular dissociation pathways of ethyl fluoroformate radical cation in the gas phase; II. Keto path. Computational and Theoretical Chemistry, 2005, 713, 153-159.	1.5	0
1755	Theoretical group 14 chemistry, Part 3. A DFT study of Ge4R6. Computational and Theoretical Chemistry, 2005, 714, 109-115.	1.5	15
1756	Vibrational spectra of phthalazine by density functional theory calculations and assignment of its metal complexes. Computational and Theoretical Chemistry, 2005, 717, 171-178.	1.5	6
1757	An ab initio (RHF) and DFT-B3LYP level spectroscopic studies of BrCCCN and the analysis of atomic polar tensors. Computational and Theoretical Chemistry, 2005, 730, 23-32.	1.5	5
1758	Structure and bonding in hexamethyldisilazane and a series of analogues, (XH3)2YH (X=C, Si, Ge and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 2005, 719, 17-30.	1.5	2
1759	Ab initio studies of gas phase asparagine conformers. Computational and Theoretical Chemistry, 2005, 719, 153-158.	1.5	32
1760	On the conformation of neat acrylamide dimersâ€”a study by ab initio calculations and vibrational spectroscopy. Computational and Theoretical Chemistry, 2005, 723, 63-68.	1.5	21
1761	Experimental and theoretical studies of the vibrational spectrum of 5-hydroxytryptamine. Computational and Theoretical Chemistry, 2005, 726, 225-232.	1.5	72

#	Article	IF	Citations
1762	Hydrogen bondings in deoxynivalenol (DON) conformationsâ€"a density functional study. Computational and Theoretical Chemistry, 2005, 726, 55-59.	1.5	37
1763	A G3(MP2) study on the concerted cycloaddition reactions between ethylene and azines as well as other related heterocyclic systems. Computational and Theoretical Chemistry, 2005, 723, 195-204.	1.5	13
1764	A theoretical study of 18+Î´ complexes. Computational and Theoretical Chemistry, 2005, 726, 149-154.	1.5	1
1765	Electronic structure and vibrational spectra of X20H20 (X=C, Si, Ge, Sn): A theoretical study. Computational and Theoretical Chemistry, 2005, 730, 171-176.	1.5	5
1766	Theoretical study of molecular nitrogen adsorption on Au clusters. Computational and Theoretical Chemistry, 2005, 755, 9-17.	1.5	30
1767	A theoretical study of potassium cation binding to prolylglycine (PG) and glycylproline (GP) dipeptide. Computational and Theoretical Chemistry, 2005, 729, 193-202.	1.5	11
1768	Semiempirical study of low molecular weight polymers of 3-phenyl-1-ureidonitrile. Computational and Theoretical Chemistry, 2005, 731, 149-155.	1.5	2
1769	Interaction of pyridine on Nb2O5. Computational and Theoretical Chemistry, 2005, 732, 1-5.	1.5	10
1770	Evaluation of Nâ€"H bond dissociation energies in some amides using ab initio and density functional methods. Computational and Theoretical Chemistry, 2005, 757, 53-59.	1.5	25
1771	Theoretical and experimental study of the inelastic neutron scattering spectra of Î²-5-Nitro-2,4-dihydro-3H-1,2,4-triazol-3-one. Computational and Theoretical Chemistry, 2005, 732, 211-218.	1.5	10
1772	Electronic structure calculated anharmonic vibrational frequencies for phenol. Computational and Theoretical Chemistry, 2005, 755, 147-150.	1.5	21
1773	Theoretical probe on the structure and properties of CnN2n (n=2â€"5) clusters. Computational and Theoretical Chemistry, 2005, 756, 205-213.	1.5	0
1774	A theoretical study of an expanding monomer and an oxirane Part 2: Oxirane and copolymer reactions. Computational and Theoretical Chemistry, 2005, 756, 195-203.	1.5	0
1775	A theoretical study of an expanding monomer and an oxirane Part 1: Expanding monomer reactions. Computational and Theoretical Chemistry, 2005, 756, 185-194.	1.5	3
1776	Amide resonance in thio- and seleno- carbamates: A theoretical study. Computational and Theoretical Chemistry, 2005, 757, 149-153.	1.5	17
1777	High resolution electron energy loss spectroscopy study of clean, air-exposed and methanol-dosed Ge(100) surface. Surface Science, 2005, 575, 51-59.	0.8	16
1778	Ethylene adsorption on the Ptâ€"Cu bimetallic catalysts. Density functional theory cluster study. Surface Science, 2005, 583, 46-59.	0.8	17
1779	Tertiary amide chemistry at the Ge(100)-2Ã—1 surface. Surface Science, 2005, 599, 41-54.	0.8	14

#	Article	IF	Citations
1780	The thermodynamic properties of 1-bromoadamantane in the gaseous state. Thermochimica Acta, 2005, 436, 56-67.	1.2	15
1781	Kinetics and mechanism of thermal gas-phase elimination of Î²-substituted carboxylic acids. Tetrahedron, 2005, 61, 5769-5777.	1.0	18
1782	Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis. Tetrahedron, 2005, 61, 7538-7545.	1.0	20
1783	Radical hydrogen abstractionâ€“cyclization with a 2-bromovinylsilyl group as a bifunctional tether. Tetrahedron, 2005, 61, 7865-7873.	1.0	5
1784	Proton affinities of ketones, vicinal diketones and Î±-keto esters: a computational study. Tetrahedron, 2005, 61, 8109-8119.	1.0	16
1785	Computational studies of benzyl-substituted halonium ions. Tetrahedron, 2005, 61, 8358-8365.	1.0	12
1786	Density-functional theory studies on standard electrode potentials of half reaction for l-adrenaline and adrenalinequinone. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 4671-4680.	1.0	26
1787	The roles of gallium hydride and BrÃ¸nsted acidity in light alkane dehydrogenation mechanisms using Ga-exchanged HZSM-5 catalysts: A DFT pathway analysis. Catalysis Today, 2005, 105, 106-121.	2.2	73
1788	DFT investigations of models related to the active site of [NiFe] and [Fe] hydrogenases. Coordination Chemistry Reviews, 2005, 249, 1620-1640.	9.5	123
1789	Observation and rovibrational analysis of the Î½2 band of HCNâ€“H35Cl. Chemical Physics, 2005, 310, 163-167.	0.9	5
1790	NIR surface enhanced Raman spectroscopy and bands assignment by DFT calculations of non-natural Î²-amino acids. Chemical Physics, 2005, 310, 189-199.	0.9	16
1791	Mechanisms of antioxidant activity: The DFT study of hydrogen abstraction from phenol and toluene by the hydroperoxyl radical. Chemical Physics, 2005, 314, 211-217.	0.9	40
1792	Experimental and DFT study of pyrazinamide. Chemical Physics, 2005, 316, 153-163.	0.9	48
1793	The heat of formation of 2-H heptafluoropropane by ab initio calculations. Chemical Physics Letters, 2005, 402, 32-36.	1.2	11
1794	Theoretical study of the kinetics of hydrogen abstraction in reactions of simple hydrogen compounds with triplet difluorocarbene. Chemical Physics Letters, 2005, 402, 460-467.	1.2	5
1795	A computational study of the water-catalyzed formation of NH2CH2OH. Chemical Physics Letters, 2005, 405, 357-363.	1.2	28
1796	Mass scaling for vibrational frequencies from ab initio calculations. Chemical Physics Letters, 2005, 403, 275-279.	1.2	5
1797	On the planarity of the tropolone molecule in the <mml:math altimg="si4.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/co	1.2	10

#	Article	IF	Citations
1798	Ab initio kinetic study on the low-energy paths of the HO+C2H4 reaction. Chemical Physics Letters, 2005, 408, 25-30.	1.2	52
1799	Linear regression correction to first principle theoretical calculations â€“ Improved descriptors and enlarged training set. Chemical Physics Letters, 2005, 409, 315-321.	1.2	9
1800	Neural network correction for heats of formation with a larger experimental training set and new descriptors. Chemical Physics Letters, 2005, 410, 125-130.	1.2	34
1801	Temperature excursion infrared (TEIR) spectroscopy used to study hydrogen bonding between water and biomolecules. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1749, 214-233.	1.1	62
1802	Bridging diimino and ene-diamido ligands in binuclear compounds: structural and electronic features. Comptes Rendus Chimie, 2005, 8, 1353-1364.	0.2	1
1803	Electron capture by HCl trimers: an ab initio study. European Physical Journal D, 2005, 35, 217-224.	0.6	4
1804	Assessment of Gaussian-3 and density-functional theories on the G3/05 test set of experimental energies. Journal of Chemical Physics, 2005, 123, 124107.	1.2	320
1805	Multidisciplinary Physicochemical Analysis of Oligothiophenes End-Capped by Nitriles:Â Electrochemistry, UVâ^'Visâ^'Near-IR, IR, and Raman Spectroscopies and Quantum Chemistry. Journal of Physical Chemistry B, 2005, 109, 10115-10125.	1.2	40
1806	Experimental (FT-IR) and theoretical (DFT-IR) studies of ketoâ€“enol tautomerism in pyruvic acid. Vibrational Spectroscopy, 2005, 39, 37-45.	1.2	53
1807	Stabilities of C3â€“C5 alkoxide species inside H-FER zeolite: a hybrid QM/MM study. Journal of Catalysis, 2005, 231, 393-404.	3.1	91
1808	Determination of the catalytically active oxidation Lewis acid sites in Sn-beta zeolites, and their optimisation by the combination of theoretical and experimental studies. Journal of Catalysis, 2005, 234, 111-118.	3.1	280
1809	Perfluorodecalin: global warming potential and first detection in the atmosphere. Atmospheric Environment, 2005, , .	1.9	12
1810	Reduced-size polarized basis sets for calculations of molecular electric properties. II. Simulation of the Raman spectra. Journal of Computational Chemistry, 2005, 26, 154-159.	1.5	27
1811	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583.	1.5	27
1812	Structure-breaking effects of solvated Rb(I) in dilute aqueous solutionâ”Anab initio QM/MM MD approach. Journal of Computational Chemistry, 2005, 26, 949-956.	1.5	45
1813	A molecular mechanics force field for biologically important sterols. Journal of Computational Chemistry, 2005, 26, 1383-1399.	1.5	45
1814	Theoretical studies on nonlinear optical properties of formaldehyde oligomers byab initio and density functional theory methods. Journal of Computational Chemistry, 2005, 26, 1543-1564.	1.5	23
1815	Lewis Acid Induced [2+2] Cycloadditions of Silyl Enol Ethers with Î±,Î²-Unsaturated Esters: A DFT Analysis. European Journal of Organic Chemistry, 2005, 2005, 3973-3979.	1.2	13

#	Article	IF	Citations
1816	Comparison of ab initio and group additive ideal gas heat capacities. AICHE Journal, 2005, 51, 292-297.	1.8	11
1817	Quantum monte carlo study of heats of formation and bond dissociation energies of small hydrocarbons. International Journal of Chemical Kinetics, 2005, 37, 583-592.	1.0	11
1818	DFT based relaxed PES scan studies and SERS of anti cancer drug, Combretastatin A-4. Laser Physics Letters, 2005, 2, 544-550.	0.6	17
1819	Proton affinity ladder for uridine and analogs: influence of the hydroxyl group on the sugar ring conformation. Journal of Mass Spectrometry, 2005, 40, 722-730.	0.7	11
1820	On the Gas-Phase Reactivity of Complexed OH+ with Halogenated Alkanes. Chemistry - A European Journal, 2005, 11, 152-159.	1.7	7
1821	Dissociation of Alkaliated Alanine in the Gas Phase: The Role of the Metal Cation. Chemistry - A European Journal, 2005, 11, 5289-5301.	1.7	10
1822	Acidity Trends in Î±,Î²-Unsaturated Sulfur, Selenium, and Tellurium Derivatives: Comparison with C-, Si-, Ge-, Sn-, N-, P-, As-, and Sb-Containing Analogues. Chemistry - A European Journal, 2005, 11, 2145-2153.	1.7	28
1823	A Multisite Molecular Mechanism for Baeyer-Villiger Oxidations on Solid Catalysts Using Environmentally Friendly H2O2 as Oxidant. Chemistry - A European Journal, 2005, 11, 6905-6915.	1.7	94
1824	Gas phase UV and IR absorption spectra of CF3CH2CH2OH and F(CF2CF2)xCH2CH2OH (x=2, 3, 4). Journal of Fluorine Chemistry, 2005, 126, 1288-1296.	0.9	19
1825	An ab initio study of ethane conversion reactions on zeolites using the complete basis set composite energy method. Journal of Molecular Catalysis A, 2005, 229, 77-85.	4.8	34
1826	Pathways for proton migration over the surface of a metal-cyclotriphosphorus cluster. Comptes Rendus Chimie, 2005, 8, 1535-1542.	0.2	1
1827	Exploring the potential energy surface of ionâ€“molecule pairs by experiment and by theory: acetaldehyde and methanol. International Journal of Mass Spectrometry, 2005, 242, 75-85.	0.7	6
1828	Thermochemistry and structures of solvated SN2 complexes and transition states in the gas phase: experiment and theory. International Journal of Mass Spectrometry, 2005, 241, 205-223.	0.7	33
1829	Ab initio model studies of copper binding to peptides containing a Hisâ€“His sequence: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2005, 10, 887-902.	1.1	54
1830	Modeling the active centers of V2O5/SiO2 and V2O5/TiO2 supported catalysts. DFT theoretical analysis of optical properties. Journal of Structural Chemistry, 2005, 46, 577-590.	0.3	10
1831	Structure effects of the protonated lincomycin molecule on the mechanism of its complexation with organic compounds. Journal of Structural Chemistry, 2005, 46, 985-990.	0.3	8
1832	Vibrational Spectroscopic Studies on the Dicycloheptylaminecobalt(II) Tetracyanonickellate(II) Hostâ€“Aromatic Guest Systems. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2005, 53, 219-229.	1.6	7
1833	Comparative quantum chemical investigation of structures and properties of diazocyclopropane and other diazoalkanes. Russian Chemical Bulletin, 2005, 54, 1100-1104.	0.4	1

#	Article	IF	Citations
1834	An ab initio Quantum-Chemical Study of C6H5S(O)CH3 and C6H5S(O)CF3. Russian Journal of General Chemistry, 2005, 75, 86-93.	0.3	7
1835	Computational study of sulfoxides of thiacyclohexane, 4-silathiacyclohexane, 4-fluoro-4-silathiacyclohexane, and 4,4-difluoro-4-silathiacyclohexane: Relative energies of conformations and sulfinyl oxygen stabilized pentacoordinate silicon in boat and twist structures. International Journal of Quantum Chemistry, 2005, 101, 40-54.	1.0	20
1836	Theoretical study of unimolecular rearrangements of vinylidenes to acetylenes. International Journal of Quantum Chemistry, 2005, 102, 189-199.	1.0	6
1837	Scaling factors for the prediction of vibrational spectra. II. The aniline molecule and several derivatives. International Journal of Quantum Chemistry, 2005, 103, 394-421.	1.0	157
1838	Infrared spectra and dissociation pathways of the linear carbon-sulfur clusters CnS and SCnS (n ? 29): Theoretical calculations. International Journal of Quantum Chemistry, 2005, 102, 795-805.	1.0	18
1839	Spectroscopic and DFT studies of donor-acceptor molecules containing phenylquinoline and phenothiazine moieties in various redox states. International Journal of Quantum Chemistry, 2005, 104, 635-644.	1.0	7
1840	Vibrational spectroscopies: Description of general analytical TDHF schemes for their simulation. International Journal of Quantum Chemistry, 2005, 104, 727-743.	1.0	4
1841	Amide I IR, VCD, and 2d IR spectra of isotope-labeled Î±-helix in liquid water: Numerical simulation studies. International Journal of Quantum Chemistry, 2005, 104, 616-634.	1.0	69
1842	Effect of the environment on vibrational infrared and circular dichroism spectra of (s)-proline. International Journal of Quantum Chemistry, 2005, 104, 744-757.	1.0	26
1843	Conformational and vibrational study of di-n-propyl and di-i-propylphosphonates by MM/QM method. International Journal of Quantum Chemistry, 2005, 103, 763-774.	1.0	4
1844	Theoretical study of kaolinite. International Journal of Quantum Chemistry, 2005, 103, 550-556.	1.0	25
1845	Calculated infrared spectra of hydrogen-bonded methanol-water, water-methanol, and methanol-methanol complexes. International Journal of Quantum Chemistry, 2005, 104, 808-815.	1.0	34
1846	Theoretical study of the structures and properties of cyclic nitramines: Tetranitrotetraazadecalin (TNAD) and its isomers. International Journal of Quantum Chemistry, 2005, 105, 48-56.	1.0	55
1847	Relative energies of conformations and sulfinyl oxygen-induced pentacoordination at silicon in 4-bromo- and 4,4-dibromo-4-silathiacyclohexane 1-oxide: A computational study. International Journal of Quantum Chemistry, 2005, 105, 313-324.	1.0	14
1848	Density functional theory study of vibrational properties of the 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) molecule: IR, Raman, and UV-vis spectra. International Journal of Quantum Chemistry, 2005, 105, 368-375.	1.0	19
1849	Density functional theory study of the relative energies and structures of the chair, twist, and boat conformations of stannacyclohexane, 1-methylstannacyclohexane, and 1,1-dimethylstannacyclohexane. International Journal of Quantum Chemistry, 2005, 105, 416-428.	1.0	5
1850	Theoretical and experimental studies on the Raman spectra of electrosynthesized polynaphthalene. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 241-251.	2.4	12
1851	Enthalpies of Formation and Reaction for Primary Reactions of Methyl- and Methylmethoxysilanes from Density Functional Theory. Plasma Processes and Polymers, 2005, 2, 669-678.	1.6	14

#	Article	IF	Citations
1852	Experimental and Theoretical Study of 1,5-Diamino-4-H-1,2,3,4-Tetrazolium Perchlorate. Propellants, Explosives, Pyrotechnics, 2005, 30, 156-163.	1.0	55
1853	DFT study of the mechanism of nitration of toluene with nitronium. Journal of Physical Organic Chemistry, 2005, 18, 62-68.	0.9	11
1854	Relative energies, stereoelectronic interactions and conformational interconversions in silathiacyclohexanes. Journal of Physical Organic Chemistry, 2005, 18, 35-48.	0.9	15
1855	Boron trifluoride activated enaminocarbonyl compounds: the influence of intermolecular interactions on theab initiodetermination of structures and vibrational spectra. Journal of Physical Organic Chemistry, 2005, 18, 217-226.	0.9	0
1856	Theoretical study of the mechanism of thermal decomposition of carbonate esters in the gas phase. Journal of Physical Organic Chemistry, 2005, 18, 134-141.	0.9	32
1857	Ab initiostudy of the effect of Î±-substituents on the acidity of cyclopropabenzene. Journal of Physical Organic Chemistry, 2005, 18, 763-772.	0.9	4
1858	Transition structures and reaction barriers in the styrene-acrylonitrile copolymerization system according to quantum mechanical calculations. Journal of Polymer Science Part A, 2005, 43, 1827-1844.	2.5	11
1859	Proton affinity of diastereoisomers of modified prolines using the kinetic method and density functional theory calculations: role of thecis/trans substituent on theendo/exo ring conformation. Rapid Communications in Mass Spectrometry, 2005, 19, 2279-2283.	0.7	13
1860	Hydrogen dissociation of naphthalene cations: a theoretical study. Astronomy and Astrophysics, 2005, 444, 629-634.	2.1	36
1861	First-principles calculations of anharmonic vibrational spectroscopy of large molecules. , 2005, , 165-194.		42
1862	G2, G3 and associated quantum chemical models for accurate theoretical thermochemistry. , 2005, , 785-812.		5
1863	Density Functional Theory Study of Solvent Effects on the Structure and Vibrational Frequencies of Tetranitrotetraazabicyclooctane â€œbicyclo-HMXâ€• Journal of the Chinese Chemical Society, 2005, 52, 405-413.	0.8	11
1864	A Theoretical Study of Substituent Effects on Allylic Ion and Ion Pair SN2 Reactions. Journal of Organic Chemistry, 2005, 70, 8486-8491.	1.7	31
1865	The structures of m-benzyne and tetrafluoro-m-benzyne. Journal of Chemical Physics, 2005, 122, 174309.	1.2	48
1866	Quantitative molecular thermochemistry based on path integrals. Journal of Chemical Physics, 2005, 123, 034103.	1.2	12
1867	Role of angular momentum conservation in unimolecular translational energy release: Validity of the orbiting transition state theory. Journal of Chemical Physics, 2005, 122, 094106.	1.2	13
1868	Infrared-visible and visible-visible double resonance spectroscopy of 1-hydroxy-9,10-anthraquinone-(H2O)nâ€Š(n=1,2) complexes. Journal of Chemical Physics, 2005, 122, 034305.	1.2	8
1869	An extended ab initio QM/MM MD approach to structure and dynamics of Zn(II) in aqueous solution. Journal of Chemical Physics, 2005, 123, 054514.	1.2	65

#	Article	IF	Citations
1870	Initial-stage oxidation mechanism ofGe(100)2Ã—1dimers. Physical Review B, 2005, 72, .	1.1	22
1871	Quantum studies of hydrogen bonding in formic acid and water ice surface. Journal of Chemical Physics, 2005, 122, 234703.	1.2	26
1872	The spectroscopic signature of the â€œall-surfaceâ€•to â€œinternally solvatedâ€•structural transition in water clusters in the n=17â€“21 size regime. Journal of Chemical Physics, 2005, 122, 194310.	1.2	79
1873	Torsional potential of 4,4â€²-bipyridine: Ab initio analysis of dispersion and vibrational effects. Journal of Chemical Physics, 2005, 123, 134309.	1.2	37
1874	Correlation energy functionals dependent on an effective number of electrons: Charged species and equilibrium geometries. Journal of Chemical Physics, 2005, 123, 144111.	1.2	0
1875	Bond and charge-density waves in(Dlâ^'DCNQI)2Ag(Dlâ^'DCNQI=2,5â^'diiodoâ^'N,Nâ€²â^'dicyanoquinediimine)studied by single-crystal infrared and Raman spectroscopy. Physical Review B, 2005, 71, .	1.1	12
1876	Benchmark correlation energies for small molecules. Molecular Physics, 2005, 103, 763-766.	0.8	48
1877	DIRECT INTERACTION ENERGY: A COMPUTATIONAL QUANTITY FOR PARAMETERIZATION OF CONDENSED-PHASE FORCE FIELDS AND ITS APPLICATION TO HYDROGEN BONDING. Journal of Theoretical and Computational Chemistry, 2005, 04, 689-705.	1.8	9
1878	H-atom abstraction dynamics of reactions between Cl atoms and heterocyclic organic molecules. Molecular Physics, 2005, 103, 1785-1796.	0.8	8
1879	A study of the isomerization and dissociation of formal [acetoneÂ–methanol]+Â· ionÂ–molecule complexes. Canadian Journal of Chemistry, 2005, 83, 1903-1912.	0.6	8
1880	Positional Isotope Effect for the Water Tetramer. Computing Letters, 2005, 1, 145-151.	0.5	0
1881	Far-Infrared Absorption of DAST: Theoretical Study. , 0, , .		0
1882	Mechanism for the Gas-Phase Reaction between Formaldehyde and Hydroperoxyl Radical. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 10786-10794.	1.1	60
1883	The Gas-Phase Acidity of 2(3H)-Oxepinone:Â A Step toward an Experimental Heat of Formation for the 2-Oxepinoxy Radical. Journal of the American Chemical Society, 2005, 127, 7466-7473.	6.6	15
1884	Câ€“Hâ‹¯O Hydrogen bonding in 4-phenyl-benzaldehyde: A comprehensive crystallographic, spectroscopic and computational study. Physical Chemistry Chemical Physics, 2005, 7, 3027.	1.3	19
1885	New Scale Factors for Harmonic Vibrational Frequencies Using the B3LYP Density Functional Method with the Triple-Î¶ Basis Set 6-311+G(d,p). Journal of Physical Chemistry A, 2005, 109, 2937-2941.	1.1	1,324
1886	Pharmacophoric Features of Biguanide Derivatives:Â An Electronic and Structural Analysis. Journal of Medicinal Chemistry, 2005, 48, 7615-7622.	2.9	114
1887	Uncertainties in Scaling Factors for ab Initio Vibrational Frequencies. Journal of Physical Chemistry A, 2005, 109, 8430-8437.	1.1	431

#	Article	IF	Citations
1888	Infrared Spectra of M(OH)1,2,4(M = Pb, Sn) in Solid Argon. Journal of Physical Chemistry A, 2005, 109, 9013-9020.	1.1	31
1889	Optically Active Seleninate Esters:Â Isolation, Absolute Configuration, Racemization Mechanism, and Transformation into Chiral Selenoxide. Journal of Organic Chemistry, 2005, 70, 5020-5027.	1.7	20
1890	Periodic Trends in Bond Dissociation Energies. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 4359-4365.	1.1	67
1891	Raman, Surface Enhanced Raman Spectroscopy, and DFT Calculations:Â A Powerful Approach for the Identification and Characterization of 5-Fluorouracil Anticarcinogenic Drug Species. Journal of Physical Chemistry A, 2005, 109, 9945-9952.	1.1	43
1892	Base-Catalyzed Hydrogenation:Â Rationalizing the Effects of Catalyst and Substrate Structures and Solvation. Journal of the American Chemical Society, 2005, 127, 2443-2454.	6.6	49
1893	Binding Affinities for Models of Biologically Available Potential Cu(II) Ligands Relevant to Alzheimer's Disease:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 8361-8370.	1.1	36
1894	Theoretical Investigation of CO Interaction with Copper Sites in Zeolites:Â Periodic DFT and Hybrid Quantum Mechanical/Interatomic Potential Function Study. Journal of Physical Chemistry B, 2005, 109, 9631-9638.	1.2	77
1895	Protonation Thermochemistry of Selected Hydroxy- and Methoxycarbonyl Molecules. Journal of Physical Chemistry A, 2005, 109, 11851-11859.	1.1	9
1896	A collisionally activated dissociation (CAD) and computational investigation of doubly and singly charged DMSO complexes of Cu2+. Canadian Journal of Chemistry, 2005, 83, 1921-1935.	0.6	8
1897	Amide I vibrational circular dichroism of polypeptides: Generalized fragmentation approximation method. Journal of Chemical Physics, 2005, 122, 174903.	1.2	51
1898	Photochemical reaction mechanisms of 2-nitrobenzyl compounds: 2-Nitrobenzyl alcohols form 2-nitroso hydrates by dual proton transfer. Photochemical and Photobiological Sciences, 2005, 4, 33-42.	1.6	87
1899	NO2 disproportionation for the IR characterisation of basic zeolites. Chemical Communications, 2005, , 1049.	2.2	20
1900	Pressure dependence for the CO quantum yield in the photolysis of acetone at 248 nm: A combined experimental and theoretical study. Physical Chemistry Chemical Physics, 2005, 7, 3342.	1.3	26
1901	Linear free energy relationship and kinetic isotope effects as measures for the transition-state variation Â— A case of the neophyl system. Canadian Journal of Chemistry, 2005, 83, 1606-1614.	0.6	2
1902	Complexation of Cu(II) Ions with the Lowest Generation Poly(amido-amine)-OH Dendrimers:â€‰ A Molecular Simulation Study. Journal of Physical Chemistry B, 2005, 109, 12480-12490.	1.2	18
1903	On the Parallel Mechanism of the Dissociation of Energy-Selected P(CH3)3+Ionsâ€. Journal of Physical Chemistry B, 2005, 109, 8393-8399.	1.2	14
1904	Isotope Effects on the Unimolecular Dissociation of Ionized 3-Methyl-2-butanol:Â Reactions via a Long-Lived Câ^'Hâ^'C Hydrogen-Bridged Ion-Neutral Complex. Journal of Physical Chemistry A, 2005, 109, 3159-3165.	1.1	5
1905	Matrix Isolation and Density Functional Theory Study of Bis(trifluoromethyl)dioxodiazine:Â A Photodimer of Trifluoronitrosomethane. Journal of Physical Chemistry A, 2005, 109, 5307-5315.	1.1	0

#	Article	IF	Citations
1906	How to Model Solvation of Peptides? Insights from a Quantum-mechanical and Molecular Dynamics Study ofN-Methylacetamide. 1. Geometries, Infrared, and Ultraviolet Spectra in Water. Journal of Physical Chemistry B, 2005, 109, 9818-9829.	1.2	91
1907	A DENSITY FUNCTIONAL STUDY OF THE STRUCTURE OF SILANE COUPLING AGENT 3â€“AMINOPROPYLTRIETHOXYSILANE. Journal of Theoretical and Computational Chemistry, 2005, 04, 117-126.	1.8	0
1908	The influence of heteroligands on the reactivity of Ni2+ in solution. Physical Chemistry Chemical Physics, 2005, 7, 1669.	1.3	22
1909	Infrared spectrum and structure of the gold dihydroxide molecule. Chemical Communications, 2005, , 4001.	2.2	12
1910	The experimental gas-phase structures of 1,3,5-trisilylbenzene and hexasilylbenzene and the theoretical structures of all benzenes with three or more silyl substituents. Dalton Transactions, 2005, , 2292.	1.6	6
1911	Gas phase synthesis and reactivity of Agn+ and Agnâ€“1H+ cluster cations. Dalton Transactions, 2005, , 2702.	1.6	52
1912	Bent and planar molecules in polymorphs of the tricyclic carbon sulfide C6S8. New Journal of Chemistry, 2005, 29, 465.	1.4	13
1913	Anharmonic vibrational spectroscopy calculations for (NH3)(HF) and (NH3)(DF): fundamental, overtone, and combination transitions. Physical Chemistry Chemical Physics, 2005, 7, 945.	1.3	15
1914	The investigation of hydrocarbon cracking reaction energetics with composite energy methods. Molecular Simulation, 2005, 31, 979-986.	0.9	4
1915	Predicting ion rearrangement reactions Â— The energetics of the internal SN2 reaction in gas-phase proton-bound molecular pairs. Canadian Journal of Chemistry, 2005, 83, 1864-1870.	0.6	3
1916	Computational studies of the properties of phenyloxenium ions Â— A comparison with phenylnitrenium and phenylcarbenium ions. Canadian Journal of Chemistry, 2005, 83, 1372-1381.	0.6	19
1917	First Singlet (n,Ï€*) Excited State of Hydrogen-Bonded Complexes between Water and Pyrimidine. Journal of Physical Chemistry A, 2005, 109, 1576-1586.	1.1	13
1918	Cubane, Cuneane, and Their Carboxylates:Â A Calorimetric, Crystallographic, Calculational, and Conceptual Coinvestigation. Journal of Organic Chemistry, 2005, 70, 5461-5470.	1.7	42
1919	Study of Singlet and Triplet 2,6-Difluorophenylnitrene by Time-Resolved Infrared Spectroscopy. Journal of Physical Chemistry A, 2005, 109, 2816-2821.	1.1	17
1920	Infrared Spectra of CH3â^'CrH, CH3â^'WH, CH2WH2, and CHâ‹®WH3Formed by Activation of CH4with Cr and W Atoms. Inorganic Chemistry, 2005, 44, 7634-7643.	1.9	44
1921	Identity Hydride-Ion Transfer from Câ^'H Donors to C Acceptor Sites. Enthalpies of Hydride Addition and Enthalpies of Activation. Comparison with CÂ·Â·Â·HÂ·Â·Â·C Proton Transfer. An ab Initio Study. Journal of the American Chemical Society, 2005, 127, 2324-2333.	6.6	40
1922	Synthesis and Characterization of a Novel Terthiophene-Based Quinodimethane Bearing a 3,4-Ethylenedioxythiophene Central Unit. Journal of Physical Chemistry B, 2005, 109, 22308-22318.	1.2	18
1923	Theoretical Study of Pyridine and 4,4â€˜-Bipyridine Adsorption on the Lewis Acid Sites of Alumina Surfaces Based on Ab Initio and Density Functional Cluster Calculations. Journal of Physical Chemistry B, 2005, 109, 13716-13728.	1.2	29

#	Article	IF	Citations
1924	Electrochemical and PM-IRRAS Studies of the Effect of the Static Electric Field on the Structure of the DMPC Bilayer Supported at a Au(111) Electrode Surface. Langmuir, 2005, 21, 330-347.	1.6	100
1926	Thermochemical and Theoretical Studies of Dimethylpyridine-2,6-dicarboxylate and Pyridine-2,3-, Pyridine-2,5-, and Pyridine-2,6-dicarboxylic Acids. Journal of Chemical & Engineering Data, 2005, 50, 1184-1191.	1.0	19
1927	Metathesis Activity and Properties of Moâ^'Alkylidene Sites Differently Located on Silica. A Density Functional Theory Study. Journal of Physical Chemistry B, 2005, 109, 20794-20804.	1.2	48
1928	Application of compound models for estimating rate constants of hydrocarbon thermal cracking reactions: The neopentyl radical Î²-scission reaction. Molecular Simulation, 2005, 31, 615-621.	0.9	7
1929	Characterization of the Conformational Probability of N-Acetyl-Phenylalanyl-NH2by RHF, DFT, and MP2 Computation and AIM Analyses, Confirmed by Jet-Cooled Infrared Data. Journal of Physical Chemistry A, 2005, 109, 5289-5302.	1.1	32
1930	Elucidating the Vibrational Spectra of Hydrogen-Bonded Aggregates in Solution:Â Electronic Structure Calculations with Implicit Solvent and First-Principles Molecular Dynamics Simulations with Explicit Solvent for 1-Hexanol inn-Hexane. Journal of the American Chemical Society, 2005, 127, 4722-4729.	6.6	54
1931	A Practical Synthesis of Isomerically Pure 1,10-Difunctionalized Derivatives of the [closo-1-CB9H10] Anion. Inorganic Chemistry, 2005, 44, 9561-9566.	1.9	28
1932	Investigations into the Stability of Tethered Palladium(II) Pincer Complexes during Heck Catalysis. Organometallics, 2005, 24, 4351-4361.	1.1	147
1933	Mapping the Triplet Potential Energy Surface of 1-Methyl-8-nitronaphthalene. Journal of Organic Chemistry, 2005, 70, 6074-6084.	1.7	1
1934	Computational Study of the Reaction of Fluorine Atom with Acetone. Journal of Physical Chemistry A, 2005, 109, 3166-3173.	1.1	7
1935	Proximity Effects in the Palladium-Catalyzed Substitution of Aryl Fluorides. Organic Letters, 2005, 7, 1011-1014.	2.4	43
1936	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrrolineN-Oxide (DMPO). 1. The Thermodynamics of Formation and Its Acidity. Journal of Physical Chemistry A, 2005, 109, 6083-6088.	1.1	53
1937	On the Relationship between the Preferred Site of Hydrogen Bonding and Protonation. Journal of Physical Chemistry A, 2005, 109, 5509-5517.	1.1	53
1938	Experimental and Computational Studies of Structure and Bonding in Parent and Reduced Forms of the Azo Dye Orange II. Journal of Physical Chemistry A, 2005, 109, 2894-2905.	1.1	69
1939	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrrolineN-Oxide (DMPO). 2. The Thermodynamics of Decay and EPR Spectral Properties. Journal of Physical Chemistry A, 2005, 109, 6089-6098.	1.1	58
1940	Conformational Analysis of 2,2â€˜-Bithiophene:Â A1H Liquid Crystal NMR Study Using the13C Satellite Spectra. Journal of Physical Chemistry A, 2005, 109, 9953-9963.	1.1	19
1941	Adsorption of 2-Aminobenzothiazole on Colloidal Silver Particles:â€‰ An Experimental and Theoretical Surface-Enhanced Raman Scattering Study. Journal of Physical Chemistry B, 2005, 109, 12861-12867.	1.2	35
1942	A Band Dispersion Mechanism for Pt Alloy Compositional Tuning of Linear Bound CO Stretching Frequencies. Journal of Physical Chemistry B, 2005, 109, 1839-1848.	1.2	32

#	Article	IF	Citations
1943	Hydride Affinities of Borane Derivatives:Â Novel Approach in Determining the Origin of Lewis Acidity Based on Triadic Formula. Inorganic Chemistry, 2005, 44, 1095-1102.	1.9	43
1944	NO+: Infrared probe for basic zeolites. Studies in Surface Science and Catalysis, 2005, 158, 663-670.	1.5	14
1945	Theoretical Study of Internal Field Effects on Peptide Amide I Modes. Journal of Physical Chemistry B, 2005, 109, 5331-5340.	1.2	19
1946	E/Z Conformation and the Vibrational Spectroscopy of Me2NN(O)NOMe. Journal of Physical Chemistry A, 2005, 109, 11317-11321.	1.1	1
1947	Infrared Spectra and Electronic Structure Calculations for the Group 2 Metal M(OH)2Dihydroxide Molecules. Journal of Physical Chemistry A, 2005, 109, 2782-2792.	1.1	40
1948	Experimental and Theoretical Surface Enhanced Raman Scattering Study of 2-Amino-4-methylbenzothiazole Adsorbed on Colloidal Silver Particles. Journal of Physical Chemistry B, 2005, 109, 22536-22544.	1.2	33
1949	A Study by Spectroelectrochemical FTIR and Density Functional Theory Calculations of the Reversible Complexing Ability of an Electroactive Tetrathiafulvalene Crown. Journal of Physical Chemistry A, 2005, 109, 1188-1195.	1.1	3
1950	Estimation, Computation, and Experimental Correction of Molecular Zero-Point Vibrational Energies. Journal of Physical Chemistry A, 2005, 109, 6779-6789.	1.1	47
1951	Infrared Spectra of the CH3â˜'CrF, CH2WHF, and CHâ‹®WH2F Molecules:â€‰ Reversible Photochemical Interconversion by Î±-Hydrogen Transfer. Organometallics, 2005, 24, 5678-5685.	1.1	26
1952	Remote Substituent Effects upon the Rearrangements of Housane Cation Radicals. Journal of Organic Chemistry, 2005, 70, 4598-4608.	1.7	17
1953	Generalized Anomeric Interpretation of the â€œHigh-Energyâ€•Nâ˜'P Bond in N-Methyl-Nâ€˜-phosphorylguanidine:â€‰ Importance of Reinforcing Stereoelectronic Effects in â€œHigh-Energyâ€•Phosphoester Bonds. Journal of the American Chemical Society, 2005, 127, 17789-17798.	6.6	20
1954	Internal Rotation in Propionic Acid:Â Near-Infrared-Induced Isomerization in Solid Argon. Journal of Physical Chemistry A, 2005, 109, 3617-3625.	1.1	72
1955	o-Phenylene Halocarbenonitrenes ando-Phenylene Chlorocarbenocarbene:Â A Combined Experimental and Computational Approach. Journal of Organic Chemistry, 2005, 70, 7744-7754.	1.7	9
1956	Reactions of Trimethylindium on TiO2Nanoparticles:Â Experimental and Computational Study. Journal of Physical Chemistry B, 2005, 109, 20858-20867.	1.2	15
1957	Comparative DFT Study of the Spin Trapping of Methyl, Mercapto, Hydroperoxy, Superoxide, and Nitric Oxide Radicals by Various Substituted Cyclic Nitrones. Journal of Physical Chemistry A, 2005, 109, 1662-1674.	1.1	36
1958	What Ion Is Generated When Ionizing Acetonitrile?. Journal of Physical Chemistry A, 2005, 109, 4425-4427.	1.1	13
1959	Photoaffinity Labeling with 8-Azidoadenosine and Its Derivatives:Â Chemistry of Closed and Opened Adenosine Diazaquinodimethanesâ€. Biochemistry, 2005, 44, 11241-11253.	1.2	20
1960	Dichlorocarbene Addition to Cyclopropenes:â€‰ A Computational Study. Journal of Organic Chemistry, 2005, 70, 1630-1635.	1.7	27

#	Article	IF	Citations
1961	Flexibility of â€œPolyunsaturated Fatty Acid Chainsâ€•and Peptide Backbones:â€‰ A Comparative ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 520-533.	1.1	13
1962	Synthesis and Characterization of Three Novel Perfluoro-oligothiophenes Ranging in Length from the Trimer to the Pentamer. Journal of Physical Chemistry B, 2005, 109, 20737-20745.	1.2	16
1963	Structure and Dynamics of Solvated Sn(II) in Aqueous Solution:Â An ab Initio QM/MM MD Approach. Journal of the American Chemical Society, 2005, 127, 14231-14238.	6.6	53
1964	Energetics of the Nâ^'O Bonds in 2-Hydroxyphenazine-di-N-oxide. Journal of Physical Chemistry B, 2005, 109, 16188-16195.	1.2	16
1965	Synthetic Applications of (Me3SiNSN)2E (E = S, Se) in Chalcogen-Nitrogen Chemistry:Â Formation and Structural Characterization of Cl2TeESN2(E = S, Se) and [PPh4]2[Pd2(Ï¼-Se2N2S)X4] (X = Cl, Br). Inorganic Chemistry, 2005, 44, 4992-5000.	1.9	9
1966	PCM Study of the Solvent and Substituent Effects on the Conformers, Intramolecular Hydrogen Bonds and Bond Dissociation Enthalpies of 2-Substituted Phenols. Journal of Physical Chemistry A, 2005, 109, 366-377.	1.1	42
1967	Dialkyl sulphur radical cations: competition between proton and methyl cation transfers to sulphur nucleophiles: anab initiostudy. Molecular Physics, 2005, 103, 1201-1209.	0.8	2
1968	Effects of Substituents on the Stability of Phosphoranyl Radicals. Journal of Physical Chemistry A, 2005, 109, 10013-10021.	1.1	15
1969	Quantum Chemical and Master Equation Simulations of the Oxidation and Isomerization of Vinoxy Radicals. Journal of Physical Chemistry A, 2005, 109, 2514-2524.	1.1	43
1970	Ultrafast Infrared Mechanistic Studies of the Interaction of 1-Hexyne with Group 6 Hexacarbonyl Complexes. Organometallics, 2005, 24, 1852-1859.	1.1	28
1971	Structures and Energetics of Hydrated Oxygen Anion Clusters. Journal of Physical Chemistry A, 2005, 109, 7418-7428.	1.1	5
1972	Saccharin: a combined experimental and computational thermochemical investigation of a sweetener and sulfonamide. Molecular Physics, 2005, 103, 221-228.	0.8	32
1973	Layer-by-Layer Growth on Ge(100) via Spontaneous Urea Coupling Reactions. Journal of the American Chemical Society, 2005, 127, 6123-6132.	6.6	127
1974	Two-Dimensional Infrared Spectroscopy of the Alanine Dipeptide in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 7511-7521.	1.2	192
1975	Understanding the Infrared Spectrum of Bare CH5+. Science, 2005, 309, 1219-1222.	6.0	194
1976	Gas-Phase Synthesis, Characterization, and Reactivity Studies of the Prototype Aromatic Phosphirenylium Ion. Organometallics, 2005, 24, 3125-3135.	1.1	12
1977	N-Alkenyl-2-aziridinylmethyl Radicals andN-Alkenylaminyl Radicals in Cascade Cyclizations to Pyrrolizidines and Indolizidines. Journal of Organic Chemistry, 2005, 70, 3674-3681.	1.7	16
1978	A Kinetic Model of the Formation of Organic Monolayers on Hydrogen-Terminated Silicon by Hydrosilation of Alkenes. Journal of Physical Chemistry B, 2005, 109, 24035-24045.	1.2	31

#	Article	IF	Citations
1979	The Reaction of Triplet Nitrenes with Oxygen:â€‰ A Computational Study. Organic Letters, 2005, 7, 549-552.	2.4	38
1980	Kinetics of Metal Organicâ^'Ammonia Adduct Decomposition:â€‰ Implications for Group-III Nitride MOCVD. Journal of Physical Chemistry A, 2005, 109, 10554-10562.	1.1	42
1981	DFT/TDDFT Studies of the Geometry, Electronic Structure and Spectra of (12S)-1,4,7,10-Tetraazadicyclo[10,3,0]-pentadecane-3,11-dione and Its Derivatives. Journal of Physical Chemistry A, 2005, 109, 2878-2886.	1.1	14
1982	A T-Shaped Three-Coordinate Nickel(I) Carbonyl Complex and the Geometric Preferences of Three-Coordinate d9Complexes. Inorganic Chemistry, 2005, 44, 7702-7704.	1.9	97
1983	Breaking of Ketene Bonds during HCl Addition to Trimethylsilylketene. Journal of Physical Chemistry A, 2005, 109, 2120-2126.	1.1	2
1984	Understanding Structural and Dynamic Properties of Well-Defined Rhenium-Based Olefin Metathesis Catalysts, Re(â‹®CR)(CHR)(X)(Y), from DFT and QM/MM Calculations. Organometallics, 2005, 24, 1586-1597.	1.1	59
1985	An Evaluation of Various Computational Methods for the Treatment of Organoselenium Compounds. Journal of Physical Chemistry A, 2005, 109, 10373-10379.	1.1	32
1986	Theoretical Methods of Potential Use for Studies of Inorganic Reaction Mechanisms. Chemical Reviews, 2005, 105, 2695-2722.	23.0	387
1987	Theoretical and Experimental Study of the Product Branching in the Reaction of Acetic Acid with OH Radicals. Journal of Physical Chemistry A, 2005, 109, 2401-2409.	1.1	43
1988	Propagation Mechanisms in Ring-Opening Polymerization of Small Phosphorus Heterocycles:Â Toward Free-Radical Polymerization of Phosphines?. Macromolecules, 2005, 38, 8902-8910.	2.2	25
1989	Cationâ^Ï€ Interactions with a Model for the Side Chain of Tryptophan:Â Structures and Absolute Binding Energies of Alkali Metal Cationâ^'Indole Complexesâ€. Journal of Physical Chemistry A, 2005, 109, 11539-11550.	1.1	71
1990	Infrared Spectra and Structures of the Coinage Metal Dihydroxide Molecules. Inorganic Chemistry, 2005, 44, 9076-9083.	1.9	39
1991	Formation and Characterization of Thorium Methylidene CH2ThHX Complexes. Inorganic Chemistry, 2005, 44, 8610-8616.	1.9	44
1992	Mechanism of the Hydrosilylation Reaction of Alkenes at Porous Silicon:â€‰ Experimental and Computational Deuterium Labeling Studies. Journal of Physical Chemistry B, 2005, 109, 12020-12031.	1.2	60
1993	Theoretical Studies of Proton-Transfer Reactions of 2-Hydroxypyridineâ^'(H2O)n (n = 0â^'2) in the Ground and Excited States. Journal of Physical Chemistry A, 2005, 109, 3983-3990.	1.1	53
1994	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	1.1	72
1995	Alternated Quinoid/Aromatic Units in Terthiophenes Building Blocks for Electroactive Narrow Band Gap Polymers. Extended Spectroscopic, Solid State, Electrochemical, and Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 16616-16627.	1.2	48
1996	The Mechanism of Photoinduced Acylation of Amines byN-Acyl-5,7-dinitroindoline as Determined by Time-Resolved Infrared Spectroscopy. Organic Letters, 2005, 7, 2845-2848.	2.4	25

#	Article	IF	Citations
1997	Trifluoromethanesulfenyl Acetate, CF3Sâ˜OC(O)CH3, and Trifluoromethanesulfenyl Trifluoroacetate, CF3Sâ˜OC(O)CF3:Â Unexpected Conformational Properties. Journal of Physical Chemistry A, 2005, 109, 3739-3744.	1.1	19
1998	Crystal Structure and Vibrational Spectra of AlVO4. A DFT Study. Journal of Physical Chemistry B, 2005, 109, 394-400.	1.2	39
1999	Modeling Î²-Scission Reactions of Peptide Backbone Alkoxy Radicals:Â Backbone Câ˜C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	2.3	6
2000	Design of Ï€-Conjugated Organic Materials for One-Dimensional Energy Transport in Nanochannels. Journal of Physical Chemistry B, 2005, 109, 4872-4880.	1.2	40
2001	Ab-initio structure, energy and stable Cr isotopes equilibrium fractionation of some geochemically relevant H-O-Cr-Cl complexes. Geochimica Et Cosmochimica Acta, 2005, 69, 851-874.	1.6	19
2002	ATR-FTIR spectroscopic characterization of coexisting carbonate surface complexes on hematite. Geochimica Et Cosmochimica Acta, 2005, 69, 1527-1542.	1.6	166
2003	Theoretical and 27Al CPMAS NMR investigation of aluminum coordination changes during aluminosilicate dissolution. Geochimica Et Cosmochimica Acta, 2005, 69, 2205-2220.	1.6	72
2004	Calculating the partitioning of the isotopes of Mo between oxidic and sulfidic species in aqueous solution. Geochimica Et Cosmochimica Acta, 2005, 69, 2981-2993.	1.6	202
2005	Boron isotopic fractionation between minerals and fluids: New insights from in situ high pressure-high temperature vibrational spectroscopic data. Geochimica Et Cosmochimica Acta, 2005, 69, 4301-4313.	1.6	57
2006	Ab initio molecular orbital calculations for boron isotope fractionations on boric acids and borates. Geochimica Et Cosmochimica Acta, 2005, 69, 3995-4006.	1.6	150
2007	Boric acid, â€œcarbonicâ€•acid, and N-containing oxyacids in aqueous solution: Ab initio studies of structure, pKa, NMR shifts, and isotopic fractionations. Geochimica Et Cosmochimica Acta, 2005, 69, 5647-5658.	1.6	52
2008	Combined Raman, electrochemical and DFT studies on a series of Î±, Î±â€²-thiophene-phosphole oligomers and their corresponding polymers. Synthetic Metals, 2005, 153, 249-252.	2.1	12
2009	Synthesis, spectroscopy and quantum chemical DFT studies on new pleiadene-based materials. Synthetic Metals, 2005, 153, 245-248.	2.1	3
2010	Experimental and Computational Studies of Substituted Terthiophene Oligomers as Electroluminescent Materials. Synthetic Metals, 2005, 153, 225-228.	2.1	6
2011	A mechanism for carbon isotope exchange between aqueous acetic acid and : An ab initio study. Organic Geochemistry, 2005, 36, 835-850.	0.9	11
2012	Structure and ultrafast dynamics of liquid water: A quantum mechanics/molecular mechanics molecular dynamics simulations study. Journal of Chemical Physics, 2005, 122, 174506.	1.2	106
2013	Searching for More Effective Agents and Conditions for the RAFT Polymerization of MMA:Â Influence of Dithioester Substituents, Solvent, and Temperature. Macromolecules, 2005, 38, 3129-3140.	2.2	214
2014	Computer Simulation of the Linear and Nonlinear Optical Susceptibilities ofp-Nitroaniline in Cyclohexane, 1,4-Dioxane, and Tetrahydrofuran in Quadrupolar Approximation. I. Molecular Polarizabilities and Hyperpolarizabilities. Journal of Physical Chemistry A, 2005, 109, 10106-10120.	1.1	33

#	Article	IF	Citations
2015	The effects of substrate orientation on the mechanism of a phosphotriesterase. Organic and Biomolecular Chemistry, 2005, 3, 4343.	1.5	32
2016	Infrared spectra and structures of the Th(OH)2 and Th(OH)4 molecules. Physical Chemistry Chemical Physics, 2005, 7, 3834.	1.3	24
2017	Vibrational energy relaxation of azulene studied by the transient grating method. II. Liquid solvents. Journal of Chemical Physics, 2005, 123, 054513.	1.2	17
2018	Gas-Phase Thermochemistry and Mechanism of Organometallic Tin Oxide CVD Precursors. Topics in Organometallic Chemistry, 2005, , 1-48.	0.7	9
2019	Examination of the Charge-Sensitive Vibrational Modes in Bis(ethylenedithio)tetrathiafulvalene. Journal of Physical Chemistry B, 2005, 109, 15226-15235.	1.2	118
2020	Raman and Theoretical Study of the Solvent Effects on the Sizable Intramolecular Charge Transfer in the Pushâ^'Pull 5-(Dimethylamino)-5â€²-nitro-2,2â€²-bithiophene. Journal of Physical Chemistry A, 2005, 109, 8724-8731.	1.1	28
2021	Incisive Structureâ^'Spectroscopic Correlation in Oligothiophenes Functionalized with (Â±) Inductive/Mesomeric Fluorine Groups:Â Joint Raman and DFT Study. Journal of the American Chemical Society, 2005, 127, 13364-13372.	6.6	29
2022	Infrared and Raman Line Shapes of Dilute HOD in Liquid H2O and D2O from 10 to 90 Â°C. Journal of Physical Chemistry A, 2005, 109, 6154-6165.	1.1	298
2023	Infrared Spectra and Structures for Group 4 Dihydroxide and Tetrahydroxide Molecules. Journal of Physical Chemistry A, 2005, 109, 10689-10701.	1.1	35
2024	Infrared Spectrum and Structure of the Hf(OH)4Molecule. Inorganic Chemistry, 2005, 44, 7189-7193.	1.9	17
2025	Secondary Alpha Isotope Effects on Deuterium Tunneling in Tripleto-Methylanthrones:Â Extraordinary Sensitivity to Barrier Width. Journal of the American Chemical Society, 2005, 127, 10178-10179.	6.6	17
2026	Oligothiophene-Containing Coumarin Dyes for Efficient Dye-Sensitized Solar Cells. Journal of Physical Chemistry B, 2005, 109, 15476-15482.	1.2	562
2027	Photochemistry of 2-(1-Naphthyl)-2H-azirines in Matrixes and in Solutions:Â Wavelength-Dependent Câ^'C and Câ^'N Bond Cleavage of the Azirine Ring. Journal of the American Chemical Society, 2005, 127, 2628-2636.	6.6	62
2028	Detailed Ab Initio Studies of the Conformers and Conformational Distributions of Gaseous Tryptophan. Journal of Physical Chemistry A, 2005, 109, 2656-2659.	1.1	75
2029	Systematic ab initio studies of the conformers and conformational distribution of gas-phase tyrosine. Journal of Chemical Physics, 2005, 122, 134313.	1.2	62
2030	Computational estimates of the gas-phase basicities, proton affinities and ionization potentials of the six isomers of dihydroxybenzoic acid. Molecular Physics, 2005, 103, 183-189.	0.8	24
2031	Intramolecular Dynamics of 1,2,3-Trifluorobenzene Radical Anions As Studied by OD ESR and Quantum-Chemical Methods. Journal of Physical Chemistry A, 2005, 109, 4404-4409.	1.1	26
2032	Gas-Phase Interaction of H2S with O2:â€‰ A Kinetic and Quantum Chemistry Study of the Potential Energy Surface. Journal of Physical Chemistry A, 2005, 109, 1057-1062.	1.1	35

#	Article	IF	Citations
2033	Progressive Systematic Underestimation of Reaction Energies by the B3LYP Model as the Number of Cå^C Bonds Increases: Why Organic Chemists Should Use Multiple DFT Models for Calculations Involving Polycarbon Hydrocarbons. Journal of Organic Chemistry, 2005, 70, 9828-9834.	1.7	214
2034	Ground and Excited State Dissociation Dynamics of Ionized 1,1-Difluoroethene. Journal of Physical Chemistry A, 2005, 109, 8225-8235.	1.1	19
2035	Vibrational Raman optical activity as a mean for revealing the helicity of oligosilanes: A quantum chemical investigation. Journal of Chemical Physics, 2005, 122, 214304.	1.2	23
2036	Spectroscopic and Computational Studies of Aqueous Ethylene Glycol Solution Surfaces. Journal of Physical Chemistry B, 2005, 109, 811-818.	1.2	46
2037	Charges of Phosphate Groups. A Role in Stabilization of 2â€²-deoxyribonucleotides. A DFT Investigation. Journal of Biomolecular Structure and Dynamics, 2005, 22, 441-454.	2.0	25
2038	Competition at Chiral Metal Surfaces:Â Fundamental Aspects of the Inversion of Enantioselectivity in Hydrogenations on Platinum. Journal of the American Chemical Society, 2005, 127, 8467-8477.	6.6	93
2039	Role of the Direct Reaction H2S + SO2in the Homogeneous Claus Reaction. Journal of Physical Chemistry A, 2005, 109, 8180-8186.	1.1	23
2040	Planar Tetracoordinate Carbons in Cyclic Hydrocarbons. Organic Letters, 2005, 7, 1509-1512.	2.4	68
2041	Development and Validation of Empirical Force Field Parameters for Netropsin. Journal of Chemical Information and Modeling, 2005, 45, 1546-1552.	2.5	31
2042	Reactivity of Alkanes on Zeolites:â€‰ A Computational Study of Propane Conversion Reactions. Journal of Physical Chemistry A, 2005, 109, 10734-10741.	1.1	45
2043	Mesitylthio-Oligothiophenes in Various Redox States. Molecular and Electronic Views as Offered by Spectroscopy and Theory. Journal of Physical Chemistry A, 2005, 109, 11275-11284.	1.1	21
2044	Infrared spectra of homogeneous and heterogeneous proton-bound dimers in the gas phase. Physical Chemistry Chemical Physics, 2005, 7, 2747.	1.3	77
2045	Theoretical Studies on the Vibrational Spectra, Thermodynamic Properties, Detonation Properties, and Pyrolysis Mechanisms for Polynitroadamantanes. Journal of Physical Chemistry A, 2005, 109, 11268-11274.	1.1	111
2046	Conformational Study of the Structure of 12-crown-4â^'Alkali Metal Cation Complexes. Journal of Physical Chemistry A, 2005, 109, 8041-8048.	1.1	21
2047	On the Binding Determinants of the Glutamate Agonist with the Glutamate Receptor Ligand Binding Domain. Biochemistry, 2005, 44, 11508-11517.	1.2	27
2048	Spectroscopy and Computations of Supported Metal Adducts. 1. DFT Study of CO and NO Adsorption and Coadsorption on Cu/SiO2. Journal of Physical Chemistry B, 2005, 109, 10291-10303.	1.2	20
2049	Quality Control of Commercially Available Essential Oils by Means of Raman Spectroscopy. Journal of Agricultural and Food Chemistry, 2006, 54, 7020-7026.	2.4	27
2050	Mechanistic Studies on the Conversion of Dicobalt Octacarbonyl into Colloidal Cobalt Nanoparticles. Langmuir, 2006, 22, 3823-3829.	1.6	44

#	Article	IF	Citations
2051	Infrared Spectra of M(OH)1,2,3 (M = Mn, Fe, Co, Ni) Molecules in Solid Argon and the Character of First Row Transition Metal Hydroxide Bonding. Journal of Physical Chemistry A, 2006, 110, 10035-10045.	1.1	80
2052	Synthesis of the CETP Inhibitor Torcetrapib:Â The Resolution Route and Origin of Stereoselectivity in the Iminium Ion Cyclization. Organic Process Research and Development, 2006, 10, 464-471.	1.3	44
2053			

#	Article	IF	Citations
2069	The absorption spectra of anisole-h8, anisole-d3 and anisole-d8. The assignment of fundamental vibrations in the S0and the S1states. Physical Chemistry Chemical Physics, 2006, 8, 2360-2377.	1.3	26
2070	Group 4 Transition-Metal Atom Reactions with CS2and OCS:Â Infrared Spectra and Density Functional Calculations of SMCS, SM-(Î·2-CS), SMCO, and OMCS in Solid Argon. Journal of Physical Chemistry A, 2006, 110, 12785-12792.	1.1	3
2071	One-electron oxidation of methionine peptides â€" Stability of the three-electron Sâ€"N(amide) bond. Canadian Journal of Chemistry, 2006, 84, 893-904.	0.6	24
2072	A Combined QM/MM Molecular Dynamics Simulations Study of Nitrate Anion (NO3-) in Aqueous Solution. Journal of Physical Chemistry A, 2006, 110, 12918-12926.	1.1	58
2073	Theoretical Investigation of Doubly Resonant IRâˆ’UV Sum-Frequency Vibrational Spectroscopy of Binaphthol Chiral Solution. Journal of Physical Chemistry B, 2006, 110, 4480-4486.	1.2	23
2074	Metal-Mediated Formation of Gas-Phase Amino Acid Radical Cationsâ€,#. Journal of Physical Chemistry A, 2006, 110, 8304-8315.	1.1	64
2075	Chemical failure modes of AlQ3-based OLEDs: AlQ3 hydrolysis. Physical Chemistry Chemical Physics, 2006, 8, 1371.	1.3	63
2076	A DFT study of the structures of pyruvic acid isomers and their decarboxylation. Organic and Biomolecular Chemistry, 2006, 4, 886.	1.5	28
2077	Theoretical study of photoacidity of HCN: the effect of complexation with water. Physical Chemistry Chemical Physics, 2006, 8, 4866-4873.	1.3	10
2078	Matrix isolation and computational study of the photochemistry of p-azidoaniline. Physical Chemistry Chemical Physics, 2006, 8, 719-727.	1.3	42
2079	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. Journal of Chemical Theory and Computation, 2006, 2, 364-382.	2.3	3,329
2080	Formation and Characterization of the Uranium Methylidene Complexes CH2UHX (X = F, Cl, and Br). Inorganic Chemistry, 2006, 45, 1847-1852.	1.9	49
2081	Mechanism of Remote Conjugate Addition of Lithium Organocuprates to Polyconjugated Carbonyl Compounds. Chemistry - an Asian Journal, 2006, 1, 322-330.	1.7	29
2082	Specific Heat of Molecular Crystals from Atomic Mean Square Displacements with the Einstein, Debye, and Nernstâ^'Lindemann Models. Journal of Physical Chemistry B, 2006, 110, 26129-26134.	1.2	20
2083	Understanding hydrogen scrambling and infrared spectrum of bare CH5+based on ab initio simulations. Physical Chemistry Chemical Physics, 2006, 8, 573-586.	1.3	80
2084	Cationâ^'Ï€ Interactions and Oxidative Effects on Cu+and Cu2+Binding to Phe, Tyr, Trp, and His Amino Acids in the Gas Phase. Insights from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 24189-24199.	1.2	77
2085	Raman spectroscopy of nanocrystalline diamond: Anab initioapproach. Physical Review B, 2006, 74, .	1.1	93
2086	Experimental and Theoretical Study of the Regiospecific Coordination of RuIIand OsIIFragments on the Lacunary Polyoxometalate [Î±-PW11O39]7-. Journal of Physical Chemistry A, 2006, 110, 6345-6355.	1.1	52

#	Article	IF	Citations
2087	Lignin Radicals in the Plant Cell Wall Probed by Kerr-Gated Resonance Raman Spectroscopy. Biophysical Journal, 2006, 90, 2978-2986.	0.2	39
2088	Design principles for Î±-tocopherol analogues. Organic and Biomolecular Chemistry, 2006, 4, 846.	1.5	24
2089	Raman scattering and FT-IR spectroscopic studies on dithienylethene switchesâ€"towards non-destructive optical readout. Organic and Biomolecular Chemistry, 2006, 4, 2387-2392.	1.5	48
2090	Chromatographic Resolution, Solution and Crystal Phase Conformations, and Absolute Configuration oftert-Butyl(dimethylamino)phenylphosphineâ^'Borane Complex. Journal of Organic Chemistry, 2006, 71, 5586-5593.	1.7	16
2091	Porphyrin-rhodanine dyads for dye sensitized solar cells. Journal of Porphyrins and Phthalocyanines, 2006, 10, 1007-1016.	0.4	59
2092	A Study of Cysteamine Ionization in Solution by Raman Spectroscopy and Theoretical Modeling. Journal of Physical Chemistry A, 2006, 110, 13394-13404.	1.1	49
2093	Proton hydration in aqueous solution: Fourier transform infrared studies of HDO spectra. Journal of Chemical Physics, 2006, 125, 204508.	1.2	41
2094	Study on the vibrational energy relaxation of p-nitroaniline, N,N-dimethyl-p-nitroaniline, and azulene by the transient grating method. Journal of Chemical Physics, 2006, 125, 194516.	1.2	17
2095	The Anharmonic Vibrational Potential and Relaxation Pathways of the Amide I and II Modes ofN-Methylacetamideâ€. Journal of Physical Chemistry B, 2006, 110, 18973-18980.	1.2	123
2096	Density functional theory and atoms-in-molecule study on the role of two-electron stabilizing interactions in retro Dielsâ€"Alder reaction of cycloadducts derived from substituted cyclopentadiene and p-benzoquinone. Organic and Biomolecular Chemistry, 2006, 4, 3923-3930.	1.5	10
2097	Transfer hydrogenation between ethane and ethene: a critical assessment of theoretical procedures. Molecular Physics, 2006, 104, 777-794.	0.8	12
2098	Matrix Preparation and Spectroscopic and Theoretical Investigations of Simple Methylidene and Methylidyne Complexes of Group 4â^'6 Transition Metals. Organometallics, 2006, 25, 4040-4053.	1.1	204
2099	Probing mechanistic photochemistry of glyoxal in the gas phase by ab initio calculations of potential-energy surfaces and adiabatic and nonadiabatic rates. Journal of Chemical Physics, 2006, 124, 054324.	1.2	13
2100	Structureâ^'Property Relationships in Pushâ^'Pull Amino/Cyanovinyl End-Capped Oligothiophenes:Â Quantum Chemical and Experimental Studies. Journal of Organic Chemistry, 2006, 71, 7509-7520.	1.7	81
2101	Primary Semiclassical Kinetic Hydrogen Isotope Effects in Identity Carbon-to-Carbon Proton- and Hydride-Transfer Reactions, an ab Initio and DFT Computational Study. Journal of Organic Chemistry, 2006, 71, 5959-5968.	1.7	15
2102	Octopolar Chromophores Based on Donor- and Acceptor-Substituted 1,3,5-Tris(phenylethynyl)benzenes:â€‰ Impact of meta-Conjugation on the Molecular and Electronic Structure by Means of Spectroscopy and Theory. Journal of Physical Chemistry B, 2006, 110, 19198-19206.	1.2	31
2103	Gaseous Arginine Conformers and Their Unique Intramolecular Interactions. Journal of Physical Chemistry A, 2006, 110, 12282-12291.	1.1	100
2104	A Photoelectron and TPEPICO Investigation of the Acetone Radical Cation. Journal of Physical Chemistry A, 2006, 110, 8663-8675.	1.1	30

#	Article	IF	Citations
2105	Electron Deficient Carbonâ˜Titanium Triple Bonds:Â Formation of Triplet XCÃ·TiX3Methylidyne Complexes. Inorganic Chemistry, 2006, 45, 9858-9863.	1.9	23
2106	Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808.	1.1	23
2107	Thermally Assisted Collision-Induced Dissociation in a Quadrupole Ion Trap Mass Spectrometer. Analytical Chemistry, 2006, 78, 4609-4614.	3.2	23
2108	IR Spectroscopy of M+(Acetone) Complexes (M = Mg, Al, Ca):â€‰Cationâ˜Carbonyl Binding Interactions. Journal of Physical Chemistry A, 2006, 110, 2325-2330.	1.1	31
2109	Combined Quantum Chemical Density Functional Theory and Spectroscopic Raman and UVâ˜visâ˜NIR Study of Oligothienoacenes with Five and Seven Rings. Journal of Physical Chemistry A, 2006, 110, 5058-5065.	1.1	39
2110	Theoretical DFT Study on the Interaction of NO and Br2with the Pt(111) Surface. Journal of Chemical Theory and Computation, 2006, 2, 801-807.	2.3	7
2111	Exploration of Ground and Excited Electronic States of Aromatic and QuinoidS,S-Dioxide Terthiophenes. Complementary Systems for Enhanced Electronic Organic Materials. Journal of the American Chemical Society, 2006, 128, 10134-10144.	6.6	55
2112	Infrared Spectra and Density Functional Calculations for the Sc(OH)2,3 and HOScO Molecules and the Sc(OH)2+ Cation in Solid Argon. Journal of Physical Chemistry A, 2006, 110, 1850-1858.	1.1	19
2113	Formation of CH2TiF2 by Câ˜F Activation and Î±-F Transfer. Organometallics, 2006, 25, 1341-1343.	1.1	16
2114	Characteristic Structure and Environment in FAD Cofactor of (6â˜4) Photolyase along Function Revealed by Resonance Raman Spectroscopy. Journal of Physical Chemistry B, 2006, 110, 16724-16732.	1.2	27
2115	Hydrogen Peroxide Clusters:Â The Role of Open Book Motif in Cage and Helical Structures. Journal of Physical Chemistry A, 2006, 110, 6294-6300.	1.1	33
2116	Oâ˜H Stretch Modes of Dodecahedral Water Clusters:Â A Statistical Ab Initio Study. Journal of Physical Chemistry A, 2006, 110, 5135-5143.	1.1	17
2117	Gas-Phase Structures, Rotational Barriers, and Conformational Properties of Hydroxyl and Mercapto Derivatives of Cyclohexa-2,5-dienone and Cyclohexa-2,5-dienthione. Journal of Physical Chemistry A, 2006, 110, 8901-8911.	1.1	8
2118	Is NO3Formed during the Decomposition of Nitramine Explosives?. Journal of Physical Chemistry A, 2006, 110, 13974-13978.	1.1	24
2119	Raman Spectroscopic Studies of Terthiophenes for Molecular Electronics. Journal of Physical Chemistry B, 2006, 110, 25671-25677.	1.2	17
2120	Fluorescence and REMPI Spectroscopy of Jet-Cooled Isolated 2-Phenylindene in the S1State. Journal of Physical Chemistry A, 2006, 110, 5017-5031.	1.1	9
2121	Saturated Hydrocarbonâ˜Benzene Complexes:Â Theoretical Study of Cooperative CH/Ï€ Interactions. Journal of Physical Chemistry A, 2006, 110, 9702-9709.	1.1	122
2122	Quantum Chemical Study of the Interaction of the Short-Chain Poly(oxyethylene)s CH3(OCH2CH2)mOCH3(C1EmC1;m= 1 and 2) with a Water Molecule in the Gas Phase and in Solutions. Journal of Physical Chemistry A, 2006, 110, 1052-1059.	1.1	14

#	Article	IF	Citations
2123	A Quantum Chemical Study of the Catalysis for Cytidine Deaminase:Â Contribution of the Extra Water Molecule. Journal of Chemical Information and Modeling, 2006, 46, 1276-1285.	2.5	23
2124	Theoretical Study of Adsorption of Sarin and Soman on Tetrahedral Edge Clay Mineral Fragments. Journal of Physical Chemistry B, 2006, 110, 21175-21183.	1.2	37
2125	Computational Study of the Reaction of Atomic Oxygen with Acetone in the Gas Phase. Journal of Physical Chemistry A, 2006, 110, 13163-13171.	1.1	4
2126	Computational Study of Antagonist/Î±1AAdrenoceptor ComplexesObservations of Conformational Variations on the Formation of Ligand/Receptor Complexes. Journal of Medicinal Chemistry, 2006, 49, 501-510.	2.9	16
2127	Vibronic Structure in the S1â^'S0 Transition of Jet-Cooled Dibenzofuran. Journal of Physical Chemistry A, 2006, 110, 10000-10005.	1.1	10
2128	Structure and Vibrational Spectra of Mononitrated Benzo[a]pyrenes. Journal of Physical Chemistry A, 2006, 110, 76-84.	1.1	39
2129	Assessing the Protonation State of Drug Molecules:Â The Case of Aztreonam. Journal of Medicinal Chemistry, 2006, 49, 3235-3243.	2.9	13
2130	Allylic H-Abstraction Mechanism:â€‰ The Potential Energy Surface of the Reaction of Propene with OH Radical. Journal of Chemical Theory and Computation, 2006, 2, 1575-1586.	2.3	66
2131	Effect of Ring Substitution on the Sâ^'H Bond Dissociation Enthalpies of Thiophenols. An Experimental and Computational Study. Journal of Physical Chemistry A, 2006, 110, 9949-9958.	1.1	25
2132	A Density Functional Theory Study of the 5-Exo Cyclization Reactions of Î±-Substituted 6,6-Diphenyl-5-hexenyl Radicals. Journal of Organic Chemistry, 2006, 71, 1984-1988.	1.7	10
2133	Formation and Decomposition of Chemically Activated Cyclopentoxy Radicals from the c-C5H9 + O Reaction. Journal of Physical Chemistry A, 2006, 110, 3165-3173.	1.1	15
2134	Infrared Spectra and Density Functional Calculations for M(OH)2,3and HOMO Molecules and M(OH)2+Cations (M = Y, La). Journal of Physical Chemistry A, 2006, 110, 4157-4168.	1.1	16
2135	IR Spectroscopic Features of Gaseous C7H7O+Ions:Â Benzylium versus Tropylium Ion Structures. Journal of Physical Chemistry A, 2006, 110, 9352-9360.	1.1	50
2136	Water-Assisted Interconversions and Dissociations of the Acetaldehyde Ion and Its Isomers. An Experimental and Theoretical Studyâ€. Journal of Physical Chemistry A, 2006, 110, 8409-8417.	1.1	6
2137	Prediction of Accurate Anharmonic Experimental Vibrational Frequencies for Water Clusters, (H2O)n, n = 2â^'5. Journal of Physical Chemistry A, 2006, 110, 303-309.	1.1	99
2138	Quantum Molecular Dynamics Study of the Reaction of O2with HOCOâ€. Journal of Physical Chemistry A, 2006, 110, 5312-5316.	1.1	23
2139	Toward a Detailed Understanding of Base Excision Repair Enzymes:â€‰ Transition State and Mechanistic Analyses of N-Glycoside Hydrolysis and N-Glycoside Transfer. Chemical Reviews, 2006, 106, 506-555.	23.0	238
2140	Experimental and Theoretical Study of the Vibrational Spectra of 12-Crown-4â^'Alkali Metal Cation Complexes. Journal of Physical Chemistry A, 2006, 110, 8676-8687.	1.1	29

#	Article	IF	Citations
2141	Quantum Chemical and Theoretical Kinetics Study of the O(3P) + C2H2Reaction:Â A Multistate Processâ€. Journal of Physical Chemistry A, 2006, 110, 6696-6706.	1.1	48
2142	Two-State Reactivity in Alkane Hydroxylation by Non-Heme Ironâ"Oxo Complexes. Journal of the American Chemical Society, 2006, 128, 8590-8606.	6.6	331
2143	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-PyrrolineN-Oxide (DMPO). 1. Carbon Dioxide Radical Anion. Journal of Physical Chemistry A, 2006, 110, 13253-13258.	1.1	84
2144	Multireference Configuration Interaction Calculation of the BÌƒ2Aâ€˜Ââ€˜â"XÌƒ2Aâ€˜Ââ€˜ Transition of Halogen- and Methyl-Substituted Vinoxy Radicals. Journal of Physical Chemistry A, 2006, 110, 12419-12426.	1.1	8
2145	Surface-Enhanced Raman Spectroscopic Study of 1,4-Phenylene Diisocyanide Adsorbed on Gold and Platinum-Group Transition Metal Electrodes. Journal of Physical Chemistry B, 2006, 110, 4782-4792.	1.2	44
2146	Density Functional Theory (DFT) Calculations of the Infrared Absorption Spectra of Acetaminophen Complexes Formed with Ethanol and Acetone Species. Journal of Physical Chemistry A, 2006, 110, 8986-9001.	1.1	17
2147	Addition-Fragmentation Kinetics of Fluorodithioformates (F-RAFT) in Styrene, Vinyl Acetate, and Ethylene Polymerization:Â An Ab Initio Investigation. Macromolecules, 2006, 39, 4585-4591.	2.2	55
2148	Spectroscopic Characterization of Ï‰-Substituted Biphenylthiolates on Gold and Their Use as Substrates for â€œOn-Topâ€•Siloxane SAM Formation. Langmuir, 2006, 22, 4170-4178.	1.6	20
2149	Proton Affinity of Canavanine and Canaline, Oxyanalogues of Arginine and Ornithine, from the Extended Kinetic Method. Journal of Physical Chemistry A, 2006, 110, 11501-11508.	1.1	14
2150	Complex Formation of Trimethylaluminum and Trimethylgallium with Ammonia:Â Evidence for a Hydrogen-Bonded Adduct. Journal of Physical Chemistry A, 2006, 110, 1094-1099.	1.1	28
2151	Molecular Orbital Studies of Gas-Phase Interactions between Complex Molecules. Journal of Physical Chemistry A, 2006, 110, 3692-3702.	1.1	5
2152	Theoretical Studies of Phosphorescence Spectra of Tris(2,2â€˜-bipyridine) Transition Metal Compounds. Inorganic Chemistry, 2006, 45, 6161-6178.	1.9	97
2153	Dissociation of Toluene Cation:â€‰ A New Potential Energy Surface. Journal of Physical Chemistry A, 2006, 110, 7655-7662.	1.1	35
2154	Nature and Role of Bridged Carbonyl Intermediates in the Ultrafast Photoinduced Rearrangement of Ru3(CO)12. Organometallics, 2006, 25, 775-784.	1.1	28
2155	Donorâ"Acceptor Heteroleptic Open Sandwiches. Inorganic Chemistry, 2006, 45, 1091-1095.	1.9	36
2156	Infrared Spectra and Density Functional Calculations of CH2MHX and CHâ‹®MH2X Complexes Prepared in Reactions of Methyl Halides with Mo and W Atoms. Journal of Physical Chemistry A, 2006, 110, 13151-13162.	1.1	13
2157	Kinetic Modeling of the Propyl Radical Î²-Scission Reaction:Â An Application of Composite Energy Methods. Industrial & Engineering Chemistry Research, 2006, 45, 530-535.	1.8	10
2158	Thermochemical Studies of Pyrazolideâ€. Journal of Physical Chemistry A, 2006, 110, 8457-8466.	1.1	41

#	Article	IF	Citations
2159	Infrared Spectra of CH3â^'NbF, CH2NbHF, and CHâ‹®NbH2F- Formed by Reaction of Methyl Fluoride with Laser-Ablated Niobium Atoms. Organometallics, 2006, 25, 477-484.	1.1	15
2160	First-Principle Kinetic Modeling of the 1-Chloroethyl Unimolecular Decomposition Reaction. Industrial & Engineering Chemistry Research, 2006, 45, 2981-2985.	1.8	2
2161	Photochemical Synthesis of the Cyanodiacetylene HC5N:â€‰ A Cryogenic Matrix Experiment. Journal of Physical Chemistry A, 2006, 110, 2371-2377.	1.1	35
2162	Combined Experimental and Computational Study of the Thermochemistry of Methylpiperidines. Journal of Organic Chemistry, 2006, 71, 3677-3685.	1.7	33
2163	Molecular Orbital Theory Study on Surface Complex Structures of Glyphosate on Goethite:â€‰ Calculation of Vibrational Frequencies. Environmental Science & Technology, 2006, 40, 3836-3841.	4.6	46
2164	Reliable Low-Cost Theoretical Procedures for Studying Additionâ^'Fragmentation in RAFT Polymerization. Journal of Physical Chemistry A, 2006, 110, 2486-2492.	1.1	85
2165	Vibrational Spectroscopy and Normal-Mode Analysis of Fe(II) Octaethylporphyrin. Journal of Physical Chemistry B, 2006, 110, 13277-13282.	1.2	17
2166	Temperature Effects on the Structural and Dynamical Properties of the Zn(II)â^'Water Complex in Aqueous Solution:Â A QM/MM Molecular Dynamics Study. Journal of Physical Chemistry B, 2006, 110, 616-621.	1.2	12
2167	Secondary Organic Aerosol Formation by Heterogeneous Reactions of Aldehydes and Ketones:Â A Quantum Mechanical Study. Environmental Science & Technology, 2006, 40, 2333-2338.	4.6	35
2168	Calculation of Electron Affinities of Polycyclic Aromatic Hydrocarbons and Solvation Energies of Their Radical Anion. Journal of Physical Chemistry A, 2006, 110, 12927-12946.	1.1	42
2169	Impact of Local and Density Fitting Approximations on Harmonic Vibrational Frequencies. Journal of Physical Chemistry A, 2006, 110, 2060-2064.	1.1	75
2170	Calculation of Relative Energies of Permethylated Oligosilane Conformers in Vapor and in Alkane Solutionâ€. Journal of Physical Chemistry B, 2006, 110, 25485-25495.	1.2	12
2171	Computational Studies of the Coordination Stereochemistry, Bonding, and Metal Selectivity of Mercuryâ€. Journal of Physical Chemistry A, 2006, 110, 452-462.	1.1	43
2172	Ab Initio/GIAOâ^'CCSD(T) Study of Propenoyl (H2CCHâ^'CO+) and Isopentenoyl ((CH3)2CCHâ^'CO+) Cations and Their Superelectrophilic Protonated Dications1. Journal of Physical Chemistry A, 2006, 110, 1041-1045.	1.1	12
2173	Hybrid Organic Semiconductors Including Chalcogen Atoms in Ï€-Conjugated Skeletons. Tuning of Optical, Redox, and Vibrational Properties by Heavy Atom Conjugation. Journal of Physical Chemistry A, 2006, 110, 7422-7430.	1.1	25
2174	Mechanism of the Cyclopropenone Decarbonylation Reaction. A Density Functional Theory and Transient Spectroscopy Study. Journal of Physical Chemistry A, 2006, 110, 1749-1757.	1.1	52
2175	Vibrational Spectroscopy of Reduced Re(I) Complexes of 1,10-Phenanthroline and Substituted Analogues. Journal of Physical Chemistry A, 2006, 110, 4880-4887.	1.1	25
2176	Silicate Glass and Mineral Dissolution:â€‰ Calculated Reaction Paths and Activation Energies for Hydrolysis of a Q3 Si by H3O+ Using Ab Initio Methods. Journal of Physical Chemistry A, 2006, 110, 198-206.	1.1	134

#	Article	IF	Citations
2177	Reactivity of Isobutane on Zeolites:â€‰ A First Principles Study. Journal of Physical Chemistry A, 2006, 110, 2455-2460.	1.1	45
2178	Photolysis of Heptanal. Journal of Organic Chemistry, 2006, 71, 6403-6408.	1.7	20
2179	Reactions of F+(3P) and F+(1D) with Silicon Oxide. Possibility of Spin-Forbidden Processes. Journal of Physical Chemistry A, 2006, 110, 7130-7137.	1.1	0
2180	Liâ^'Biphenylâ^'1,2-Dimethoxyethane Solution:Â Calculation and Its Application. Journal of Physical Chemistry B, 2006, 110, 10341-10347.	1.2	20
2181	Two-Metal-Ion Mechanism for Hammerhead-Ribozyme Catalysis. Journal of Physical Chemistry B, 2006, 110, 3395-3409.	1.2	34
2182	Boric acid adsorption on humic acids: Ab initio calculation of structures, stabilities, 11B NMR and 11B,10B isotopic fractionations of surface complexes. Geochimica Et Cosmochimica Acta, 2006, 70, 5089-5103.	1.6	43
2183	Origins of Stereoselectivity in Dielsâ^'Alder Cycloadditions Catalyzed by Chiral Imidazolidinones. Journal of the American Chemical Society, 2006, 128, 3543-3553.	6.6	126
2184	Butatrienes as Extended Alkenes:Â Barriers to Internal Rotation and Substitution Effects on the Stabilities of the Ground States and Transition States. Journal of Physical Chemistry A, 2006, 110, 7237-7246.	1.1	23
2185	The correlation consistent composite approach (ccCA): An alternative to the Gaussian-n methods. Journal of Chemical Physics, 2006, 124, 114104.	1.2	269
2187	Stability of Complexes of Phenylacetylides and Benzyl Alkoxides with Methanol in the Gas Phase. Acidâ€“Base Correlation in the Ionic Hydrogen-Bond Strength. Bulletin of the Chemical Society of Japan, 2006, 79, 1118-1125.	2.0	2
2188	Geometrical Isomerism and Stability of Mono- and Dichalcogenide Analogs of Carbamic Acid H2NC(=X)YH (X, Y = O, S, Se). Bulletin of the Chemical Society of Japan, 2006, 79, 1869-1875.	2.0	10
2190	Equilibrium Conditions in Laser-Desorbed Plumes: Thermodynamic Properties of Î±-Cyano-4-Hydroxycinnamic Acid and Protonation of Amino Acids. European Journal of Mass Spectrometry, 2006, 12, 359-367.	0.5	20
2191	Theoretical Investigation of the Proton Affinity and Gas-Phase Basicity of Neutral x,y-Dihydroxybenzoic Acid and its Derivatives. European Journal of Mass Spectrometry, 2006, 12, 385-396.	0.5	7
2192	Hula-twist photoisomerization of a styrene derivative examined by argon-matrix-infrared-spectroscopic method. Molecular Physics, 2006, 104, 1009-1015.	0.8	3
2193	Quantum Monte Carlo study of small hydrocarbon atomization energies. Molecular Physics, 2006, 104, 467-475.	0.8	0
2194	Density Functional Theory Study on the Nitration of Halobenzene by Nitronium Ion. Journal of the Chinese Chemical Society, 2006, 53, 1005-1015.	0.8	2
2195	Studies of polycrystalline pentacene thin-film transistors at the microscopic level. , 2006, , .		2
2196	Calculation of low-frequency vibrational modes of biologically important isomers. , 2006, 6416, 59.		0

#	Article	IF	Citations
2198	Anisotropic displacement parameters for H atoms using an ONIOM approach. Acta Crystallographica Section B: Structural Science, 2006, 62, 875-888.	1.8	69
2199	Electrospray ionization mass spectrometric studies of some imidazole amidoximes and nitrolic acids and their esters. Rapid Communications in Mass Spectrometry, 2006, 20, 1071-1076.	0.7	6
2200	Minimum proton affinity for efficient ionization with atmospheric pressure desorption/ionization on silicon mass spectrometry. Rapid Communications in Mass Spectrometry, 2006, 20, 3669-3673.	0.7	23
2201	Reaction of trimethylsilylketene with HCl: Mechanistic study. International Journal of Quantum Chemistry, 2006, 106, 719-726.	1.0	0
2202	Use of vibrational spectroscopy to study protein and DNA structure, hydration, and binding of biomolecules: A combined theoretical and experimental approach. International Journal of Quantum Chemistry, 2006, 106, 1160-1198.	1.0	73
2203	Potential energy surface of thionylimide. International Journal of Quantum Chemistry, 2006, 106, 1237-1249.	1.0	11
2204	IR and Raman spectra, density functional computations of vibrational spectrum, molecular geometry, atomic charges, and some molecular properties of 3-aminobenzonitrile molecule. International Journal of Quantum Chemistry, 2006, 106, 1885-1901.	1.0	11
2205	Singletâ€“triplet gaps and insertion reactions of aminocyanocarbenes: A computational study of hydrogen cyanide covalent dimers. International Journal of Quantum Chemistry, 2006, 106, 2379-2389.	1.0	6
2206	Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity. International Journal of Quantum Chemistry, 2006, 106, 3097-3107.	1.0	17
2207	[2,3]-sigmatropic rearrangements of hydrogen and alkyl 3-propenyl sulfoxides: A computational study. International Journal of Quantum Chemistry, 2006, 106, 2390-2397.	1.0	8
2208	Conformational and vibrational study of di-n-butyl and di-sec-butylphosphonates by MM/QM method. International Journal of Quantum Chemistry, 2006, 106, 2633-2642.	1.0	2
2209	Thermochemistry of oxabicycloheptenes: enthalpy of formation, entropy and heat capacity. Journal of Physical Organic Chemistry, 2006, 19, 93-103.	0.9	13
2210	On the stability of non-conventional Ï€-complexes between Ni+ and toluene, phenyl-silane and phenyl-germane. Journal of Physical Organic Chemistry, 2006, 19, 495-502.	0.9	3
2211	Molecular aggregation in neat 2-methoxyethanol and in 2-methoxyethanol/acrylamide solutionsâ€”A study by Raman spectroscopy and ab initio calculations. Vibrational Spectroscopy, 2006, 42, 302-308.	1.2	10
2212	Structureâ€“activity relationship study of flavone compounds with anti-HIV-1 integrase activity: A density functional theory study. Bioorganic and Medicinal Chemistry, 2006, 14, 7105-7112.	1.4	39
2213	Infrared spectroscopy used to evaluate glycosylation of proteins. Analytical Biochemistry, 2006, 348, 40-48.	1.1	101
2214	Spectral investigations of unsymmetrical Ï€-donor ethylenedithio-dithiadiselenafulvalene iodomercurate, (EDT-DTDSF)4Hg3I8. Chemical Physics, 2006, 323, 161-168.	0.9	7
2215	The dynamics of the solvation of Pb(II) in aqueous solution obtained by an ab initio QM/MM MD approach. Chemical Physics, 2006, 323, 473-478.	0.9	9

#	Article	IF	Citations
2216	Optical properties of the conducting salt (DOEO)4HgBr4Â·TCE. Chemical Physics, 2006, 326, 551-562.	0.9	13
2217	A simple method to generate B(N3)3. Chemical Physics Letters, 2006, 419, 213-216.	1.2	7
2218	The relationship between thermodynamic stabilities of carbenium ions in the gas phase and in aqueous solution: A wide scope study. Chemical Physics Letters, 2006, 420, 493-496.	1.2	5
2219	A time-dependent density functional study of vibrationally resolved excitation, emission, and ionization spectra of the S1 state of phenol. Chemical Physics Letters, 2006, 420, 459-464.	1.2	13
2220	Unimolecular dissociation of CH3SH+ near threshold: A theoretical study. Chemical Physics Letters, 2006, 421, 589-594.	1.2	2
2221	First-principles vibrational studies of pentaerythritol crystal under hydrostatic pressure. Chemical Physics Letters, 2006, 422, 397-401.	1.2	15
2222	Terahertz phonon modes of an intermolecular network of hydrogen bonds in an anhydrous Î²-d-glucopyranose crystal. Chemical Physics Letters, 2006, 423, 439-444.	1.2	38
2223	Interplay between theory and experiment in the quest for silica with reduced dimensionality grown on a Mo(112) surface. Chemical Physics Letters, 2006, 424, 115-119.	1.2	27
2224	TDDFT investigation of the optical properties of cyanine dyes. Chemical Physics Letters, 2006, 425, 105-109.	1.2	93
2225	A QM/MM MD simulation study of hydrated Pd2+. Chemical Physics Letters, 2006, 426, 301-305.	1.2	17
2226	Theoretical study of the global potential energy surface of the [CH3,N,C,S] system in singlet and triplet states. Chemical Physics Letters, 2006, 430, 13-20.	1.2	6
2227	Application of the linear/exponential hybrid force field scaling scheme to the bond length alternation modes of polyacetylene. Chemical Physics Letters, 2006, 432, 356-361.	1.2	4
2228	Spectral and structural study of two acceptor-substituted pyridinium-betaines of squaric acid: Promising chromophores for nonlinear optical applications. Chemical Physics, 2006, 324, 489-496.	0.9	16
2229	Structure and dynamics of La(III) in aqueous solution â€“ An ab initio QM/MM MD approach. Chemical Physics, 2006, 327, 31-42.	0.9	34
2230	Adsorption of 2-amino-6-methylbenzothiazole on colloidal silver particles: Quantum chemical calculations and surface enhanced Raman scattering study. Chemical Physics, 2006, 330, 172-183.	0.9	22
2231	Electron affinities of polynuclear aromatic hydrocarbons and negative-ion chemical-ionization sensitivities. International Journal of Mass Spectrometry, 2006, 255-256, 123-129.	0.7	7
2232	Conformational study of ketoprofen by combined DFT calculations and Raman spectroscopy. International Journal of Pharmaceutics, 2006, 307, 56-65.	2.6	70
2233	Probing the basicity of zeolite frameworks with N2O4: A DFT approach. Microporous and Mesoporous Materials, 2006, 90, 370-376.	2.2	14

#	Article	IF	Citations
2234	A computational study of methane catalytic reactions on zeolites. Journal of Molecular Catalysis A, 2006, 246, 1-10.	4.8	32
2235	Hydrogen bonding in liquid water: An ab initio QM/MM MD simulation study. Journal of Molecular Liquids, 2006, 123, 61-67.	2.3	63
2236	Vibrational spectra of imidazolium tetrafluoroborate ionic liquids. Journal of Molecular Liquids, 2006, 124, 84-95.	2.3	266
2237	Conformational analysis of the potential anticancer agent ethyl trihydroxycinnamateâ€"A combined raman spectroscopy and ab initio study. Journal of Molecular Structure, 2006, 783, 122-135.	1.8	17
2238	Raman experimental and DFT theoretical studies on the adsorption behavior of benzoic acid on silver nanoparticles. Journal of Molecular Structure, 2006, 789, 157-161.	1.8	15
2239	Quantum-mechanical calculations and spectroscopic characteristics of magnesium glutamateâ€"glycine and magnesium glutamateâ€"arginine. Journal of Molecular Structure, 2006, 792-793, 186-193.	1.8	2
2240	Are 1,5- and 1,7-dihydrodiimidazo[4,5-b:4â€²,5â€²-e]pyrazine the main products of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) alkaline hydrolysis? A DFT study of vibrational spectra. Journal of Molecular Structure, 2006, 794, 288-302.	1.8	11
2241	X-ray and ab initio studies of the structure and vibrational spectra of 4-carboxy-1-methylpyridinium chloride. Journal of Molecular Structure, 2006, 797, 66-81.	1.8	16
2242	An experimental and theoretical study on the adsorption behaviors of MHBA ions on silver nano-particles. Journal of Molecular Structure, 2006, 797, 40-43.	1.8	9
2243	Characterisation of aliphatic chains in vacuum residues (VRs) of asphaltenes and resins using molecular modelling and FTIR techniques. Fuel Processing Technology, 2006, 87, 325-333.	3.7	78
2244	Photoexcitation of tetrathiafulvalene radical cations in a storage ring: Kinetics and energetics of the dissociation process. International Journal of Mass Spectrometry, 2006, 248, 47-55.	0.7	5
2245	Gas-phase titration of C7H9+ ion mixtures by FT-ICR mass spectrometry: Semiquantitative determination of ion populations generated by CI-induced protonation of C7H8 isomers and by EI-induced fragmentation of some monoterpenes. International Journal of Mass Spectrometry, 2006, 249-250, 340-352.	0.7	20
2246	Cu+ association to some Phâ€"X (X=OH, NH2, CHO, COOH, CF3) phenyl derivatives.. International Journal of Mass Spectrometry, 2006, 255-256, 20-27.	0.7	27
2247	The unexpected decarbonylation of ionized 2,3-pentanedione and related diketones. International Journal of Mass Spectrometry, 2006, 249-250, 222-229.	0.7	6
2248	IR spectroscopy of protonated toluene: Probing ring hydrogen shifts in gaseous arenium ions. International Journal of Mass Spectrometry, 2006, 249-250, 149-154.	0.7	49
2249	The unimolecular dissociation of protonated glyoxylic acid: Structure and dynamics of a step-by-step process. International Journal of Mass Spectrometry, 2006, 255-256, 177-184.	0.7	5
2250	Why ketonization is favored over enolization in 5-membered ring H-transfers by CH3C(OH+)CH2CH2 and in 6-membered ring H-transfers by CH3(COH+)CH2CH2CH2. International Journal of Mass Spectrometry, 2006, 249-250, 120-129.	0.7	5
2251	The mass spectrometry-induced cyclization of protonated N-[2-(benzoyloxy)phenyl]-benzamide: A gas-phase analog of a solution reaction. International Journal of Mass Spectrometry, 2006, 249-250, 21-30.	0.7	10

#	Article	IF	Citations
2252	Dissociation reactions of protonated anthracycline antibiotics following electrospray ionization-tandem mass spectrometry. International Journal of Mass Spectrometry, 2006, 255-256, 130-138.	0.7	24
2253	On the dehydrogenation of N,Nâ€²-substituted p-phenylenediamine antioxidants. I. N-Phenyl-Nâ€²-isopropyl-p-phenylenediamine (IPPD). Polymer Degradation and Stability, 2006, 91, 1775-1780.	2.7	20
2254	Structure and piezoelectric properties of poly(vinylidene fluoride) studied by density functional theory. Polymer, 2006, 47, 7988-7996.	1.8	69
2255	Intramolecular hydrogen bonding in chiral alcohols: The microwave spectrum of the chloropropanols. Journal of Molecular Spectroscopy, 2006, 236, 1-10.	0.4	19
2256	Electronic differentiations in palladium-catalyzed allylic substitutions. Journal of Organometallic Chemistry, 2006, 691, 4508-4513.	0.8	20
2257	Ab-initio calculations of Raman, IR-active vibrational modes in isotopically modified B12 icosahedral clusters. Journal of Solid State Chemistry, 2006, 179, 2927-2933.	1.4	10
2258	Theoretical survey of the NH+CH3 potential energy surface in relation to Titan atmospheric chemistry. Planetary and Space Science, 2006, 54, 181-187.	0.9	22
2259	Theoretical study of the changes in the vibrational characteristics arising from the hydrogen bonding between Vitamin C (l-ascorbic acid) and H2O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 427-437.	2.0	18
2260	Low frequency internal modes of 1,2,4,5-tetramethylbenzene, tetramethylpyrazine and tetramethyl-1,4-benzoquinone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 766-773.	2.0	25
2261	Fourier transform-infrared and Raman spectra, ab initio calculations and assignments for 6-methyl-4-bromomethylcoumarin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 301-307.	2.0	27
2262	The molecular structure and vibrational spectra of corrolazine metal complexes (CzM) by density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 795-800.	2.0	6
2263	Calculation of standard electrode potential of half reaction for benzoquinone and hydroquinone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 333-339.	2.0	14
2264	Density functional theoretical (DFT) study for the prediction of spectroscopic parameters of ClCCCN. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 874-881.	2.0	2
2265	Theoretical study of the syn and anti thiophene-2-aldehyde conformers using density functional theory and normal coordinate analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 935-945.	2.0	15
2266	Ab initio and DFT studies of the vibrational spectra of benzofuran and some of its derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 1125-1130.	2.0	11
2267	Electron capture dissociation of peptides metalated with alkaline-earth metal ions. Journal of the American Society for Mass Spectrometry, 2006, 17, 757-771.	1.2	54
2268	Ab initio and DFT investigation of fluorinated methyl hydroperoxides: Structures, rotational barriers, and thermochemical properties. Journal of Fluorine Chemistry, 2006, 127, 54-62.	0.9	11
2269	Adsorption of 1-hexene on Î³-alumina (110C). Journal of Molecular Catalysis A, 2006, 248, 76-83.	4.8	7

#	Article	IF	Citations
2270	Cation-terminated structural clusters as a model for the interpretation of zeolite vibrational spectra. Journal of Molecular Structure, 2006, 792-793, 163-169.	1.8	12
2271	A spectroscopic and computational study of stereochemistry in 2-hydroxymutilin. Journal of Molecular Structure, 2006, 797, 5-24.	1.8	12
2272	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	0.8	43
2273	Comparative studies for selective deprotection of the N-arylideneamino moiety from heterocyclic amides: kinetic and theoretical studies. Tetrahedron, 2006, 62, 1182-1192.	1.0	13
2274	A DFT study of the Dielsâ€“Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. Tetrahedron, 2006, 62, 5502-5509.	1.0	35
2275	Comparative studies for selective deprotection of the N-arylideneamino moiety from heterocyclic amides: kinetic and theoretical studies. Part 2. Tetrahedron, 2006, 62, 6214-6221.	1.0	9
2276	Ab initio, DFT vibrational calculations and SERRS study of Rhodamine 123 adsorbed on colloidal silver particles. Vibrational Spectroscopy, 2006, 41, 90-96.	1.2	40
2277	Analysis of the VROA signals of helical heptasilanes using an atomistic approach. Vibrational Spectroscopy, 2006, 42, 309-316.	1.2	12
2278	Infrared, Raman spectra and DFT calculations of chlorine substituted anilines. Vibrational Spectroscopy, 2006, 42, 397-402.	1.2	41
2279	Vibrational circular dichroism DFT study on bicyclo[3.3.0]octane derivatives. Tetrahedron: Asymmetry, 2006, 17, 3203-3218.	1.8	12
2280	Theoretical study of the propagation barrier of ethylene polymerization with TiR2 (R=OCH3 or CN): The importance of the Î²-agostic interactions. Computational and Theoretical Chemistry, 2006, 762, 9-15.	1.5	5
2281	Substituent and solvent effects on the rotational barriers in selenoamides: A theoretical study. Computational and Theoretical Chemistry, 2006, 759, 41-49.	1.5	26
2282	MÃ¸llerâ€“Plesset perturbation theory calculations of the pKa values for a range of carboxylic acids. Computational and Theoretical Chemistry, 2006, 758, 275-278.	1.5	35
2283	Exploration of the full conformational landscapes of gaseous aromatic amino acid phenylalanine: An ab initio study. Computational and Theoretical Chemistry, 2006, 758, 195-202.	1.5	70
2284	A computational and conceptual DFT approach to the kinetics of acid zeolite catalyzed electrophilic aromatic substitution reactions. Computational and Theoretical Chemistry, 2006, 762, 69-78.	1.5	18
2285	Calculation of two-electron reduction potentials for some quinone derivatives in aqueous solution using MÃ¸llerâ€“Plesset perturbation theory. Computational and Theoretical Chemistry, 2006, 759, 245-247.	1.5	21
2286	A computational study of bond dissociation enthalpies in haloethenes. Computational and Theoretical Chemistry, 2006, 760, 121-129.	1.5	7
2287	Scaling factors for vibrational frequencies and zero-point vibrational energies of some recently developed exchange-correlation functionals. Computational and Theoretical Chemistry, 2006, 760, 189-192.	1.5	108

#	Article	IF	Citations
2288	Ab initio studies of the conformers and conformational distribution of the gaseous hydroxyamino acid threonine. Computational and Theoretical Chemistry, 2006, 760, 159-166.	1.5	27
2289	DFT studies and vibrational spectra of trans 1,2-bis(4-pyridyl)ethylene and its zinc(II)halide complexes. Computational and Theoretical Chemistry, 2006, 761, 113-118.	1.5	3
2290	The study of isotope effects of chloroform and chloromethane using vibrational frequencies. Computational and Theoretical Chemistry, 2006, 765, 105-114.	1.5	4
2291	A computational study of the thermodynamic properties of sinapic and ferulic acids and their corresponding radical cations. Computational and Theoretical Chemistry, 2006, 766, 137-141.	1.5	7
2292	The effect of solvent on the stereoselectivity of reactions between hydroxyalkyl azides and ketones. Computational and Theoretical Chemistry, 2006, 766, 105-112.	1.5	5
2293	The two hydrogen transfer dissociation channels of nicotine molecule in the gas phase. Computational and Theoretical Chemistry, 2006, 767, 95-101.	1.5	2
2294	Structure and electronic properties for a newly synthesized red fluorescent material. Computational and Theoretical Chemistry, 2006, 770, 73-77.	1.5	3
2295	Calculations on the structure, vibrational spectrum, and enthalpy of formation of pentafluoronitrosulfane, SF5NO2. Computational and Theoretical Chemistry, 2006, 767, 155-158.	1.5	1
2296	Conformational changes and S1â†S0 origin transition energies: Polychlorinated biphenyls (PCBs). Computational and Theoretical Chemistry, 2006, 772, 31-37.	1.5	1
2297	A study of the dependence of substituted N,N-acyl defended keto stabilized sulfur ylides structure on their transformations by means of quantum chemistry. Computational and Theoretical Chemistry, 2006, 774, 29-32.	1.5	4
2298	First-principle studies of gaseous aromatic amino acid histidine. Computational and Theoretical Chemistry, 2006, 801, 7-20.	1.5	35
2299	Theoretical studies on heats of formation, group interactions, and bond dissociation energies in neopentyl difluoroamino compounds. Computational and Theoretical Chemistry, 2006, 801, 55-62.	1.5	30
2300	An ab initio study of the SN2 reaction of 1- and 3-methyltriazene with halide ions. Computational and Theoretical Chemistry, 2006, 801, 21-28.	1.5	4
2301	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. Journal of Chemical Physics, 2006, 125, 194101.	1.2	4,175
2302	Radical Stabilityâ€"AÂTheoretical Perspective. , 0, , 163-189.		165
2303	An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene. Journal of Physical Chemistry A, 2006, 110, 8942-8951.	1.1	70
2304	Theoretical Studies on the Structures, Thermodynamic Properties, Detonation Properties, and Pyrolysis Mechanisms of Spiro Nitramines. Journal of Physical Chemistry A, 2006, 110, 3797-3807.	1.1	144
2305	The Photochemistry of 4-Azidopyridine-1-oxide. Journal of Organic Chemistry, 2006, 71, 9023-9029.	1.7	11

#	Article	IF	Citations
2306	Dissociative photoionization of mono-, di- and trimethylamine studied by a combined threshold photoelectron photoion coincidence spectroscopy and computational approach. Physical Chemistry Chemical Physics, 2006, 8, 613-623.	1.3	23
2307	Role of carbon clusters in pyrolysis of iodomethanes. Russian Journal of General Chemistry, 2006, 76, 245-250.	0.3	0
2308	Quantum-chemical study of the structure and reactivity of 4,5-dihydropyrazol-5-ones and their thio and seleno analogs: VIII. Solvation effects and tautomerism of 4,5-dihydropyrazol-5-ones and their thio and seleno analogs. Russian Journal of General Chemistry, 2006, 76, 1117-1122.	0.3	1
2309	Synthesis, structure, and properties of phosphorus-containing bis(amidrazones). Russian Journal of General Chemistry, 2006, 76, 1219-1225.	0.3	5
2310	Quantum-chemical study of nitrosonium complexes derived from nitrogen-containing heterocycles. Russian Journal of Organic Chemistry, 2006, 42, 1551-1562.	0.3	0
2312	Low-frequency resonance Raman studies of the H(M202)G cavity mutant of bacterial photosynthetic reaction centers. Photosynthesis Research, 2006, 88, 31-41.	1.6	3
2313	Structural characterization of agmatine at physiological conditions. Structural Chemistry, 2006, 17, 163-175.	1.0	18
2314	Structural studies of spiroarsoranes derived from 2-aminophenols. Structural Chemistry, 2006, 17, 359-366.	1.0	2
2315	Experimental and density functional studies on two structurally similar antipyrine derivatives:Â4-(2-hydroxy-5-nitrobenzylidene-amino)-1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one and 4-(3-bromo-5-chloro-2-hydroxybenzylideneamino)-1,2-dihydro-1,5-dimethyl-2-phenylpyrazol-3-one. Structural Chemistry, 2006, 17, 655-665.	1.0	21
2316	Ab initio vibrational analysis of hexafluoroethane C2F6. Journal of Structural Chemistry, 2006, 47, 232-240.	0.3	2
2317	Ab initio computational insight into the ion-pair SN2 reaction of lithium isothiocyanate and methyl fluoride in the gas phase and in acetone solution. Journal of Molecular Modeling, 2006, 12, 182-189.	0.8	7
2318	Umpolung catalysts: comparative assessments on reactivities. Journal of Molecular Modeling, 2006, 12, 591-595.	0.8	27
2319	Valence isomerization of 2-phospha-4-silabicyclo[1.1.0]butane: a high-level ab initio study. Journal of Molecular Modeling, 2006, 12, 531-536.	0.8	14
2320	FTIR in situ transmission studies on the kinetics of paper degradation via hydrolytic and oxidative reaction paths. Applied Physics A: Materials Science and Processing, 2006, 83, 597-603.	1.1	52
2321	Acceleration of Correlation-corrected Vibrational Self-consistent Field Calculation Times for Large Polyatomic Molecules. Theoretical Chemistry Accounts, 2006, 117, 69-72.	0.5	38
2322	Low temperature adsorption of oxygen on reduced V2O3(0001) surfaces. Surface Science, 2006, 600, 1497-1503.	0.8	55
2323	Ab initio studies on the tri- and diphosphate fragments of adenosine triphosphate. Biophysical Chemistry, 2006, 119, 127-136.	1.5	16
2324	Lattice dynamics of TTFâ€“CA across the neutralâ€“ionic transition. Chemical Physics, 2006, 325, 71-77.	0.9	20

#	Article	IF	Citations
2325	Accurate ab initio prediction of propagation rate coefficients in free-radical polymerization: Acrylonitrile and vinyl chloride. Chemical Physics, 2006, 324, 96-110.	0.9	136
2326	Infrared spectroscopic investigation of higher diamondoids. Journal of Molecular Spectroscopy, 2006, 238, 158-167.	0.4	45
2327	Do alkali and alkaline earth acetates form organometallates via decarboxylation?. International Journal of Mass Spectrometry, 2006, 255-256, 45-52.	0.7	46
2328	Methane loss from (CH3)3O+: An asynchronous, concerted 1,2-alkane elimination. International Journal of Mass Spectrometry, 2006, 248, 103-107.	0.7	4
2329	Competing rearrangement reactions in small gas-phase ionic complexes: The internal SN2 and nitro-nitrite rearrangements in nitroalkane proton-bound pairs. International Journal of Mass Spectrometry, 2006, 255-256, 93-101.	0.7	5
2330	Dehydrogenation of formic acid catalyzed by magnesium hydride anions, HMgL2â˜ (L=Cl and HCO2). International Journal of Mass Spectrometry, 2006, 254, 145-151.	0.7	26
2331	Experimental and computational thermochemistry of the dihydroxypyridine isomers. Journal of Chemical Thermodynamics, 2006, 38, 450-454.	1.0	11
2332	Acetone: isomerization and aggregation. Frontiers of Physics in China, 2006, 1, 275-282.	1.0	2
2333	Elucidation of the absolute configuration of JNJ-27553292, a CCR2 receptor antagonist, by vibrational circular dichroism analysis of two precursors. Chirality, 2006, 18, 609-620.	1.3	8
2334	Low-Pressure Pyrolysis oftBu2SO: Synthesis and IR Spectroscopic Detection of HSOH. Chemistry - A European Journal, 2006, 12, 832-844.	1.7	40
2335	Nucleophilicityâ€"Periodic Trends and Connection to Basicity. Chemistry - A European Journal, 2006, 12, 1127-1136.	1.7	67
2336	A Counterintuitive Structural Effect of Metalâ€“Metal Bond Protonation and Its Electronic Underpinnings. Chemistry - A European Journal, 2006, 12, 4691-4701.	1.7	17
2337	Tuning of Electronic Properties in Thienyl-Phosphole Ï€-Conjugated Systems through P-Functionalization Monitored by Raman Spectroscopy. Chemistry - A European Journal, 2006, 12, 3759-3767.	1.7	26
2338	Ab Initio and Experimental Thermodynamic and Kinetic Study of Proton-Assisted Bond Activation in Gaseous Hydrocarbons: Deconvolution of Reaction Efficiencies in the Case of Adamantane. Chemistry - A European Journal, 2006, 12, 5505-5513.	1.7	10
2339	One-Electron Oxidation Pathways during Î²-Cyclodextrin-Modified TiO2 Photocatalytic Reactions. Chemistry - A European Journal, 2006, 12, 7585-7594.	1.7	30
2340	Synthesis and Structure of Ultrathin Aluminosilicate Films. Angewandte Chemie - International Edition, 2006, 45, 7636-7639.	7.2	45
2341	Bonding Trends in Lewis Acid Adducts of S4N4 â€“ X-ray Structure of TeCl4Â·S4N4. European Journal of Inorganic Chemistry, 2006, 2006, 2951-2958.	1.0	6
2342	Energetic Nitrate, Perchlorate, Azide and Azolate Salts of Hexamethylenetetramine. European Journal of Inorganic Chemistry, 2006, 2006, 2959-2965.	1.0	57

#	Article	IF	Citations
2343	The Mechanism of Semibullvalene Bromination. European Journal of Organic Chemistry, 2006, 2006, 738-745.	1.2	7
2344	Theoretical studies on electron delocalization in diaminoguanidine. Journal of Computational Chemistry, 2006, 27, 334-343.	1.5	8
2345	New model potentials for sulfurâ€“copper(I) and sulfurâ€“mercury(II) interactions in proteins: Fromab initio to molecular dynamics. Journal of Computational Chemistry, 2006, 27, 837-856.	1.5	20
2346	Quantum mechanical calculation of the effects of stiff and rigid constraints in the conformational equilibrium of the alanine dipeptide. Journal of Computational Chemistry, 2006, 27, 1733-1747.	1.5	15
2347	Characterization of the structure and reactivity of monocopper-oxygen complexes supported by Î²-diketiminate and anilido-imine ligands. Journal of Computational Chemistry, 2006, 27, 1950-1961.	1.5	54
2348	Theoretical Study on the High Energy Density Compound Hexanitrohexaazatricyclotetradecanedifuroxan. Chinese Journal of Chemistry, 2006, 24, 1538-1546.	2.6	11
2349	Ab Initio Study of Free-Radical Polymerization: Polyethylene Propagation Kinetics. ChemPhysChem, 2006, 7, 131-140.	1.0	60
2350	Raman Spectroscopy of Short-Lived Terthiophene Radical Cations Generated by Photochemical and Chemical Oxidation. ChemPhysChem, 2006, 7, 1276-1285.	1.0	8
2351	Remarkably Stable Icosahedral Fulleranes: C80H80 and C180H180. ChemPhysChem, 2006, 7, 1661-1663.	1.0	43
2352	Computationally-Assisted Approach to the Vibrational Spectra of Molecular Crystals: Study of Hydrogen-Bonding and Pseudo-Polymorphism. ChemPhysChem, 2006, 7, 2150-2161.	1.0	71
2353	Theoretical Determination of the Vibrational Raman Optical Activity Signatures of Helical Polypropylene Chains. ChemPhysChem, 2006, 7, 2366-2376.	1.0	37
2354	Rearrangements in Model Peptide-Type Radicalsvia Intramolecular Hydrogen-Atom Transfer. Helvetica Chimica Acta, 2006, 89, 2254-2272.	1.0	39
2355	A facile synthesis of pyrazolo[3,4â€D]pyridazines Via the 1,3â€dipolar cycloaddition of 3â€arylsydnones. Synthesis and computational studies of 1â€arylâ€4,5â€dihydroâ€1Hâ€pyrazolo[3,4â€D]pyridazineâ€3,6â€diones and their 3,6â€dichloro derivatives.. Journal of Heterocyclic Chemistry, 2006, 43, 827-834.	1.4	8
2356	Experimental and theoretical Raman investigation on interactions of Cu(II) with histamine. Journal of Raman Spectroscopy, 2006, 37, 291-298.	1.2	27
2357	Raman, FT-IR and DFT studies ofortho-,meta- andpara-pyridinomethylene substituted di(4-hydroxy-coumarin) and their Ce(III), La(III) and Nd(III) complexes. Journal of Raman Spectroscopy, 2006, 37, 742-754.	1.2	15
2358	On the Raman spectrum of Maya blue. Journal of Raman Spectroscopy, 2006, 37, 1046-1053.	1.2	61
2359	Computational Studies of RAFT Polymerizationâ€“Mechanistic Insights and Practical Applications. Macromolecular Rapid Communications, 2006, 27, 473-497.	2.0	122
2360	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. Advanced Functional Materials, 2006, 16, 531-536.	7.8	42

#	Article	IF	Citations
2361	Kinetic modeling oftert-butyl radical decomposition reaction. AICHE Journal, 2006, 52, 3216-3221.	1.8	3
2362	Experimental and theoretical investigation of the Raman and hyper-Raman spectra of acetonitrile and its derivatives. Journal of Chemical Physics, 2006, 124, 244312.	1.2	39
2363	Vibrational dynamics of DNA. II. Deuterium exchange effects and simulated IR absorption spectra. Journal of Chemical Physics, 2006, 125, 114509.	1.2	53
2364	The correlation-consistent composite approach: Application to the G3/99 test set. Journal of Chemical Physics, 2006, 125, 104111.	1.2	134
2365	Conformational Study of Monomeric 2,3-Butanediols by Matrix-Isolation Infrared Spectroscopy and DFT Calculations. Journal of Physical Chemistry A, 2006, 110, 4169-4179.	1.1	72
2366	Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. Journal of Chemical Physics, 2006, 124, 094704.	1.2	103
2367	Sr(II) in Water:Â A Labile Hydrate with a Highly Mobile Structure. Journal of Physical Chemistry B, 2006, 110, 20409-20417.	1.2	49
2368	Modeling carbon nanostructures with the self-consistent charge density-functional tight-binding method: Vibrational spectra and electronic structure of C28, C60, and C70. Journal of Chemical Physics, 2006, 125, 214706.	1.2	40
2369	The effect of oxidation on the structure of styryl-substituted sexithiophenes: A resonance Raman spectroscopy and density functional theory study. Journal of Chemical Physics, 2006, 124, 164501.	1.2	17
2370	A theoretical study of the interactions of water with gallic acid and a PEO/TGG complex. Molecular Simulation, 2006, 32, 17-27.	0.9	5
2371	A theoretical study of the chiroptical properties of molecules with isotopically engendered chirality. Journal of Chemical Physics, 2006, 124, 174301.	1.2	52
2372	Infrared multiphoton spectra from metal dication complexes in the gas phase. Journal of Chemical Physics, 2006, 124, 201103.	1.2	5
2373	Vibrational dynamics of DNA. I. Vibrational basis modes and couplings. Journal of Chemical Physics, 2006, 125, 114508.	1.2	70
2374	Converged vibrational energy levels and quantum mechanical vibrational partition function of ethane. Journal of Chemical Physics, 2006, 124, 184310.	1.2	15
2375	Atomic structure of a thin silica film on aMo(112)substrate: A combined experimental and theoretical study. Physical Review B, 2006, 73, .	1.1	61
2376	THz Fingerprinting of Biomolecules Supported by Ab Initio Molecular Modelling. , 2006, , .		0
2377	Phenol-benzene complexation dynamics: Quantum chemistry calculation, molecular dynamics simulations, and two dimensional IR spectroscopy. Journal of Chemical Physics, 2006, 125, 244508.	1.2	49
2378	STRUCTURAL AND ELECTRONIC PROPERTIES OF DIPROPYL SULFIDE: A THEORETICAL INVESTIGATION. International Journal of Modern Physics C, 2006, 17, 1179-1190.	0.8	1

#	Article	IF	Citations
2379	Conformational and vibrational study of platinum(II) anticancer drugs: cis-diamminedichloroplatinum (II) as a case study. Journal of Chemical Physics, 2007, 127, 185104.	1.2	57
2380	Experimental and Theoretical Study of the Electrochemical Behavior ofoâ€Benzoquinone and Pyrocatechol. Spectroscopy Letters, 2007, 40, 811-833.	0.5	2
2381	Vibrational fingerprint of the structural tuning in push-pull organic chromophores with quinoid or proaromatic spacers. Journal of Chemical Physics, 2007, 126, 074701.	1.2	7
2382	Vibrational dynamics of DNA: IV. Vibrational spectroscopic characteristics of A-, B-, and Z-form DNAâ€™s. Journal of Chemical Physics, 2007, 126, 145102.	1.2	36
2383	Interaction of alkali metals with perylene-3,4,9,10-tetracarboxylic-dianhydride thin films studied by IR spectroscopy. Journal of Chemical Physics, 2007, 126, 164709.	1.2	13
2384	Lagrangian approach to molecular vibrational Raman intensities using time-dependent hybrid density functional theory. Journal of Chemical Physics, 2007, 126, 201104.	1.2	77
2385	In search of definitive signatures of the elusive NCCO radical. Journal of Chemical Physics, 2007, 127, 014306.	1.2	19
2386	Electronic and quantum dynamical insight into the ultrafast proton transfer of 1-hydroxy-2-acetonaphthone. Journal of Chemical Physics, 2007, 127, 084318.	1.2	22
2387	Unraveling the structure of hydrogen bond stretching mode infrared absorption bands: An anharmonic density functional theory study on 7-azaindole dimers. Journal of Chemical Physics, 2007, 127, 054309.	1.2	55
2388	Ab initiostudies of aspartic acid conformers in gas phase and in solution. Journal of Chemical Physics, 2007, 127, 154314.	1.2	44
2389	Titanium, Zirconium, and Hafnium Metal Atom Reactions with CF4, CCl4, and CF2Cl2:Â A Matrix Isolation Spectroscopic and DFT Investigation of Triplet XCÃ·MX3Complexes. Organometallics, 2007, 26, 2519-2527.	1.1	42
2390	IR-UV double resonance spectroscopy of xanthine. Physical Chemistry Chemical Physics, 2007, 9, 4587.	1.3	40
2391	Comparing electronic structure predictions for the ground state dissociation of vinoxy radicals. Journal of Chemical Physics, 2007, 127, 094309.	1.2	7
2392	MO Calculations Involving Î¼-Hydrido Cation Intermediates Relevant to the Heptane to Toluene Dehydrocyclization Reaction. ACS Symposium Series, 2007, , 268-296.	0.5	0
2393	NadyktoetÂal.Reply:. Physical Review Letters, 2007, 98, .	2.9	9
2394	Charge ordered state and frustration of site charges in(ET)5Te2I6and(BETS)5Te2I6. Physical Review B, 2007, 75, .	1.1	3
2395	Molecular behavior in the vibronic and excitonic properties of hydrogenated silicon nanoparticles. Physical Review B, 2007, 76, .	1.1	33
2396	Towards a Better Understanding of 'Delocalized Charge' in Ionic Liquid Anions. Australian Journal of Chemistry, 2007, 60, 15.	0.5	79

#	Article	IF	Citations
2397	Quantitative Structure-Activity Relationship Analysis of the Anticancer Activity of Chloroethylnitrosourea Derivatives. , 2007, , .		0
2398	Radical Ring-Opening Polymerization of Phosphorus Heterocycles: Computational Design of Suitable Phosphetane Monomers. Australian Journal of Chemistry, 2007, 60, 744.	0.5	7
2399	Computing protein infrared spectroscopy with quantum chemistry. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2007, 365, 2799-2812.	1.6	14
2400	Quantum Mechanics for Organic Chemistry. , 0, , 1-41.		1
2401	Tetrathiafulvalene-Based Materials for Organic Field Effect Transistors. Inspection of Their Semiconductor Properties by Means of Molecular Spectroscopy and Quantum Chemistry. Journal of Physical Chemistry C, 2007, 111, 10110-10118.	1.5	20
2402	Energetics of naphthalene derivatives, IV+: a calorimetric and calculational thermochemical study of the isomeric naphthalenemethanols. Molecular Physics, 2007, 105, 1789-1796.	0.8	6
2403	Vibrational and Surface-Enhanced Raman Spectra of 1,6-Diphenyl-1,3,5-hexatriene. Applied Spectroscopy, 2007, 61, 1001-1006.	1.2	5
2404	Resonance-Assisted Hydrogen Bonds:Â A Critical Examination. Structure and Stability of the Enols of Î²-Diketones and Î²-Enaminones. Journal of Physical Chemistry A, 2007, 111, 3585-3591.	1.1	142
2405	Gas-phase reaction thermodynamics in preparation of pyrolytic carbon by propylene pyrolysis. Computational Materials Science, 2007, 40, 504-524.	1.4	11
2406	Modeling and spectroscopic studies of bisphosphonateâ€“bone interactions. The Raman, NMR and crystallographic investigations of Caâ€“HEDP complexes. Bone, 2007, 41, 668-678.	1.4	51
2407	Molecular structures of 3,6-di(hexylthioureido)acridine conformers, their protonation, 1H NMR and IR analyses: Theoretical and experimental studies. Journal of Molecular Structure, 2007, 832, 16-25.	1.8	1
2408	Density Functional Theory Study of the Reaction Mechanism and Energetics of the Reduction of Hydrogen Peroxide by Ebselen, Ebselen Diselenide, and Ebselen Selenol. Journal of Physical Chemistry A, 2007, 111, 3152-3160.	1.1	51
2409	Synthesis and Pharmacological Evaluation of Fluorescent and Photoactivatable Analogues of Antiplasmodial Naphthylisoquinolines. Journal of Medicinal Chemistry, 2007, 50, 6104-6115.	2.9	16
2410	Infrared Spectrum and Bonding in Uranium Methylidene Dihydride, CH2UH2. Inorganic Chemistry, 2007, 46, 4917-4925.	1.9	73
2411	A Combined Experimental and Theoretical Study of Uranium Polyhydrides with New Evidence for the Large Complex UH4(H2)6. Journal of Physical Chemistry A, 2007, 111, 6383-6387.	1.1	39
2412	Structural Analysis of the Anti-Malaria Active Agent Chloroquine under Physiological Conditions. Journal of Physical Chemistry B, 2007, 111, 1815-1822.	1.2	46
2413	Influence of the Interaction between Hydrogen Sulfide and Ionic Liquids on Solubility:â€‰ Experimental and Theoretical Investigation. Journal of Physical Chemistry B, 2007, 111, 13014-13019.	1.2	148
2414	After 20 Years, Theoretical Evidence That â€œAuF7â€•Is Actually AuF5Â·F2. Inorganic Chemistry, 2007, 46, 5338-5342.	1.9	57

#	Article	IF	Citations
2415	Resolution of Identity Density Functional Theory Augmented with an Empirical Dispersion Term (RI-DFT-D):Â A Promising Tool for Studying Isolated Small Peptides. Journal of Physical Chemistry A, 2007, 111, 1146-1154.	1.1	66
2416	Synthesis and Ab Initio/DFT Studies on 2-(4-methoxyphenyl)benzo[d]thiazole. International Journal of Molecular Sciences, 2007, 8, 760-776.	1.8	53
2417	Theoretical Study of Structure, Vibrational Frequencies, and Electronic Spectra of Dibenzofuran and Its Polychlorinated Derivatives. Journal of Physical Chemistry A, 2007, 111, 1339-1350.	1.1	11
2418	Photochemistry of Sulfilimine-Based Nitrene Precursors:â€‰ Generation of Both Singlet and Triplet Benzoylnitrene. Journal of Organic Chemistry, 2007, 72, 6848-6859.	1.7	42
2419	Linear and Nonlinear Optical Properties of Pyridine-Based Octopolar Chromophores Designed for Chemical Sensing. Joint Spectroscopic and Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 18778-18784.	1.5	25
2420	Dendrimerâ˜Tetrachloroplatinate Precursor Interactions. 1. Hydration of Pt(II) Species and PAMAM Outer Pockets. Journal of Physical Chemistry A, 2007, 111, 932-944.	1.1	18
2421	Assessment of the exchange-correlation functionals for the physical description of spin transition phenomena by density functional theory methods: All the same?. Journal of Chemical Physics, 2007, 126, 014105.	1.2	102
2422	Density functional study of the conformations and intramolecular proton transfer in thiohydroxamic acids. Organic and Biomolecular Chemistry, 2007, 5, 547-557.	1.5	13
2423	Thiophene- and Selenophene-Based Heteroacenes:â€‰ Combined Quantum Chemical DFT and Spectroscopic Raman and UVâ˜Visâ˜NIR Study. Journal of Physical Chemistry B, 2007, 111, 7488-7496.	1.2	32
2424	UV Near-Resonance Raman Spectroscopic Study of 1,1â€˜-Bi-2-naphthol Solutions. Journal of Physical Chemistry A, 2007, 111, 4767-4775.	1.1	11
2425	Intermediates in Dioxygen Activation by Methane Monooxygenase:Â A QM/MM Study. Journal of the American Chemical Society, 2007, 129, 3135-3147.	6.6	106
2426	Theoretical and Spectroscopic Study of Nickel(II) Porphyrin Derivatives. Journal of Physical Chemistry A, 2007, 111, 2706-2714.	1.1	65
2427	Structural, Energetic, and Infrared Spectra Insights into Methanol Clusters (CH3OH)n, for n = 2â˜12, 16, 20. ONIOM as an Efficient Method of Modeling Large Methanol Clusters. Journal of Chemical Theory and Computation, 2007, 3, 1073-1082.	2.3	53
2428	Dual-basis self-consistent field methods: 6-31G* calculations with a minimal 6-4G primary basis. Molecular Physics, 2007, 105, 2455-2473.	0.8	25
2429	4-Aryl-1,3,2-oxathiazolylium-5-olates as pH-Controlled NO-Donors:Â The Next Generation ofS-Nitrosothiols. Journal of the American Chemical Society, 2007, 129, 5503-5514.	6.6	14
2430	Ab Initio Study of the Penultimate Effect for the ATRP Activation Step Using Propylene, Methyl Acrylate, and Methyl Methacrylate Monomers. Macromolecules, 2007, 40, 5985-5994.	2.2	84
2431	Chlorineâ€“benzene complexesâ€”the reliability of density functionals for non-covalent radical complexes. Physical Chemistry Chemical Physics, 2007, 9, 5649.	1.3	13
2432	Bond Dissociation Energies and Radical Stabilization Energies:â€‰ An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	1.1	101

#	Article	IF	Citations
2433	Applications of Quantum Chemical Methods in Zeolite Science. Studies in Surface Science and Catalysis, 2007, , 701-XXI.	1.5	16
2434	Modeling elementary reactions in coke formation from first principles. Molecular Simulation, 2007, 33, 879-887.	0.9	32
2435	Gas-Phase Diastereoselectivity of Secondary 5-Substituted (X)-Adamant-2-yl (X = F, Si(CH3)3) Cations. Journal of Organic Chemistry, 2007, 72, 4077-4083.	1.7	10
2436	Hydrogenation of Simple Aromatic Molecules: A Computational Study of the Mechanism. Journal of the American Chemical Society, 2007, 129, 924-933.	6.6	47
2437	Infrared Spectroscopic Observation of the Group 13 Metal Hydroxides, M(OH)1,2,3 (M =Al, Ga, In, and Tl) and HAl(OH)2. Journal of Physical Chemistry A, 2007, 111, 1860-1868.	1.1	35
2438	Computational Studies of Radicals Relevant to Nucleic Acid Damage. Advances in Quantum Chemistry, 2007, 52, 89-120.	0.4	20
2439	Vibronic Interaction in Metalloporphyrin Ï€-Anion Radicals. Journal of Physical Chemistry A, 2007, 111, 852-857.	1.1	12
2440	N-Acyloxy-N-alkoxyamides â€“ structure, properties, reactivity and biological activity. Advances in Physical Organic Chemistry, 2007, , 35-123.	0.5	11
2441	DNA hybridization detection by porous silicon-based DNA microarray in conjugation with infrared microspectroscopy. Journal of Applied Physics, 2007, 102, 014303.	1.1	20
2442	An exploratory ab initio study of the S_N2 reaction of 1,3,3-trimethyltriazene with halide ions. Canadian Journal of Chemistry, 2007, 85, 958-963.	0.6	2
2443	Spectroscopic and Theoretical Studies of a New Cerium (III) Complex with 3,3â€²â€²(orthoâ€Pyridinomethylene)diâ€[4â€hydroxycoumarin]. Spectroscopy Letters, 2007, 40, 65-81.	0.5	10
2444	Comprehensive theoretical studies on the CF3H dissociation mechanism and the reactions of CF3H with OH and H free radicals. Journal of Chemical Physics, 2007, 126, 034307.	1.2	28
2445	Activation of the Câ€“I and Câ€“OH bonds of 2-iodoethanol by gas phase silver cluster cations yields subvalent silver-iodide and -hydroxide cluster cations. Dalton Transactions, 2007, , 3149-3157.	1.6	18
2446	Oxidation of some cage hydrocarbons by dioxiranes. Nature of the transition structure for the reaction of Câ€“H bonds with dimethyldioxirane: a comparison of B3PW91 density functional theory with experiment. Organic and Biomolecular Chemistry, 2007, 5, 2302-2310.	1.5	12
2447	Synthesis, photophysics and molecular structures of luminescent 2,5-bis(phenylethynyl)thiophenes (BPETs). New Journal of Chemistry, 2007, 31, 841-851.	1.4	41
2448	An Epoxide Intermediate in Nucleophilic Acylations by Thiazolium Precursors. Organic Letters, 2007, 9, 3065-3068.	2.4	20
2449	Gas-Phase Reactivity of 2,7-Dimethyl-[1,2,4]-triazepine Thio Derivatives toward Cu+ Cation:â€‰ A DFT Study. Journal of Physical Chemistry A, 2007, 111, 2213-2219.	1.1	12
2450	Application of a Novel Linear/Exponential Hybrid Force Field Scaling Scheme to the Longitudinal Raman Active Mode of Polyyne. Journal of Physical Chemistry A, 2007, 111, 2434-2441.	1.1	56

#	Article	IF	Citations
2451	Electronic Spectroscopy of an Isolated Halocarbocation:â€‰ The Iodomethyl Cation CH₂I⁺ and Its Deuterated Isotopomers. Journal of Physical Chemistry A, 2007, 111, 10562-10566.	1.1	9
2452	Effect of Ni(ii), Cu(ii) and Zn(ii) association on the keto-enol tautomerism of thymine in the gas phase. Physical Chemistry Chemical Physics, 2007, 9, 2531-2537.	1.3	30
2453	Synthesis and NMR characterization of the cis and trans isomers of [Ptii(N9-adeH)2(pz)2] and X-ray crystallography of the trans isomer. Dalton Transactions, 2007, , 3966.	1.6	9
2454	Water/cyanobutadiyne complexes: an infrared matrix isolation and theoretical study. Physical Chemistry Chemical Physics, 2007, 9, 3985-3991.	1.3	8
2455	Experimental and theoretical studies of the reaction of the OH radical with alkyl sulfides: 2. Kinetics and mechanism of the OH initiated oxidation of methylethyl and diethyl sulfides; observations of a two channel oxidation mechanism. Physical Chemistry Chemical Physics, 2007, 9, 4370.	1.3	12
2456	A comparison of the reactivity of germylene and dimethylgermylene with some methylgermanes. Direct kinetic and quantum chemical studies. Physical Chemistry Chemical Physics, 2007, 9, 4395.	1.3	14
2457	Kinetics and mechanism of the gas phase reaction of chlorine atoms with i-propanol. Physical Chemistry Chemical Physics, 2007, 9, 4211.	1.3	15
2458	Theoretical Characterization of a Tridentate Photochromic Pt(II) Complex Using Density Functional Theory Methods. Journal of Chemical Theory and Computation, 2007, 3, 2198-2209.	2.3	14
2459	Density Functional Theory Investigation of Competitive Free-Radical Processes during the Thermal Cracking of Methylated Polyaromatics: Estimation of Kinetic Parameters. Journal of Physical Chemistry A, 2007, 111, 3082-3090.	1.1	21
2460	Ultrasensitivein situTracing of the Alkaloid Dioncophylline A in the Tropical LianaTriphyophyllum peltatumby Applying Deep-UV Resonance Raman Microscopy. Analytical Chemistry, 2007, 79, 986-993.	3.2	46
2461	Pushâ^'Pull Bithienyl Chromophore with an Unusual Transverse Path of Conjugation. Journal of Physical Chemistry A, 2007, 111, 841-851.	1.1	5
2462	Methane Activation by Laser-Ablated Group 3 Metal Atoms:Â Infrared Spectra and Structures of the CH3â^'MH and CH2â^'MH2Complexes. Organometallics, 2007, 26, 633-643.	1.1	50
2463	Ultrafast Spectroscopic and Matrix Isolation Studies ofp-Biphenylyl,o-Biphenylyl, and 1-Naphthylnitrenium Cations. Journal of the American Chemical Society, 2007, 129, 8380-8388.	6.6	38
2464	Reaction of Hydrogen Atoms with Propyne at High Temperatures:Â An Experimental and Theoretical Studyâ€. Journal of Physical Chemistry A, 2007, 111, 3812-3818.	1.1	35
2465	Thermal Control of Amide Product Distributions at the Ge(100)-2Ã—1 Surface. Journal of Physical Chemistry C, 2007, 111, 411-419.	1.5	11
2466	Infrared Spectra and Theoretical Calculations of Lithium Hydride Clusters in Solid Hydrogen, Neon, and Argon. Journal of Physical Chemistry A, 2007, 111, 6008-6019.	1.1	25
2467	Determining the Structure of Silica-Supported Monomeric Vanadium Oxide Catalysts Based on Synthesis Method and Spectral Data from Theoretical Calculations. Journal of Physical Chemistry C, 2007, 111, 7071-7077.	1.5	12
2468	Normal Vibrational Analysis of a trans-Planar Syndiotactic Polystyrene Chain. Journal of Physical Chemistry B, 2007, 111, 6327-6335.	1.2	47

#	Article	IF	Citations
2469	Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. Journal of Chemical Physics, 2007, 126, 224513.	1.2	61
2470	Infrared Spectroscopy of thetert-Butyl Cation in the Gas Phase. Journal of the American Chemical Society, 2007, 129, 13782-13783.	6.6	48
2471	Group 4 Metal Atom Reactions with CF₃Cl, CFCl₃, CF₃Br, and CF₃I:â€‰ A Matrix Infrared Spectroscopic and DFT Investigation of Competitive Î±-Halogen Transfer to Form Triplet XCÃ·MX₃ Complexes. Organometallics, 2007, 26, 4152-4159.	1.1	15
2472	Computational Studies of Intramolecular Hydrogen Atom Transfers in the Î²-Hydroxyethylperoxy and Î²-Hydroxyethoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 5032-5042.	1.1	37
2473	Signature of the Conformational Preferences of Small Peptides:â€‰ a Theoretical Investigation. Journal of Physical Chemistry A, 2007, 111, 8650-8658.	1.1	21
2474	Calculation of Entropy and Heat Capacity of Organic Compounds in the Gas Phase. Evaluation of a Consistent Method without Adjustable Parameters. Applications to Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 4464-4477.	1.1	16
2475	Methylidyne XCâ‹®MX₃ (M = Cr, Mo, W; X = H, F, Cl) Diagnostic Câ^'H and Câ^'X Stretching Absorptions and Methylidene CH₂MX₂ Analogues. Organometallics, 2007, 26, 6373-6387.	1.1	45
2476	On the Perturbation of the Intramolecular H-Bond in Diols by Supercritical CO2:â€‰ A Theoretical and Spectroscopic Study. Journal of Physical Chemistry A, 2007, 111, 4181-4187.	1.1	30
2477	Matrix Infrared Spectroscopic Studies of the MHâ^'C2H3 and MH2â^'C2H2 Intermediates in the Reactions of Ethylene with Laser-Ablated Group 5 Metal Atoms. Journal of Physical Chemistry A, 2007, 111, 5201-5210.	1.1	19
2478	Atmospheric Chemistry of Linear Perfluorinated Aldehydes:Â Dissociation Kinetics of CnF2n+1CO Radicals. Journal of Physical Chemistry A, 2007, 111, 2555-2562.	1.1	23
2479	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	1.2	149
2480	A Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Isolated Vanadate Species Supported on Silica. Journal of Physical Chemistry C, 2007, 111, 14753-14761.	1.5	74
2481	Icosahedral Polysilane Nanostructures. Journal of Physical Chemistry C, 2007, 111, 2545-2547.	1.5	41
2482	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-Pyrroline N-Oxide (DMPO). 2. Carbonate Radical Anion. Journal of Physical Chemistry A, 2007, 111, 384-391.	1.1	78
2483	Alkylation Effects on Strong Collisions of Highly Vibrationally Excited Alkylated Pyridines with CO2â€. Journal of Physical Chemistry A, 2007, 111, 4073-4080.	1.1	8
2484	Icosahedral Polygermane and Polystannane Nanostructures. Journal of Physical Chemistry C, 2007, 111, 6318-6320.	1.5	6
2485	Covalent and Ionic Nature of the Dative Bond and Account of Accurate Ammonia Borane Binding Enthalpies. Journal of Physical Chemistry A, 2007, 111, 13472-13483.	1.1	41
2486	Sodium Hydride Clusters in Solid Hydrogen and Neon:Â Infrared Spectra and Theoretical Calculations. Journal of Physical Chemistry A, 2007, 111, 7098-7104.	1.1	11

#	Article	IF	Citations
2487	Toward Selective Reactions with CH Bonds:â€‰ A Rationale for the Regio- and Stereochemistry of Dichlorocarbene Insertions into Cyclic Hydrocarbons. Journal of Organic Chemistry, 2007, 72, 10211-10219.	1.7	10
2488	Thermochemical and Kinetic Analysis of the Thermal Decomposition of Monomethylhydrazine:ÂAn Elementary Reaction Mechanismâ€. Journal of Physical Chemistry A, 2007, 111, 3748-3760.	1.1	31
2489	Thermochemical Properties of Polycyclic Aromatic Hydrocarbons (PAH) from G3MP2B3 Calculations. Journal of Physical Chemistry A, 2007, 111, 6510-6520.	1.1	49
2490	Computational Study of the Curtius-like Rearrangements of Phosphoryl, Phosphinyl, and Phosphinoyl Azides and Their Corresponding Nitrenes. Journal of Organic Chemistry, 2007, 72, 9426-9438.	1.7	28
2491	Thermochemistry of 2- and 3-Acetylthiophenes:â€‰ Calorimetric and Computational Study. Journal of Physical Chemistry A, 2007, 111, 11084-11092.	1.1	34
2492	CalculatedVersusâ€œExperimentalâ€•Force Fields: The Influence in the Structure Determination of Benzene by NMR Spectroscopy in Liquid Crystal Solvents. Molecular Crystals and Liquid Crystals, 2007, 465, 289-299.	0.4	7
2493	IR Spectroscopy of Nb+(N2)nComplexes:Â Coordination, Structures, and Spin States. Journal of the American Chemical Society, 2007, 129, 2297-2307.	6.6	51
2494	Proton-Bound Homodimers:Â How Are the Binding Energies Related to Proton Affinities?. Journal of the American Chemical Society, 2007, 129, 12197-12199.	6.6	43
2495	Dissociation Reactions of Free Tetrapyridinium Tetracations and of Their Catenanes. Journal of the American Chemical Society, 2007, 129, 10141-10148.	6.6	22
2496	Structural Characteristics of Hydrocarbon Cages:â€‰ From Fulleranes to Icosahedral Diamondoids. Journal of Physical Chemistry C, 2007, 111, 18118-18126.	1.5	10
2497	2-Amino-4-nitroaniline, a Known Compound with Unexpected Properties. Journal of Physical Chemistry A, 2007, 111, 10084-10089.	1.1	24
2498	chapter 2 Obtaining Molecular Thermochemistry from Calculations. Comprehensive Chemical Kinetics, 2007, , 7-42.	2.3	2
2499	Quantum Chemical and Statistical Rate Investigation of the CF2(a3B1) + NO(X2Î) Reaction:Â A Fast Chemical Quenching Processâ€. Journal of Physical Chemistry A, 2007, 111, 6628-6636.	1.1	1
2500	Time dependent density functional theory investigation of the resonance Raman properties of the julolidinemalononitrile push-pull chromophore in various solvents. Journal of Chemical Physics, 2007, 127, 164507.	1.2	93
2501	Possible Dual-Charge-Carrier Mechanism of Surface Conduction on Î³-Alumina. Journal of Physical Chemistry C, 2007, 111, 5506-5513.	1.5	11
2502	Protonation Processes and Electronic Spectra of Histidine and Related Ions. Journal of Physical Chemistry A, 2007, 111, 4340-4352.	1.1	61
2503	Stability of Different Zinc(II)â^'Diamine Complexes in Aqueous Solution with Respect to Structure and Dynamics:Â A QM/MM MD Study. Journal of Physical Chemistry B, 2007, 111, 151-158.	1.2	21
2504	Thermochemical Properties, Î”fHÂ°(298), SÂ°(298), and CpÂ°(T), for n-Butyl and n-Pentyl Hydroperoxides and the Alkyl and Peroxy Radicals, Transition States, and Kinetics for Intramolecular Hydrogen Shift Reactions of the Peroxy Radicals. Journal of Physical Chemistry A, 2007, 111, 6361-6377.	1.1	58

#	Article	IF	Citations
2505	Helically Annelated and Cross-Conjugated Î²-Oligothiophenes:Â A Fourier Transform Raman Spectroscopic and Quantum Chemical Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 4854-4860.	1.5	14
2506	The Protonation of Allene and Some Heteroallenes, a Computational Study. Journal of Organic Chemistry, 2007, 72, 6343-6352.	1.7	18
2507	Exploration of Mechanisms for the Transformation of 8-Hydroxy Guanine Radical to FAPyG by Density Functional Theory. Chemical Research in Toxicology, 2007, 20, 432-444.	1.7	46
2508	Synthesis and reaction mechanism of a photoremovable protecting group based on 1,4-naphthoquinone. Photochemical and Photobiological Sciences, 2007, 6, 865.	1.6	12
2509	Chemisorption of Hydrogen Atoms on the Sidewalls of Armchair Single-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2007, 111, 7376-7383.	1.5	79
2510	Uncatalyzed Transfer Hydrogenation of Quinones and Related Systems:â€‰ A Theoretical Mechanistic Study. Journal of Physical Chemistry A, 2007, 111, 6456-6467.	1.1	20
2511	The First Photoexcitation Step of Ruthenium-Based Models for Artificial Photosynthesis Highlighted by Resonance Raman Spectroscopy. Journal of Physical Chemistry B, 2007, 111, 6078-6087.	1.2	57
2512	Formation of HCâ‹®ReH₃ in Methane Activation by Rhenium Atoms: Observation of the Elusive Methylidyne Câ‹®H Stretching Absorption. Organometallics, 2007, 26, 4098-4101.	1.1	32
2513	A Spectroscopic and Computational Study of the Neutral and Radical Cation Species of Conjugated Aryl-Substituted 2,5-Bis(2-thien-2-ylethenyl)thiophene-Based Oligomers. Journal of Physical Chemistry A, 2007, 111, 7171-7180.	1.1	31
2514	Should Contemporary Density Functional Theory Methods Be Used to Study the Thermodynamics of Radical Reactions?. Journal of Physical Chemistry A, 2007, 111, 10754-10768.	1.1	140
2515	Infrared and DFT Investigations of the XCâ‹®ReX₃ and HCâ‹®ReX₃ Complexes:â€‰ Jahnâ‹®Teller Distortion and the Methylidyne Câ‹®X(H) Stretching Absorptions. Inorganic Chemistry, 2007, 46, 8728-8738.	1.9	22
2516	In situUV Resonance Raman Micro-spectroscopic Localization of the Antimalarial Quinine in Cinchona Bark. Journal of Physical Chemistry B, 2007, 111, 4171-4177.	1.2	50
2517	Group 4 Transition Metal CH2MF2, CHFMF2, and HCÃ·MF3Complexes Formed by Câ‹®F Activation and Î±-Fluorine Transfer. Inorganic Chemistry, 2007, 46, 4799-4808.	1.9	27
2518	Reactivity of Superoxide Radical Anion with Cyclic Nitrones:Â Role of Intramolecular H-Bond and Electrostatic Effects. Journal of the American Chemical Society, 2007, 129, 8177-8191.	6.6	70
2519	The Lowest Singlet (n,Ï€*) and (Ï€,Ï€*) Excited States of the Hydrogen-Bonded Complex between Water and Pyrazine. Journal of Physical Chemistry A, 2007, 111, 954-962.	1.1	25
2520	High-Resolution Microwave Studies of Ring-Structured Complexes between Trifluoroacetic Acid and Water. Journal of Physical Chemistry A, 2007, 111, 6165-6175.	1.1	53
2521	Computational Study of CO2Reduction by Aminesâ€. Journal of Physical Chemistry A, 2007, 111, 3719-3726.	1.1	19
2522	Structure and Morphology of Hydroxylated Amorphous Alumina Surfaces. Journal of Physical Chemistry C, 2007, 111, 7422-7429.	1.5	53

#	Article	IF	Citations
2523	Ligand Binding Energies in Cationic Platinum(II) Complexes:â€‰ A Quantitative Study in the Gas Phase. Organometallics, 2007, 26, 1523-1530.	1.1	32
2524	Electronic Structure Investigation of Surfaceâ^'Adsorbate and Adsorbateâ^'Adsorbate Interactions in Multilayers of CH4on MgO(100). Journal of Physical Chemistry C, 2007, 111, 966-976.	1.5	14
2525	Effects of Substituents on the Stabilities of Phosphonyl Radicals and their Hydroxyphosphinyl Tautomers. Journal of Physical Chemistry A, 2007, 111, 8229-8240.	1.1	9
2526	Modulation of Electronic Properties in Neutral and Oxidized Oligothiophenes Substituted with Conjugated Polyaromatic Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 2385-2397.	1.1	7
2527	First Infrared Spectroscopic Detection of the Monobridged Diboranyl Radical (B2H5,C2v) and Its D5-Isotopomer in Low-Temperature Diborane Ices. Inorganic Chemistry, 2007, 46, 5739-5743.	1.9	9
2528	Quantum-Chemical Study of the Adsorption of DMMP and Sarin on Î³-Al2O3. Journal of Physical Chemistry C, 2007, 111, 3719-3728.	1.5	74
2529	Photoinduced Î²-Hydrogen Elimination and Radical Formation with CpW(CO)3(CH2CH3):â€‰ Ultrafast IR and DFT Studies. Organometallics, 2007, 26, 1424-1432.	1.1	14
2530	Foiled Carbenes Revisited:Â When Ïƒ-Stabilization Surpasses Ï€-Stabilizationâ€. Journal of Organic Chemistry, 2007, 72, 263-268.	1.7	11
2531	Boron Rings Enclosing Planar Hypercoordinate Group 14 Elements. Journal of the American Chemical Society, 2007, 129, 14767-14774.	6.6	129
2532	Synthesis and Characterization ofmeso-Triarylsubporphyrins. Journal of the American Chemical Society, 2007, 129, 8271-8281.	6.6	146
2533	Intramolecular Vibrational Force Fields for Linear Carbon Chains through an Adaptative Linear Scaling Scheme. Journal of Physical Chemistry A, 2007, 111, 11645-11651.	1.1	45
2534	The Guanine Tautomer Puzzle:â€‰ Quantum Chemical Investigation of Ground and Excited States. Journal of Physical Chemistry A, 2007, 111, 1545-1553.	1.1	169
2535	THEORETICAL AND EXPERIMENTAL STUDY OF ELECTRICAL AND ELECTROCHEMICAL PROPERTIES OF (E)-3-(4,) Tj ETQq0 0 0 rgBT /Overlo of Theoretical and Computational Chemistry, 2007, 06, 255-268.	1.8	33
2536	Characterization of a Genuine Iron(V)â^'Nitrido Species by Nuclear Resonant Vibrational Spectroscopy Coupled to Density Functional Calculations. Journal of the American Chemical Society, 2007, 129, 11053-11060.	6.6	70
2537	One-Electron Oxidation and Reduction Potentials of Nitroxide Antioxidants:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 13595-13605.	1.1	141
2538	Regioselectivity and Mechanism of Dihalocarbene Addition to Benzocyclopropene. Journal of Organic Chemistry, 2007, 72, 7574-7580.	1.7	12
2539	Experimental Vibrational Zero-Point Energies: Diatomic Molecules. Journal of Physical and Chemical Reference Data, 2007, 36, 389-397.	1.9	336
2540	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. Journal of Chemical Theory and Computation, 2007, 3, 1927-1946.	2.3	136

#	Article	IF	Citations
2541	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264
2542	Accurate Calculation of Absolute One-Electron Redox Potentials of Some para-Quinone Derivatives in Acetonitrile. Journal of Physical Chemistry A, 2007, 111, 7227-7232.	1.1	99
2543	Secondary Deuterium Isotope Effects on the Acidity of Carboxylic Acids and Phenols. Journal of the American Chemical Society, 2007, 129, 4490-4497.	6.6	55
2544	Liquid crystalline behavior of tetraaryl derivatives of benzo[c]cinnoline, tetraazapyrene, phenanthrene, and pyrene: the effect of heteroatom and substitution pattern on phase stability. Journal of Materials Chemistry, 2007, 17, 1399.	6.7	43
2545	Sublimation of Ammonium Salts:â€‰ A Mechanism Revealed by a First-Principles Study of the NH₄Cl System. Journal of Physical Chemistry C, 2007, 111, 13831-13838.	1.5	38
2546	Thermodynamic Properties and Hydrogen Accumulation Ability of Fullerene Hydride C₆₀H₃₆. Fullerenes Nanotubes and Carbon Nanostructures, 2007, 15, 227-247.	1.0	14
2547	The Structure, Stability, and Reactivity of Mo-oxo Species in H-ZSM5 Zeolites:â€‰ Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 2081-2091.	1.5	20
2548	Theoretical Methods for Computing Enthalpies of Formation of Gaseous Compounds. Reviews in Computational Chemistry, 2007, , 147-211.	1.5	31
2549	An Infrared Spectroscopic and Theoretical Study of Group 4 Transition Metal CH2MCl2and HCÃ·MCl3Complexes. Organometallics, 2007, 26, 332-339.	1.1	19
2550	Densityâ€functional Theory on the Oxidation Potentials and Geometry Parameters of Thioxanthen Derivatives: Theory and Experiment. Analytical Letters, 2007, 40, 2574-2588.	1.0	7
2551	Remote Position Substituents as Modulators of Conformational and Reactive Properties of Quinones. Relevance of the Ï€/Ï€ Intramolecular Interaction. Journal of Organic Chemistry, 2007, 72, 1883-1894.	1.7	20
2552	Vibrational analysis of deoxy-andrographolide using MM/QM methods. Spectroscopy, 2007, 21, 279-292.	0.8	1
2553	Electronic differentiation competes with transition state sensitivity in palladium-catalyzed allylic substitutions. Beilstein Journal of Organic Chemistry, 2007, 3, 36.	1.3	5
2554	The Molecular Structure and Vibrational Spectrum of 6-bromo-8-thia-1,4-epoxybicyclo[4.3.0]non-2-ene. International Journal of Molecular Sciences, 2007, 8, 1064-1082.	1.8	9
2556	Activation of the Disulfide Bond and Chalcogenâ€“Chalcogen Interactions: An Experimental (FTICR) and Computational Study. Chemistry - A European Journal, 2007, 13, 1796-1803.	1.7	25
2557	DNA Base Trimers: Empirical and Quantum Chemical Ab Initio Calculations versus Experiment in Vacuo. Chemistry - A European Journal, 2007, 13, 2067-2077.	1.7	28
2558	Icosahedral and Ring-Shaped Allotropes of Phosphorus. Chemistry - A European Journal, 2007, 13, 5232-5237.	1.7	46
2559	How Important Is Molecular Rigidity for the Complex Stability of Artificial Hostâ€“Guest Systems? A Theoretical Study on Self-Assembly of Gas-Phase Arginine. Chemistry - A European Journal, 2007, 13, 6644-6653.	1.7	21

#	Article	IF	Citations
2560	Infrared Spectrum and Structure of Thorimine (HNï£¾ThH2). Chemistry - A European Journal, 2007, 13, 5601-5606.	1.7	33
2561	Organometallic Polymers Assembled from Cationâ€“Ï€ Interactions: Use of Ferrocene as a Ditopic Linker Within the Homologous Series [{(Me3Si)2NM}2â‹…(Cp2Fe)]âˆž (M=Na, K, Rb, Cs; Cp=cyclopentadienyl). Chemistry - A European Journal, 2007, 13, 4418-4432.	1.7	55
2562	Forceâ€Field Development and Molecular Dynamics Simulations of Ferroceneâ€“Peptide Conjugates as a Scaffold for Hydrogenase Mimics. Chemistry - A European Journal, 2007, 13, 8139-8152.	1.7	30
2563	The Activation of Hydrogen by Li Atoms To Form [(LiH)2]. Angewandte Chemie - International Edition, 2007, 46, 2602-2606.	7.2	16
2564	The Activation of Hydrogen by Li Atoms To Form [(LiH)2]. Angewandte Chemie, 2007, 119, 2656-2660.	1.6	4
2567	A Smart Supramolecular Hydrogel Exhibiting pH-Modulated Viscoelastic Properties. Advanced Functional Materials, 2007, 17, 1837-1843.	7.8	91
2568	Thicknessâ€Dependent Structural Evolutions and Growth Models in Relation to Carrier Transport Properties in Polycrystalline Pentacene Thin Films. Advanced Functional Materials, 2007, 17, 3639-3649.	7.8	164
2569	Optical Bandgaps of Ï€-Conjugated Organic Materials at the Polymer Limit: Experiment and Theory. Advanced Materials, 2007, 19, 173-191.	11.1	566
2570	Quantum mechanical/molecular mechanical simulations of the Tl(III) ion in water. Journal of Computational Chemistry, 2007, 28, 1057-1067.	1.5	9
2571	Tl(I)-the strongest structure-breaking metal ion in water? A quantum mechanical/molecular mechanical simulation study. Journal of Computational Chemistry, 2007, 28, 1006-1016.	1.5	17
2572	Quantum mechanical charge field molecular dynamics simulation of the TiO2+ ion in aqueous solution. Journal of Computational Chemistry, 2007, 28, 1704-1710.	1.5	22
2573	Structure and bonding of Ag(I)-DNA base complexes and Ag(I)-adenine-cytosine mispairs: An ab Initio study. Journal of Computational Chemistry, 2007, 28, 2299-2308.	1.5	32
2574	Hydroxylic Solvents as Hydrogen Atom Donors in Radical Reactions. European Journal of Organic Chemistry, 2007, 2007, 5817-5820.	1.2	24
2575	Anionic ring-opening polymerization of small phosphorus heterocycles and their borane adducts: An ab initio investigation. Heteroatom Chemistry, 2007, 18, 118-128.	0.4	10
2576	Ab Initio Study of Poly(vinyl chloride) Propagation Kinetics: Head-to-Head versus Head-to-Tail Additions. ChemPhysChem, 2007, 8, 541-552.	1.0	26
2577	Fourier Transform Raman and DFT Study of Three Annulated Oligothiophenes with Different Molecular Shapes. ChemPhysChem, 2007, 8, 745-750.	1.0	6
2578	The Importance of Tetrahedrally Coordinated Molecules for the Explanation of Liquid Water Properties. ChemPhysChem, 2007, 8, 938-943.	1.0	39
2579	Gas-Phase Reactions Between Thiourea and Ca2+: New Evidence for the Formation of [Ca(NH3)]2+ and Other Doubly Charged Species. ChemPhysChem, 2007, 8, 1330-1337.	1.0	25

#	Article	IF	Citations
2580	Contraâ€thermodynamic Behavior in Intermolecular Hydrogen Transfer of Alkylperoxy Radicals. ChemPhysChem, 2007, 8, 1969-1978.	1.0	4
2581	Micro-Hydration of the MgNO3+ Cation in the Gas Phase. ChemPhysChem, 2007, 8, 1629-1639.	1.0	70
2582	Nonâ€Resonanceâ€Assisted Hydrogen Bonding in Hydroxymethylene and Aminomethylene Cyclobutanones and Cyclobutenones and Their Nitrogen Counterparts.. ChemPhysChem, 2007, 8, 1950-1958.	1.0	82
2583	Icosahedral and Ringâ€Shaped Allotropes of Arsenic. ChemPhysChem, 2007, 8, 2373-2378.	1.0	17
2584	Gasâ€phase basicities of polyfunctional molecules. Part 1: Theory and methods. Mass Spectrometry Reviews, 2007, 26, 775-835.	2.8	111
2585	Thermochemistry of methyl and ethyl esters from vegetable oils. International Journal of Chemical Kinetics, 2007, 39, 481-491.	1.0	54
2586	Spectroscopic and computational studies on self-assembly complexes of bis(pyrrol-2-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td (ylm 483-495.	1.2	6
2587	FTIR and FTâ€Raman spectra and density functional computations of the vibrational spectra, molecular geometry and atomic charges of the biomolecule: 5â€bromouracil. Journal of Raman Spectroscopy, 2007, 38, 1227-1241.	1.2	79
2588	Surface-enhanced Raman scattering study of the red dye laccaic acid. Journal of Raman Spectroscopy, 2007, 38, 1259-1266.	1.2	35
2589	Vibrational spectra and quantum chemical calculations of uracilylâ€“pyridinium mesomeric betaine. Journal of Raman Spectroscopy, 2007, 38, 1500-1509.	1.2	5
2590	Vibrational spectroscopy of the seselin crystal. Journal of Raman Spectroscopy, 2007, 38, 1615-1621.	1.2	3
2591	A DFT study of the chemisorption of methoxy on clean and low oxygen precovered Ru(0001) surfaces. Surface Science, 2007, 601, 2473-2485.	0.8	14
2592	Structure modification of maltol (3-hydroxy-2-methyl-4H-pyran-4-one) upon cation and anion formation studied by vibrational spectroscopy and quantum-mechanical calculations. Vibrational Spectroscopy, 2007, 43, 344-350.	1.2	10
2593	HF and DFT studies and vibrational spectra of 1,2-bis(2-pyridyl)ethylene and its zinc (II) halide complexes. Vibrational Spectroscopy, 2007, 43, 335-343.	1.2	6
2594	Calculating the vibrational spectra of molecules: An introduction for experimentalists with contemporary examples. Vibrational Spectroscopy, 2007, 43, 26-37.	1.2	41
2595	On the dehydrogenation of N,Nâ€²-substituted p-phenylenediamine antioxidants. Vibrational Spectroscopy, 2007, 44, 1-8.	1.2	20
2596	Vibrational spectra and theoretical studies of tautomerism and hydrogen bonding in the violuric acid and 6-amino-5-nitrosouracil system. Vibrational Spectroscopy, 2007, 44, 133-141.	1.2	25
2597	A spectroelectrochemical study of the electrosorption of 4-isopropylsulfanylmethyl-1,2,3-triazole on gold. Vibrational Spectroscopy, 2007, 44, 142-153.	1.2	15

#	Article	IF	Citations
2598	Synthesis of hetero- and carbocycles by nucleophilic substitution at sp2 carbon. Tetrahedron, 2007, 63, 5940-5953.	1.0	26
2599	A comparison between entropies of aromatic compounds from quantum mechanical calculations and experiment. Computational and Theoretical Chemistry, 2007, 802, 23-34.	1.5	8
2600	Theoretical study of hydrogen bond interactions of felodipine with polyvinylpyrrolidone and polyethyleneglycol. Computational and Theoretical Chemistry, 2007, 803, 29-38.	1.5	38
2601	Theoretical study of CH bond dissociation energies of HC(X)R {X=O, S, Se; R=H, CH3, Cl, NH2}. Computational and Theoretical Chemistry, 2007, 803, 95-101.	1.5	7
2602	Ab initio and density functional study of a caffeic acid amide. Computational and Theoretical Chemistry, 2007, 804, 57-63.	1.5	2
2603	Calculating gas phase energies of an Î±(1â€“4) linked disaccharide: electronic structure theory and classical atomistic simulation. Computational and Theoretical Chemistry, 2007, 806, 9-22.	1.5	1
2604	Calculation of the relative stability of molecular alumoxanes. Computational and Theoretical Chemistry, 2007, 805, 101-109.	1.5	10
2605	Substituent effects on the proton affinities of selenoamides: A theoretical study. Computational and Theoretical Chemistry, 2007, 805, 119-125.	1.5	7
2606	Conformational study of isolated pindolol by HF, DFT and MP2 calculations. Computational and Theoretical Chemistry, 2007, 806, 231-238.	1.5	9
2607	Sulfurâ€“sulfur bond dissociation enthalpies: A high-level ab initio study. Computational and Theoretical Chemistry, 2007, 807, 87-92.	1.5	17
2608	Study of mechanisms of sulfonium keto ylides intramolecular cyclization. Computational and Theoretical Chemistry, 2007, 807, 55-60.	1.5	6
2609	A multivariate study on flavonoid compounds scavenging the peroxynitrite free radical. Computational and Theoretical Chemistry, 2007, 808, 25-33.	1.5	36
2610	Can the CH2BH2 and CH3BH radicals, cations and anions be observed by experiment?. Computational and Theoretical Chemistry, 2007, 811, 303-312.	1.5	2
2611	A comparative study on the nature and strength of Oâ€“O, Sâ€“S, and Seâ€“Se bond. Computational and Theoretical Chemistry, 2007, 810, 31-37.	1.5	19
2612	Electronic structure, charge distribution and vibrational characteristics of glycine/NMDA receptor antagonists. Computational and Theoretical Chemistry, 2007, 813, 9-19.	1.5	2
2613	Uncatalyzed 1,4-hydrogenation of polycyclic aromatic hydrocarbons: A computational study. Computational and Theoretical Chemistry, 2007, 811, 13-17.	1.5	10
2614	Conformational equilibria of citral. Computational and Theoretical Chemistry, 2007, 814, 33-41.	1.5	25
2615	Ab initio and DFT study of the molecular conformations and the thermochemistry of the CH2CHC(O)OONO2 (APAN) atmospheric molecule and of the CH2CHC(O)OO and CH2CHC(O)O radicals. Computational and Theoretical Chemistry, 2007, 814, 51-60.	1.5	9

#	Article	IF	Citations
2616	A density functional theory study of the cyclization and ring opening reactions of selected 2,2-diphenyl-cyclopropyl radicals. Computational and Theoretical Chemistry, 2007, 811, 135-140.	1.5	1
2617	A computational study of regioisomers formed from the Ïƒ-dimerisation of asymmetric terthiophenes. Computational and Theoretical Chemistry, 2007, 815, 135-143.	1.5	2
2618	A study of cobalt and nickel complexes formation with aromatic Schiffâ€™s bases. Computational and Theoretical Chemistry, 2007, 819, 21-25.	1.5	3
2619	An ab initio study of the SN2 reaction of 1,3- and 3,3-dimethyltriazene with halide ions. Computational and Theoretical Chemistry, 2007, 821, 166-170.	1.5	2
2620	NBO analysis of halogen bridging in 4-halo-1-buten-3-yl cations. Computational and Theoretical Chemistry, 2007, 822, 8-11.	1.5	5
2621	Solvent effects on vibrational spectra of hydrogen-bonded complexes of propanedinitrile (malononitrile) and dimethyl sulfoxide (DMSO): Ab initio and DFT studies. Computational and Theoretical Chemistry, 2007, 823, 65-73.	1.5	5
2622	Theoretical study on the structure and properties of crenulatin molecule in herb Rhodiola crenulata. Computational and Theoretical Chemistry, 2007, 847, 59-67.	1.5	8
2623	Origin and occurrence of selenium in some Australian coals. International Journal of Coal Geology, 2007, 72, 72-80.	1.9	21
2624	Isomerization and dissociation of ethylbenzene and xylene molecular ions: A DFT study. Chemical Physics Letters, 2007, 435, 39-44.	1.2	17
2625	Theoretical study of N2O adsorption on clean and partially oxidized Si(1 0 0)-(2 Ã— 1) small clusters. Chemical Physics Letters, 2007, 436, 263-267.	1.2	5
2626	Novel detection of the C2v isomer of carbon tetraoxide (CO4). Chemical Physics Letters, 2007, 440, 105-109.	1.2	22
2627	First detection of the C2 symmetric isomer of carbon pentaoxide (CO5) at 10K. Chemical Physics Letters, 2007, 443, 49-54.	1.2	17
2628	An effective scaling frequency factor method for scaling of harmonic vibrational frequencies: theory and preliminary application to toluene. Chemical Physics Letters, 2007, 446, 191-198.	1.2	27
2629	Computational approach to the basicity of a series of Î±1-adrenoceptor ligands in aqueous solution. Bioorganic and Medicinal Chemistry, 2007, 15, 2850-2855.	1.4	16
2630	Ideal-gas heat capacities of dimethylsiloxanes from speed-of-sound measurements and ab initio calculations. Fluid Phase Equilibria, 2007, 257, 102-113.	1.4	29
2631	Combining computational and in situ spectroscopies joint with molecular modeling for determination of reaction intermediates of deNOx processâ€”CuZSM-5 catalyst case study. Catalysis Today, 2007, 126, 103-111.	2.2	25
2632	The vibrational spectra of N-phenylpyrrole in the gas phase, in argon matrices and in single crystals. Chemical Physics, 2007, 333, 168-178.	0.9	9
2633	On the calculations of the vibrational Raman spectra of small water clusters. Chemical Physics, 2007, 342, 163-172.	0.9	26

#	Article	IF	Citations
2634	Electrochemical and spectroscopic characterisation of amphetamine-like drugs: Application to the screening of 3,4-methylenedioxymethamphetamine (MDMA) and its synthetic precursors. Analytica Chimica Acta, 2007, 596, 231-241.	2.6	43
2635	Vacuum electrospray ionization study of the ionic liquid, [Emim][Im]. International Journal of Mass Spectrometry, 2007, 265, 146-158.	0.7	67
2636	Dehydrogenation of hydroxymatairesinol to oxomatairesinol over carbon nanofibre-supported palladium catalysts. Journal of Molecular Catalysis A, 2007, 274, 42-49.	4.8	31
2637	Structure and vibrational assignment of 3,4-diacetyl-2,5-hexanedione. A density functional theoretical study. Journal of Molecular Structure, 2007, 827, 176-187.	1.8	39
2638	A luminescent silver-saccharinato complex with S,S-diphenylsulfimide: Synthesis, spectroscopic, thermal, structural and DFT computational studies. Journal of Molecular Structure, 2007, 828, 181-187.	1.8	18
2639	Microwave studies of 4-methyl-1-pentyne. Journal of Molecular Structure, 2007, 837, 86-91.	1.8	5
2640	Vibrational spectra of oligothienyl-vinylenes with donor-Ï€-donor and donor-Ï€-acceptor substitution patterns. Journal of Molecular Structure, 2007, 834-836, 374-379.	1.8	1
2641	Vibrational spectra of nonlinear optical chromophores based on octopolar C3-symmetric 1,3,5 trisalkynylbenzenes. Journal of Molecular Structure, 2007, 834-836, 369-373.	1.8	2
2642	Formation of N,N,Nâ€²,Nâ€²-tetramethylformamidinium disulphide from the chemical and electrochemical oxidation of tetramethylthiourea: Vibrational spectra and crystal structure of the chloride dihydrate salt. Journal of Molecular Structure, 2007, 871, 131-139.	1.8	5
2643	X-ray and ab initio studies of the structure, vibrational and NMR spectra of 1-methyl-3-hydroxypyridinium chloride. Journal of Molecular Structure, 2007, 844-845, 102-114.	1.8	8
2644	Structure of 1-methylpyridinium-4-carboxylate monohydrate studied by X-ray, FT-IR, Raman, NMR and ab initio methods. Journal of Molecular Structure, 2007, 844-845, 140-156.	1.8	17
2645	DFT calculations and vibrational (FT-IR, FT-Raman) spectra on an uracilyl-pyridinium salt. Journal of Molecular Structure, 2007, 834-836, 311-317.	1.8	14
2646	Vibrational frequencies and structural determination of 2,2â€²-biquinoline. Journal of Molecular Structure, 2007, 834-836, 555-560.	1.8	11
2647	An analysis of stable forms of CL-20: A DFT study of conformational transitions, infrared and Raman spectra. Journal of Molecular Structure, 2007, 843, 14-25.	1.8	72
2648	cis- and trans-Bis(pyridine)chromium(III) complexes containing mixed-valence chrysenesemiquinonateâ€“chrysenecatecholate ligands: Synthesis, characterization and interpretation of the electronic absorption spectra using ZINDO/S method. Polyhedron, 2007, 26, 2550-2558.	1.0	3
2649	Metal ion complexes of thioformin: A density functional study. Polyhedron, 2007, 26, 5301-5308.	1.0	8
2650	Structure and electric properties of poly(vinylidene fluorideâ€“tetrafluoroethylene) copolymer studied with density functional theory. Polymer, 2007, 48, 7145-7155.	1.8	28
2651	Spectroscopic properties and electronic structures of 17-electron half-sandwich ruthenium acetylide complexes, [Ru(CCAr)(L2)Cpâ€²]+ (Ar=phenyl, p-tolyl, 1-naphthyl, 9-anthryl; L2=(PPh3)2, Cpâ€²=Cp; L2=dppe;) Tj ET Q q 1 1 0 0 7 8 4 3 1 4 r g		

#	Article	IF	Citations
2652	Exciting flavins: Absorption spectra and spinâ€“orbit coupling in lightâ€“oxygenâ€“voltage (LOV) domains. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 290-300.	2.0	43
2653	An in situ SFG and SERS investigation into the electrodeposition of Au from and solutions. Journal of Electroanalytical Chemistry, 2007, 602, 61-69.	1.9	30
2654	Ab initio and density functional computations of the vibrational spectrum, molecular geometry and some molecular properties of the antidepressant drug sertraline (Zoloft) hydrochloride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 405-412.	2.0	25
2655	Surface-enhanced vibrational spectra of 2-nitrofluorene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 474-479.	2.0	7
2656	The vibrational spectra, assignments and ab initio/DFT analysis for 3-chloro, 4-chloro and 5-chloro-2-methylphenyl isocyanates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 150-159.	2.0	18
2657	A DFT conformational analysis and VCD study on methyl tetrahydrofuran-2-carboxylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 402-411.	2.0	31
2658	DFT and ab initio calculations of the vibrational frequencies and visible spectra of triazenes derived from cyclic amines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 437-443.	2.0	14
2659	Theoretical studies on electrochemistry of p-aminophenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 611-618.	2.0	40
2660	FT-IR and NMR investigation of 1-phenylpiperazine: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 793-801.	2.0	52
2661	Theoretical studies of molecular structure and vibrational spectra of O-ethyl benzoylthiocarbamate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 936-943.	2.0	52
2662	Density functional theory studies on the electronic and vibrational spectra of octaethylporphyrin diacid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 1382-1391.	2.0	8
2663	FT-IR and NMR investigation of 2-(1-cyclohexenyl)ethylamine: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 55-62.	2.0	14
2664	Experimental and density functional theory and ab initio Hartreeâ€“Fock study on the vibrational spectra of 2-(4-fluorobenzylideneamino)-3-mercaptopropanoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 85-93.	2.0	7
2665	DFT calculations on the cyclic ethers hydrogen-bonded complexes: Molecular parameters and the non-linearity of the hydrogen bond. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 626-631.	2.0	25
2666	FT-Raman and infrared spectra and vibrational assignments for 3-chloro-4-methoxybenzaldehyde, as supported by ab initio, hybrid density functional theory and normal coordinate calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 710-717.	2.0	44
2667	HF, MP2 and DFT calculations and spectroscopic study of the vibrational and conformational properties of N-diethylendiamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 942-947.	2.0	32
2668	The molecular structure and vibrational spectra of 2-chloro-N-(diethylcarbamothioyl)benzamide by Hartreeâ€“Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 1347-1355.	2.0	96
2669	Preparation, properties and infrared spectral studies of N-(p-ethylphenyl)thiobenzohydroxamic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 1362-1369.	2.0	3

#	Article	IF	Citations
2670	Isomeric differentiation of green tea catechins using gas-phase hydrogen/deuterium exchange reactions. Journal of the American Society for Mass Spectrometry, 2007, 18, 1749-1759.	1.2	21
2671	Ionic-liquid-like copolymer stabilized nanocatalysts in ionic liquids I. Platinum catalyzed selective hydrogenation of o-chloronitrobenzene. Journal of Catalysis, 2007, 250, 25-32.	3.1	60
2672	Vanadia-based SCR catalysts supported on tungstated and sulfated zirconia: Influence of doping with potassium. Journal of Catalysis, 2007, 251, 459-473.	3.1	91
2673	Surface complexes of phthalic acid at the hematite/water interface. Journal of Colloid and Interface Science, 2007, 307, 124-134.	5.0	63
2674	Using density functional theory to postulate a mechanism for zinc sulfide formation in a CVD reactor. Journal of Crystal Growth, 2007, 307, 440-447.	0.7	7
2675	Geometrical parameters, vibrational wavenumbers, and relationships established with six difluorobenzonitriles. International Journal of Quantum Chemistry, 2007, 107, 1099-1114.	1.0	16
2676	A computational study into the reactivity of epichlorohydrin and epibromohydrin under basic conditions in the gas phase and solution. Journal of Physical Organic Chemistry, 2007, 20, 19-29.	0.9	7
2677	Experimental and theoretical push-pull Chemo- and regioselectivity in 1,3-Dipolar cycloaddition reactions: the case of benzotriazepin-5-one with mesitylnitrile oxide. Journal of Physical Organic Chemistry, 2007, 20, 245-254.	0.9	7
2678	Brotherversusbrother: competitive stabilization of carbocationic centers by flanking cyclopropanes andÏ€-systems. Journal of Physical Organic Chemistry, 2007, 20, 384-394.	0.9	10
2679	Physical imagevsstructure relation: part 12 - structure of 2,2,5,5-tetramethyl-dihydro-furan-3-one oxime and its protonated forms through isomerization and NMR spectra. Journal of Physical Organic Chemistry, 2007, 20, 422-430.	0.9	8
2680	Initiation of petroleum formation and antioxidant function â€“ a DFT study of sulfurï£¿sulfur bond dissociation enthalpies. Journal of Physical Organic Chemistry, 2007, 20, 754-763.	0.9	4
2681	Substituent effect of diarylethenes on IR spectra for application of nonâ€destructive readout of photochromic recording. Journal of Physical Organic Chemistry, 2007, 20, 998-1006.	0.9	18
2682	A computational study into the reactivity of epichlorohydrin and epibromohydrin under acidic conditions in the gas phase and aqueous solution. Journal of Physical Organic Chemistry, 2007, 20, 1058-1071.	0.9	5
2683	Ab initio study on N,Nâ€²,Nâ€³â€triaminoguanidine. Journal of Physical Organic Chemistry, 2007, 20, 1072-1080.	0.9	3
2684	Structural and spectral studies on 3-(6-benzoyl-5-chloro-2-benzoxazolinon-3-yl) propanoic acid. Vibrational Spectroscopy, 2007, 44, 248-255.	1.2	24
2685	Quantum DFT and DFâ€“DFT study of vibrational spectra of sulfuric acid, sulfuric acid monohydrate, formic acid and its cyclic dimer. Vibrational Spectroscopy, 2007, 44, 286-296.	1.2	28
2686	DFT calculation and Raman excitation profile studies of benzophenone molecule. Vibrational Spectroscopy, 2007, 44, 331-342.	1.2	29
2687	Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite. European Journal of Soil Science, 2007, 58, 932-944.	1.8	102

#	Article	IF	Citations
2688	Catalytic isomerization of 1-pentene to cis-2-pentene over zeolites: A quantum mechanical study. Materials Chemistry and Physics, 2007, 106, 394-398.	2.0	3
2689	Theoretical and experimental studies of the electrochemistry of p-aminophenol on a golden electrode. Russian Journal of Physical Chemistry A, 2007, 81, 1669-1676.	0.1	2
2690	Quantum-chemical study of the structure and reactivity of pyrazol-5-ones and their thio and seleno analogs: X. 1-methylpyrazol-5-one and its thio and seleno analogs in H-complex formation reactions in the gas phase and in solutions. Russian Journal of General Chemistry, 2007, 77, 1628-1634.	0.3	1
2691	Reactions of heterocumulenes with organometallic reagents: XIII. Quantum-chemical study on the mechanisms of syn-(Z)/anti-(E)-isomerization of methyl 2-methoxy-N-methylbuta-2,3-dienimidothioate. Russian Journal of Organic Chemistry, 2007, 43, 1585-1594.	0.3	3
2692	Reactions of heterocumulenes with organometallic reagents: XIV. Quantum-chemical study on the mechanism of unusual thermally induced transformation of methyl N-Methylbuta-2,3-dienimidothioates into iminocyclobutenes with migration of the methylsulfanyl group. Russian Journal of Organic Chemistry, 2007, 43, 1595-1603.	0.3	0
2693	Stereochemistry of seven-membered heterocycles: XLVI. Synthesis and dynamic 13C NMR spectroscopy of spiro[cyclohexane-1,4â€²-[3,5]dioxabicyclo[5.1.0]octanes]. DFT calculations of structurally related formaldehyde and acetone acetals. Russian Journal of Organic Chemistry, 2007, 43, 1846-1853.	0.3	2
2694	Thermodynamics of reversible gas adsorption on alkali-metal exchanged zeolitesâ€"the interplay of infrared spectroscopy and theoretical calculations. Physical Chemistry Chemical Physics, 2007, 9, 1421-1437.	1.3	96
2695	Bicyclic proline analogues as organocatalysts for stereoselective aldol reactions: an in silico DFT study. Organic and Biomolecular Chemistry, 2007, 5, 1287.	1.5	65
2696	Harmonic vibrational frequency scaling factors for the new NDDO Hamiltonians: RM1 and PM6. Molecular Physics, 2007, 105, 2597-2605.	0.8	33
2697	Oligothiophene- and Oligopyrrole-Mediated Aggregation of Gold Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 5886-5892.	1.5	18
2698	Identification of a Vibrational Frequency Corresponding to H-atom Translocation in HypericinÂ¶. Photochemistry and Photobiology, 2007, 74, 157-163.	1.3	1
2699	Molecular structure of cotinine studied by gas electron diffraction combined with theoretical calculations. Journal of Molecular Structure, 2007, 841, 13-21.	1.8	4
2700	Retro-Dielsâ^'Alder Reaction of 4H-1,2-Benzoxazines to Generate o-Quinone Methides:â€‰ Involvement of Highly Polarized Transition States. Journal of Organic Chemistry, 2007, 72, 10088-10095.	1.7	38
2701	The Application of Composite Energy Methods to n-butyl Radical Î²-scission Reaction Kinetic Estimations. Theoretical Chemistry Accounts, 2007, 117, 207-212.	0.5	7
2702	Relative Raman Intensities in C6H6, C6D6, and C6F6: A Comparison of Different Computational Methods. Theoretical Chemistry Accounts, 2007, 117, 283-290.	0.5	53
2703	A study of influence of temperature and N, N-acyl protected keto ylides structure on their predominant transformations. Theoretical Chemistry Accounts, 2007, 118, 363-369.	0.5	1
2704	The 1-D hindered rotor approximation. Theoretical Chemistry Accounts, 2007, 118, 881-898.	0.5	168
2705	Study of hydrogen-bonded clusters of 2-methoxyphenolâ€"water. Theoretical Chemistry Accounts, 2007, 118, 947-957.	0.5	8

#	Article	IF	Citations
2706	Raman spectroscopic investigation of the antimalarial agent mefloquine. Analytical and Bioanalytical Chemistry, 2007, 387, 1749-1757.	1.9	41
2707	Spectroscopic and electrochemical studies of cocaineâ€“opioid interactions. Analytical and Bioanalytical Chemistry, 2007, 388, 1799-1808.	1.9	34
2708	Structure, bioactivity and theoretical study of 1-cyano-N-p-tolylcyclo-propanecarboxamide. Structural Chemistry, 2007, 18, 563-568.	1.0	9
2709	Experimental and theoretical spectral properties of ethyl 2-(7-hydroxy-2-oxo-2H-chromen-4-yl)acetate doped sol-gel materials: new materials with potential optical application. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2007, 59, 167-176.	1.6	4
2710	Quantum chemical study of the effect of N,N-acyl group nature on the structure and Gibbs free energy of the sulfur ketoylides and products of their transformations. Journal of Structural Chemistry, 2007, 48, 37-45.	0.3	0
2711	Ab initio modelling of the structure and redox behaviour of copper(I) bound to a Hisâ€“His model peptide: relevance to the Î²-amyloid peptide of Alzheimerâ€™s disease. Journal of Biological Inorganic Chemistry, 2007, 12, 147-164.	1.1	48
2712	Accurate gas phase acidities of carboxylic acids estimated by scaling the vibrational contribution of ab initio gibbs free energies. Journal of Molecular Modeling, 2007, 13, 801-808.	0.8	7
2713	In situ FTIR spectra at the Cu electrode/propylene carbonate solution interface. Electrochimica Acta, 2007, 52, 2710-2715.	2.6	49
2714	Transition state ring sizes in H-transfers in closed shell aliphatic cations. International Journal of Mass Spectrometry, 2007, 266, 8-14.	0.7	2
2715	Characterization by theory of H-transfers and onium reactions of CH3CH2CH2N+H=CH2. Journal of the American Society for Mass Spectrometry, 2007, 18, 270-278.	1.2	21
2716	Protonated nitro group as a gas-phase electrophile: Experimental and theoretical study of the cyclization of o-nitrodiphenyl ethers, amines, and sulfides. Journal of the American Society for Mass Spectrometry, 2007, 18, 2204-2217.	1.2	6
2717	Vibrational dynamics and molecular structure of 1H- and 3H-1,2,3-triazolo[4,5-b]pyridine and its methyl-derivatives based on DFT chemical quantum calculations. Chemical Physics, 2007, 334, 90-108.	0.9	4
2718	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of biomolecule 5-aminouracil. Chemical Physics, 2007, 340, 17-31.	0.9	98
2719	Structure, phase transition and electric properties of poly(vinylidene fluoride-trifluoroethylene) copolymer studied with density functional theory. Polymer, 2007, 48, 3226-3236.	1.8	32
2720	Identification of lamivudine conformers by Raman scattering measurements and quantum chemical calculations. Journal of Pharmaceutical and Biomedical Analysis, 2007, 43, 1885-1889.	1.4	14
2721	Gas-phase proton affinities of guanidines with heteroalkyl side chains. International Journal of Mass Spectrometry, 2008, 270, 39-46.	0.7	36
2722	Synthesis of a novel benzyl-octahydropyrazino[1,2-a]pyrimidin-6-one derivative as a convenient internal bicyclic peptidomimetic. Tetrahedron Letters, 2008, 49, 2316-2319.	0.7	14
2723	1,2-O-(1-Ethylpropylidene)-Î±-d-glucofuranose, a low molecular mass organogelator: benzene gel formation and their thermal stabilities. Tetrahedron Letters, 2008, 49, 6685-6689.	0.7	15

#	Article	IF	Citations
2724	Two theoretical simulations of hydrocarbons thermal cracking: Reactive force field and density functional calculations. Computational and Theoretical Chemistry, 2008, 852, 62-70.	1.5	16
2725	Quantum chemical study of the atmospheric C2H5C(O)OONO2 (PPN) molecule and of the C2H5C(O)OO and C2H5C(O)O radicals. Computational and Theoretical Chemistry, 2008, 856, 59-70.	1.5	8
2726	A theoretical study on NH bond dissociation enthalpies of oxo, thio and seleno carbamates and their N-protonated and N-deprotonated species. Computational and Theoretical Chemistry, 2008, 858, 94-100.	1.5	8
2727	The molecular structure of disulfiram and its complexation with silica. A quantum chemical study. Computational and Theoretical Chemistry, 2008, 861, 57-61.	1.5	11
2728	Molecular structure, vibrational spectra and NBO analysis of phenylisothiocyanate by density functional method. Computational and Theoretical Chemistry, 2008, 863, 44-49.	1.5	20
2729	Molecular structure, barriers to internal rotation, and the enthalpy of formation of cumene hydroperoxide PhCMe2OOH: a DFT study. Russian Chemical Bulletin, 2008, 57, 1179-1186.	0.4	2
2730	FT-Raman, FT-IR and NMR spectra, vibrational assignments and density functional studies of 1,3-bis(benzimidazol-2-yl)-2-thiapropane ligand and its Zn(II) halide complexes. Structural Chemistry, 2008, 19, 21-32.	1.0	9
2731	Calculating molecular vibrational spectra beyond the harmonic approximation. Theoretical Chemistry Accounts, 2008, 120, 23-35.	0.5	61
2732	A microsolvation approach to the prediction of the relative enthalpies and free energies of hydration for ammonium ions. Theoretical Chemistry Accounts, 2008, 120, 5-22.	0.5	6
2733	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. Theoretical Chemistry Accounts, 2008, 120, 215-241.	0.5	23,928
2734	Global warming potential predictions for hydrofluoroethers with two carbon atoms. Theoretical Chemistry Accounts, 2008, 119, 369-381.	0.5	42
2735	The interconversion mechanism between TcO3+ and TcO2 + core of 99mTc labeled amine-oxime (AO) complexes. Theoretical Chemistry Accounts, 2008, 121, 271-278.	0.5	11
2736	Density functional theory study of vibrational spectra, and assignment of fundamental modes of dacarbazine. Journal of Chemical Sciences, 2008, 120, 315-324.	0.7	90
2737	Hydroxy-1,2,5-oxadiazolyl moiety as bioisoster of the carboxy function. A computational study on Î³-aminobutyric acid (GABA) related compounds. Journal of Molecular Modeling, 2008, 14, 279-291.	0.8	15
2738	Molecular geometry, vibrations and electrode potentials of 2-(4,5-dihydroxy-2-methylphenyl)-2-phenyl-2H-indene-1,3-dione; experimental and theoretical attempts. Journal of Molecular Modeling, 2008, 14, 325-333.	0.8	8
2739	Molecular structure and vibrational and chemical shift assignments of 5-(2-Hydroxyphenyl)-4-(p-tolyl)-2,4-dihydro-1,2,4-triazole-3-thione by DFT and ab initio HF calculations. Journal of Molecular Modeling, 2008, 14, 823-832.	0.8	35
2740	Accurate thermochemistry from quantum chemical calculations?. Monatshefte FÃ¼r Chemie, 2008, 139, 309-318.	0.9	29
2741	Periodic density functional theory calculations of bulk and the (010) surface of goethite. Geochemical Transactions, 2008, 9, 4.	1.8	72

#	Article	IF	Citations
2742	Effect of aqueous solvation on the structures of pyruvic acid isomers and their reactions in solution: a computational study. Journal of Physical Organic Chemistry, 2008, 21, 23-29.	0.9	18
2743	Computational study of the mechanism of thermal decomposition of xanthates in the gas phase (the) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	18
2744	The hydroxyacetone (CH₃COCH₂(OH)) torsional potential and isomerization: A theoretical study. International Journal of Quantum Chemistry, 2008, 108, 279-288.	1.0	4
2745	Intra and intermolecular hydrogen bonding in formohydroxamic acid. International Journal of Quantum Chemistry, 2008, 108, 119-134.	1.0	15
2746	Theoretical investigation on the detailed mechanism of the OHâ€initiated atmospheric photooxidation of oâ€xylene. International Journal of Quantum Chemistry, 2008, 108, 954-966.	1.0	13
2747	Understanding selenocysteine through conformational analysis, proton affinities, acidities and bond dissociation energies. International Journal of Quantum Chemistry, 2008, 108, 983-991.	1.0	23
2748	Improvement of scale factors for harmonic vibrational frequency calculations using new polarization functions. International Journal of Quantum Chemistry, 2008, 108, 1036-1043.	1.0	16
2749	Tautomeric preferences and electron delocalization in biurets, thiobiurets, and dithiobiurets: Anab initiostudy. International Journal of Quantum Chemistry, 2008, 108, 1277-1286.	1.0	19
2750	A DFT study of infrared spectrum of sphingomyelin lipid molecule with calcium cation. International Journal of Quantum Chemistry, 2008, 108, 2935-2942.	1.0	7
2751	Factors influencing the Cï£¿ON bond strength of the alkoxyamines in the styreneâ€“acrylonitrileâ€“TEMPO copolymerization system. Journal of Polymer Science Part A, 2008, 46, 1165-1177.	2.5	13
2752	Ni⁺ reactions with aminoacetonitrile, a potential prebiological precursor of glycine. Journal of Mass Spectrometry, 2008, 43, 317-326.	0.7	9
2753	Conformational Stability of Ibuprofen: Assessed by DFT Calculations and Optical Vibrational Spectroscopy. Journal of Pharmaceutical Sciences, 2008, 97, 845-859.	1.6	87
2754	Antioxidant phenolic esters with potential anticancer activity: A Raman spectroscopy study. Journal of Raman Spectroscopy, 2008, 39, 95-107.	1.2	43
2755	Vibrational and optical properties of a oneâ€dimensional organicâ€“inorganic crystal [C₆H₁₄N]PbI₃. Journal of Raman Spectroscopy, 2008, 39, 786-792.	1.2	25
2756	Spectroscopic, structural and theoretical studies of 2â€methylâ€4â€nitroaniline (MNA) crystal. Electronic transitions in IR. Journal of Raman Spectroscopy, 2008, 39, 849-862.	1.2	24
2757	The vibrational assignment of phenanthridine molecule based on normal coordinate analysis and DFT. Journal of Raman Spectroscopy, 2008, 39, 1878-1889.	1.2	7
2758	Pseudopolymorphic transitions of niclosamide monitored by Raman spectroscopy. Journal of Raman Spectroscopy, 2008, 39, 1915-1924.	1.2	17
2759	Thermodynamic properties of the species resulting from the phenyl radical with O₂ reaction system. International Journal of Chemical Kinetics, 2008, 40, 583-604.	1.0	33

#	Article	IF	Citations
2760	Coâ€oxidation of ammonia and ethanol in supercritical water, part 2: Modeling demonstrates the importance of H₂NNO_x. International Journal of Chemical Kinetics, 2008, 40, 653-662.	1.0	19
2761	Joziknipholones A and B: The First Dimeric Phenylanthraquinones, from the Roots of Bulbine frutescens. Chemistry - A European Journal, 2008, 14, 1420-1429.	1.7	30
2762	Infrared Study of Intercomponent Interactions in a Switchable Hydrogenâ€Bonded Rotaxane. Chemistry - A European Journal, 2008, 14, 1935-1946.	1.7	45
2763	Bonding in Tropolone, 2â€Aminotropone, and Aminotroponimine: No Evidence of Resonanceâ€Assisted Hydrogenâ€Bond Effects. Chemistry - A European Journal, 2008, 14, 4225-4232.	1.7	80
2764	Reactions of Uranium Atoms with Ammonia: Infrared Spectra and Quasiâ€Relativistic Calculations of the U:NH₃, H₂Nï£¿UH, and HNï£¾UH₂ Complexes. Chemistry - A European Journal, 2008, 14, 9192-9201.	1.7	40
2765	The Role of Noninnocent Solvent Molecules in Organocatalyzed Asymmetric Michael Addition Reactions. Chemistry - A European Journal, 2008, 14, 10472-10485.	1.7	51
2766	A Theoretical Evaluation of the pK_{HB} and Î”$H{{{,ominus}hfill atop {m HB}hfill}}}$ Hydrogenâ€Bond Scales of Nitrogen Bases. Chemistry - A European Journal, 2008, 14, 10656-10669.	1.7	25
2767	Use of Raman spectroscopy as an In Situ Tool to Obtain Kinetic Data for Organic Transformations. Chemistry - A European Journal, 2008, 14, 9943-9950.	1.7	37
2768	Origin of Diastereocontrol in the Oxyâ€Michael Reactions of Î´â€Lactol Anions: A Computational and Experimental Study. Chemistry - A European Journal, 2008, 14, 9607-9612.	1.7	4
2769	Strength of Câ€“H Bonds at Nitrogen Î±â€Position:Implication for Metabolic Stability of Nitrogenâ€containing Drug Molecules. Chinese Journal of Chemistry, 2008, 26, 787-793.	2.6	8
2770	nâ€Butane Monomolecular Cracking on Acidic Zeolites: A Density Functional Study. Chinese Journal of Chemistry, 2008, 26, 1173-1180.	2.6	14
2771	Theoretical Study on the Vibrational Spectra and Thermodynamic Properties for Nitro Derivatives of Benzene and Anilines. Chinese Journal of Chemistry, 2008, 26, 1357-1362.	2.6	19
2772	Structure-Antioxidant Activity Relationships in a Series of NO-Donor Phenols. ChemMedChem, 2008, 3, 1443-1448.	1.6	6
2773	IRMPD Spectroscopy of a Protonated, Phosphorylated Dipeptide. ChemPhysChem, 2008, 9, 2564-2573.	1.0	33
2774	A DFTâ€Based Investigation of Hydrogen Abstraction Reactions from Methylated Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2008, 9, 2349-2358.	1.0	27
2775	Theoretical studies on fourâ€membered ring compounds with NF₂, ONO₂, N₃, and NO₂ groups. Journal of Computational Chemistry, 2008, 29, 505-513.	1.5	70
2776	Colleâ€Salvettiâ€type correction for electronâ€“nucleus correlation in the nuclear orbital plus molecular orbital theory. Journal of Computational Chemistry, 2008, 29, 735-740.	1.5	36
2777	Fundamental vibrational frequencies and dominant resonances in methylamine isotopologues by ab initio and density functional theory methods. Journal of Computational Chemistry, 2008, 29, 1268-1276.	1.5	16

#	Article	IF	Citations
2778	Additive empirical force field for hexopyranose monosaccharides. Journal of Computational Chemistry, 2008, 29, 2543-2564.	1.5	483
2779	Reactions of Thorium Atoms with Polyhalomethanes: Infrared Spectra of the CH2=ThX2, HCÃ·ThX3, and XCÃ·ThX3 Molecules. European Journal of Inorganic Chemistry, 2008, 2008, 1047-1058.	1.0	37
2780	Infrared Spectra of Insertion, Methylidene, and Methylidyne Complexes in Reactions of Laser-Ablated Ruthenium Atoms with Halomethanes and Methane. European Journal of Inorganic Chemistry, 2008, 2008, 2537-2549.	1.0	28
2781	Reactions of Carbenes with Ethers: The Role of Noncovalent Interactions. European Journal of Organic Chemistry, 2008, 2008, 3363-3368.	1.2	11
2782	Palladiumâ€Catalysed Isomerisation of 2â€Vinylidenehydrofurans to 1,3â€Dienes and Some Aspects of Their Reactivity. European Journal of Organic Chemistry, 2008, 2008, 4446-4453.	1.2	8
2783	Thiolâ€“thione tautomeric forms recognition on the example of 4â€[3â€(2â€methylâ€furanâ€3â€yl)â€5â€thioxoâ€1,2,4â€triazolinâ€4â€yl]acetic acid. Heteroatom Chemistry, 2008, 19, 337-344.	0.4	26
2784	In Situ Synchrotronâ€Based IR Microspectroscopy To Study Catalytic Reactions in Zeolite Crystals. Angewandte Chemie - International Edition, 2008, 47, 3543-3547.	7.2	88
2785	Unraveling the Mechanism of the Soai Asymmetric Autocatalytic Reaction by Firstâ€Principles Calculations: Induction and Amplification of Chirality by Selfâ€Assembly of Hexamolecular Complexes. Angewandte Chemie - International Edition, 2008, 47, 6832-6835.	7.2	91
2786	Gasâ€Phase Formation of the Gombergâ€“Bachmann Magnesium Ketyl. Angewandte Chemie - International Edition, 2008, 47, 9118-9121.	7.2	38
2787	Mechanism of the Nucleophilic Substitution of Acyl Electrophiles using Lithium Organocuprates. Advanced Synthesis and Catalysis, 2008, 350, 1063-1072.	2.1	27
2791	Elimination of H₂ from CH₃CH=N⁺HCH₃: A synchronous, concerted 1,4-H₂ elimination. Journal of the American Society for Mass Spectrometry, 2008, 19, 27-32.	1.2	2
2792	Quantitative aspects of and ionization mechanisms in positive-ion atmospheric pressure chemical ionization mass spectrometry. Journal of the American Society for Mass Spectrometry, 2008, 19, 1926-1941.	1.2	40
2793	Can Î±- and Î²-Alanine Containing Peptides Be Distinguished Based on the CID Spectra of Their Protonated Ions?. Journal of the American Society for Mass Spectrometry, 2008, 19, 1743-1754.	1.2	6
2794	Structural characterization and properties of an azopolymer arranged in Langmuir and Langmuirâ€“Blodgett films. Journal of Colloid and Interface Science, 2008, 319, 277-286.	5.0	10
2795	Experimental and theoretical thermochemistry of Î²-tetralone. Journal of Chemical Thermodynamics, 2008, 40, 1552-1557.	1.0	9
2796	Thermal fragmentation of the guanidinato aluminum amide precursor [Me2NC(NiPr)2]Al(NMe2)2: An investigation of reactive species by matrix-isolation FTIR spectroscopy and time-of-flight mass spectrometry. Polyhedron, 2008, 27, 1832-1840.	1.0	13
2797	Possible reasons that piezoelectricity has not been found in bulk polymer of polyvinylidene cyanide. Polymer, 2008, 49, 2542-2547.	1.8	17
2798	The Oâ€“HÂ·Â·Â·O, Oâ€“HÂ·Â·Â·N and Câ€“HÂ·Â·Â·O hydrogen bonds in 1,4-dimethylpiperazine mono-betaine monohydrate. Journal of Molecular Structure, 2008, 880, 69-76.	1.8	6

#	Article	IF	Citations
2799	Theoretical and experimental study of vibrational spectra of two polymorphic 4-hydroxy-1-methylpiperidine betaine hydrochlorides. Journal of Molecular Structure, 2008, 887, 100-116.	1.8	1
2800	X-ray, FT-Raman, FT-IR spectra and ab initio HF, DFT calculations of 2-[(5-methylisoxazol-3-yl)amino]-2-oxo-ethyl methacrylate. Journal of Molecular Structure, 2008, 886, 148-157.	1.8	67
2801	X-ray, DFT, NMR, FTIR and Raman study of 1-methylquinolinium-3-carboxylate monohydrate. Journal of Molecular Structure, 2008, 889, 394-407.	1.8	14
2802	Investigation of thermodynamic properties of gaseous SiC(XÂ and aÂ) with accurate model chemistry calculations. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 5440-5456.	1.2	14
2803	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 5-chloro-10-oxa-3-thia-tricyclo[5.2.1.01,5]dec-8-ene-3,3-dioxide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 105-112.	2.0	10
2804	DFT and ab initio study of structure of dyes derived from 2-hydroxy and 2,4-dihydroxy benzoic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 449-459.	2.0	55
2805	Synthesis, spectroscopic and structural elucidation of 3-ethylamino-2-(4-nitro-benzoyl)-but-2-enoic acid phenylamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 559-565.	2.0	2
2806	Solâ€"gel materials doped with 3-(3-(4-(dimethylamino)phenyl)propenoyl)-2H-chromen-2-one: Spectroscopic and structural elucidation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 587-591.	2.0	4
2807	Vibrational study of phase transition in N-benzyl methyl ammonium dihydrogenmonophosphate monohydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 743-747.	2.0	6
2808	2-Bromohydroquinone: Structures, vibrational assignments and RHF, B- and B3-based density functional calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 926-932.	2.0	9
2809	Experimental and density functional theory and ab initio Hartreeâ€"Fock study on the vibrational spectra of 2-(4-fluorobenzylideneamino)-3-(4-hydroxyphenyl) propanoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 682-687.	2.0	2
2810	Structural study of 2-(1-oxo-1 H-inden-3-yl)-2H-indene-1,3-dione by DFT calculations, NMR and IR spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 94-98.	2.0	45
2811	Vibrational spectra and ab initio molecular orbital calculations of the novel anti-cancer drug combretastatin A-4 prodrug. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 1208-1216.	2.0	45
2812	Phototransformation studies of halo-substituted cinnamates by Raman spectrometry and quantum-chemical computations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 147-152.	2.0	0
2813	Vibrational spectrum, ab initio calculations, conformational stabilities and assignment of fundamentals of the Ci conformer of 1,4-dichlorobutane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 436-448.	2.0	3
2814	Simulation of IR and Raman spectral based on scaled DFT force fields: A case study of 2-amino 4-hydroxy 6-trifluoromethylpyrimidine, with emphasis on band assignment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 449-457.	2.0	112
2815	Vibrational assignments for 7-methyl-4-bromomethylcoumarin, as aided by RHF and B3LYP/6-31G* calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 688-694.	2.0	56
2816	Theoretical study on the geometry and vibration of 1-{6-(4-Chlorophenyl)-1-[(6-chloropyridin-3-yl)methyl]-2-[(6-chloropyridin-3-yl)methylsulfanyl]-4-methyl-1,6-dihydropyrimidin-5-yl}etha Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 943-952.	2.0	5

#	Article	IF	Citations
2817	Monoclinic and triclinic polymorphs of 2-{5,5-dimethyl-3-[2-(2,4,6-trimethoxyphenyl)vinyl]cyclohex-2-enylidene}malononitrileâ€"Solid-state linear-polarized IR-spectroscopy, DFT calculations and vibrational analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 786-793.	2.0	5
2818	Synthesis, crystal structure, insecticidal activity and DFT study on the geometry and vibration of O-(E)-1-{1-[(6-chloropyridin-3-yl)methyl]-5-methyl-1H-1,2,3-triazol-4-yl}ethyleneamino-O-ethyl-O-phenylphosphorothioate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1011-1020.	2.0	10
2819	Theoretical surface-enhanced Raman spectra study of substituted benzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1049-1055.	2.0	34
2820	Theoretical surface-enhanced Raman spectra study of substituted benzenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1074-1079.	2.0	15
2821	Synthesis, IR, UV/vis-, 1H NMR and DFT study of chelatophore functionalized 1,3-benzoxazinone spiropyrans. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1146-1152.	2.0	14
2822	Experimental and quantum chemical study on the IR, UV and electrode potential of 6-(2,3-dihydro-1,3-dioxo-2-phenyl-1H-inden-2-yl)-2,3-dihydroxybenzaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1390-1396.	2.0	33
2823	Vibrational spectroscopy of triacetone triperoxide (TATP): Anharmonic fundamentals, overtones and combination bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1438-1445.	2.0	30
2824	Magnetic anisotropy and spin fluctuations in the paramagnetic dimer : MÃ¶ssbauer spectroscopy and ab initio calculations. Journal of Magnetism and Magnetic Materials, 2008, 320, 898-905.	1.0	1
2825	An experimental and a DFT study on the synthesis, spectroscopic characterization, and reactivity of the adducts of dimethyl- and diphenyltin(IV) dichlorides with Î³-pyrones [4H-pyran-4-one (PYR) and 2,6-dimethyl-4H-pyran-4-one (DMP)]: Crystal structure of Ph2SnCl2(PYR). Journal of Organometallic Chemistry, 2008, 693, 1203-1214.	0.8	4
2826	anti-Markovnikov addition of tellurium tetrachloride to trimethyl ethynyl silane. Journal of Organometallic Chemistry, 2008, 693, 2509-2513.	0.8	14
2827	The photophysics of flavins: What makes the difference between gas phase and aqueous solution?. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 198, 221-231.	2.0	93
2828	Electron affinity and redox potential of tetrafluoro-p-benzoquinone: A theoretical study. Journal of Fluorine Chemistry, 2008, 129, 222-225.	0.9	24
2829	Strain energies of cubane derivatives with different substituent groups. Journal of Hazardous Materials, 2008, 151, 255-260.	6.5	54
2830	Density functional theory study of piperidine and diazocine compounds. Journal of Hazardous Materials, 2008, 156, 342-347.	6.5	47
2831	DFT study of the interaction between 3-nitro-1,2,4-triazole-5-one and hydrogen fluoride. Journal of Hazardous Materials, 2008, 160, 51-55.	6.5	5
2832	Adsorption behavior of terephthalic acid on Au(100), Au(111) and Au(110) electrodes in neutral solution. Electrochimica Acta, 2008, 53, 5456-5463.	2.6	12
2833	First detection of the Cs symmetric isomer of carbon hexaoxide (CO6) at 10K. Chemical Physics Letters, 2008, 450, 312-317.	1.2	12
2834	Observation of transition state in Raman triggered oxidation of chloroform in the ground state by real-time vibrational spectroscopy. Chemical Physics Letters, 2008, 457, 421-426.	1.2	11

#	Article	IF	Citations
2835	On the formation of higher carbon oxides in extreme environments. Chemical Physics Letters, 2008, 465, 1-9.	1.2	17
2836	An effective scaling frequency factor method for harmonic vibrational frequencies: The factorsâ€™ transferability problem. Chemical Physics Letters, 2008, 465, 290-294.	1.2	14
2837	Surface enhanced Raman scattering of trans-3-hydroxycinnamic acid adsorbed on silver nanoparticles. Chemical Physics Letters, 2008, 467, 101-104.	1.2	8
2838	Deactivation via ring opening: A quantum chemical study of the excited states of furan and comparison to thiophene. Chemical Physics, 2008, 349, 269-277.	0.9	58
2839	Quantum mechanical simulation studies of molecular vibrations and dynamics of oxo-anions in water. Chemical Physics, 2008, 346, 182-185.	0.9	36
2840	Infrared and Raman spectroscopic study of BDA-TTP [2,5-bis(1,3-dithian-2-ylidene)â€“1,3,4,6-tetrathiapentalene] and its charge-transfer salts. Solid State Communications, 2008, 147, 484-489.	0.9	6
2841	A statistical thermodynamic approach to sonochemical reactions. Ultrasonics Sonochemistry, 2008, 15, 78-88.	3.8	7
2842	Vibrational and DFT study of 5-(3-pyridyl-methylidene)-thiazolidine-2-thione-4-one. Vibrational Spectroscopy, 2008, 48, 289-296.	1.2	45
2843	Spectroscopic and theoretical studies of dofetilide. Vibrational Spectroscopy, 2008, 48, 297-301.	1.2	8
2844	Pre-resonance Raman and IR absorption spectroscopy of imidazophenazine and its derivatives: Experimental and ab initio study. Vibrational Spectroscopy, 2008, 47, 71-81.	1.2	3
2845	FRET-derived ratiometric fluorescence sensor for Cu2+. Tetrahedron, 2008, 64, 1294-1300.	1.0	121
2846	Accurate conformation analysis in solution: NMR and DFT/PCM study ofÂthe S-3-(1-naphthoyl)-4-isopropyl-2,2-dimethyloxazolidin-5-one inÂCDCl3. Tetrahedron, 2008, 64, 1743-1752.	1.0	14
2847	Umpolung catalysis: assessment of catalyst and substrate reactivities in acyloin type reactions. Tetrahedron, 2008, 64, 1648-1653.	1.0	19
2848	Mechanistic insights on the site selectivity in successive 1,3-dipolar cycloadditions to meso-tetraarylporphyrins. Tetrahedron, 2008, 64, 7937-7943.	1.0	28
2849	Synthesis, characterization, and DFT studies of a novel azo dye derived from racemic or optically active binaphthol. Tetrahedron, 2008, 64, 11776-11782.	1.0	24
2850	Computational and experimental studies on the IR spectral and structural changes caused by the conversion of 5,5-diethyl(1H, 3H, 5H)-pyrimidinetrione into azanion and diazanion. Computational and Theoretical Chemistry, 2008, 848, 9-15.	1.5	8
2851	Computational investigations of the gas phase reactions between hydrogen chloride and protonated alkyl chlorides. Computational and Theoretical Chemistry, 2008, 848, 128-138.	1.5	6
2852	The prediction of gas-phase and aqueous basicities for alkyl amines. Computational and Theoretical Chemistry, 2008, 849, 84-97.	1.5	9

#	Article	IF	Citations
2853	Hartreeâ€“Fock and density functional theory calculations of the molecular structure and the vibrational spectra of 2-tert-butyldithio-5-methyl-1,3,4-thiadiazole. Computational and Theoretical Chemistry, 2008, 852, 87-92.	1.5	8
2854	A semi-empirical and ab initio combined approach for the full conformational searches of gaseous lysine and lysineâ€“H2O complex. Computational and Theoretical Chemistry, 2008, 858, 52-65.	1.5	39
2855	Hydrogen-bonding interactions in monomeric dimethylcuprates. A theoretical study. Computational and Theoretical Chemistry, 2008, 861, 85-96.	1.5	3
2856	Thermodynamic investigation of the gas-phase reactions in the chemical vapor deposition of boron carbide with BCl3â€“CH4â€“H2 precursors. Computational and Theoretical Chemistry, 2008, 861, 103-116.	1.5	25
2857	Scaling factors for fundamental vibrational frequencies and zero-point energies obtained from HF, MP2, and DFT/DZP and TZP harmonic frequencies. Computational and Theoretical Chemistry, 2008, 864, 20-25.	1.5	55
2858	Conformational stability, barriers to internal rotation of 2-aminothiophenol (d0 and d3): A combined vibrational and theoretical approach. Computational and Theoretical Chemistry, 2008, 865, 14-24.	1.5	16
2859	DFT studies toward the design and properties of high-energy density hydrocarbon fuel. Computational and Theoretical Chemistry, 2008, 866, 63-74.	1.5	15
2860	A theoretical study on the structure and properties of DPO (2,5-dipicryl-1,3,4-oxadiazole). Computational and Theoretical Chemistry, 2008, 869, 98-104.	1.5	7
2861	In situ FTIR study of the Cu electrode/ethylene carbonate+dimethyl carbonate solution interface. Electrochimica Acta, 2008, 53, 3663-3669.	2.6	56
2862	Development of the TraPPE-UA force field for ethylene oxide. Fluid Phase Equilibria, 2008, 274, 44-49.	1.4	30
2863	Hydrogenation of Dicyclopentadiene over amorphous nickel alloy catalyst SRNA-4. Fuel, 2008, 87, 3655-3659.	3.4	62
2864	Methane and methyl halide activation by Sc atoms: Infrared spectra and DFT calculations for the CH3â€“ScX and CH2â€“ScHX complexes. Inorganica Chimica Acta, 2008, 361, 551-559.	1.2	11
2865	Structure of Co2(CO)6(dppm) and Co2(CO)5(CHCO2Et)(dppm) (dppm=Ph2PCH2PPh2) and exchange reaction with 13CO: An experimental and computational study. Inorganica Chimica Acta, 2008, 361, 1832-1842.	1.2	6
2866	Computational and experimental exploration of the gas-phase chemistry of alkyloxalate ions ROCOCOOâ¯ (R=H, CH3, C2H5, i-C3H7, and t-C4H9). International Journal of Mass Spectrometry, 2008, 269, 62-70.	0.7	9
2867	Gas-phase chemistry of alkylcarbonate anions and radicals. International Journal of Mass Spectrometry, 2008, 270, 68-80.	0.7	5
2868	Theoretical and experimental investigations of organic acids/cyclodextrin complexes and their consequences upon the formation of miconazole/cyclodextrin/acid ternary inclusion complexes. International Journal of Pharmaceutics, 2008, 347, 62-70.	2.6	19
2869	Theoretical and experimental vibrational study of miconazole and its dimers with organic acids: Application to the IR characterization of its inclusion complexes with cyclodextrins. International Journal of Pharmaceutics, 2008, 350, 155-165.	2.6	14
2870	Experimental and theoretical determination of the antioxidant properties of isoespintanol (2-isopropyl-3,6-dimethoxy-5-methylphenol). Journal of Molecular Structure, 2008, 877, 1-6.	1.8	51

#	Article	IF	Citations
2871	Spectroscopic and structural elucidation of alanyl-containing dipeptides and their hydrogensquarates. Journal of Molecular Structure, 2008, 877, 79-88.	1.8	4
2872	Synthesis, spectroscopic and theoretical study of isoquinoline alkaloid dehydrosalsolinol base and its triacetylated derivative. Journal of Molecular Structure, 2008, 878, 1-9.	1.8	1
2873	Structure and vibrational spectra of 1,4-dimethylpiperazine di-betaine dihydrate. Journal of Molecular Structure, 2008, 887, 92-99.	1.8	9
2874	Surface-enhanced Raman scattering and DFT computational studies of a benzotriazole derivative. Journal of Molecular Structure, 2008, 888, 2-6.	1.8	5
2875	Comparative ab initio/GIAO-CCSD(T) study of protonated propionaldehyde, isobutyraldehyde and pivalaldehyde cations and their superelectrophilic diprotonated dications. Journal of Molecular Structure, 2008, 890, 9-17.	1.8	4
2876	Density functional theory and two-dimensional correlation polarized infrared spectroscopy studies on the anti-ferroelectric liquid crystal (1-methylheptyl)4-(4â€²-decyloxy-4-biphenyl) oxymethylene benzoate. Journal of Molecular Structure, 2008, 889, 45-53.	1.8	2
2877	Molecular structure of trans-cinnamaldehyde as determined by gas electron diffraction aided by DFT calculations. Journal of Molecular Structure, 2008, 892, 158-162.	1.8	8
2878	DFT and time-resolved IR investigation of electron transfer between photogenerated 17- and 19-electron organometallic radicals. Journal of Molecular Structure, 2008, 890, 328-338.	1.8	10
2879	Thermodynamic properties of the most stable gaseous small silicon-carbon clusters in their ground states. European Physical Journal D, 2008, 49, 21-35.	0.6	22
2880	Interaction of Hydronium Ion with Dibenzo-18-crown-6: NMR, IR, and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 10236-10243.	1.1	104
2881	Comparison of the Standard 6-31G and Binning-Curtiss Basis Sets for Third Row Elements. Journal of Chemical Theory and Computation, 2008, 4, 86-100.	2.3	24
2882	Thermodynamic Stability Versus Kinetic Lability of ZnS₄ Core. Chemistry - an Asian Journal, 2010, 5, 1445-1454.	1.7	8
2883	Excited states of thiophene: ring opening as deactivation mechanism. Physical Chemistry Chemical Physics, 2008, 10, 380-392.	1.3	86
2884	Quantum-chemical study of intramolecular photocyclization in bis(thioxopropenyl) sulfide systems. Russian Journal of General Chemistry, 2008, 78, 295-300.	0.3	2
2885	Quantum-chemical study on the mechanism of formation of geminal hydroxy thiols by reaction of 1,3-dihalopropan-2-ones with hydrogen sulfide. Russian Journal of Organic Chemistry, 2008, 44, 31-37.	0.3	3
2886	Solid-state linear polarized IR-spectroscopy of croconic and rhodizonic acids. Open Chemistry, 2008, 6, 393-399.	1.0	8
2887	Raman, surface-enhanced Raman scattering and DFT study of para-nitro-aniline. Vibrational Spectroscopy, 2008, 48, 210-214.	1.2	41
2888	FT-IR and Raman spectroscopic and quantum chemical studies of zinc halide complexes with 2,2â€²-biquinoline. Vibrational Spectroscopy, 2008, 48, 238-245.	1.2	6

#	Article	IF	Citations
2889	A vibrational spectroscopic investigation on benzocaine molecule. Vibrational Spectroscopy, 2008, 48, 215-228.	1.2	43
2890	Analysis of the reactivities of organic compounds in hydrogen atom abstraction from their C-H bonds by the sulfate radical anion SO 4 Â·â˜. Kinetics and Catalysis, 2008, 49, 202-211.	0.3	12
2891	Isotope effect on metalâ€“insulator transition of (EDO-TTF)2XF6 (X = P, As) with multi-instability of metallic state. Solid State Sciences, 2008, 10, 1780-1785.	1.5	10
2892	Infrared Spectroscopy of Gas Phase Benzenium Ions: Protonated Benzene and Protonated Toluene, from 750 to 3400 cm^{â€“1}. Journal of Physical Chemistry A, 2008, 112, 4869-4874.	1.1	108
2893	Ab Initio Study of Acrylate Polymerization Reactions: Methyl Methacrylate and Methyl Acrylate Propagation. Journal of Physical Chemistry A, 2008, 112, 6772-6782.	1.1	73
2894	Kinetic Study of the Copolymerization of Methyl Methacrylate and Methyl Acrylate Using Quantum Chemistry. Macromolecules, 2008, 41, 8242-8251.	2.2	45
2895	A Î²-Naphthaleneimide-Modified Terthiophene Exhibiting Charge Transfer and Polarization Through the Short Molecular Axis. Joint Spectroscopic and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 6732-6740.	1.1	27
2896	Infrared spectroscopy of gas phase C3H5+: The allyl and 2-propenyl cations. Journal of Chemical Physics, 2008, 128, 021102.	1.2	42
2897	Formation of C 7H 7 + from Benzyl Chloride and Chlorotoluene Molecular Ions: A Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 6190-6197.	1.1	18
2898	Theoretical Studies for Lewis Acidâ˜Base Interactions and Câ˜HÂ·Â·Â·O Weak Hydrogen Bonding in Various CO₂ Complexes. Journal of Physical Chemistry A, 2008, 112, 1596-1603.	1.1	56
2899	The Self-Assembly of Metaboric Acid Molecules into Bowls, Balls and Sheets. Journal of Physical Chemistry A, 2008, 112, 8107-8115.	1.1	7
2900	Preparation of Aza-Polycyclic Aromatic Compounds via Superelectrophilic Cyclizations. Journal of Organic Chemistry, 2008, 73, 3654-3657.	1.7	35
2901	The importance of the oxidative character of doubly charged metal cations in binding neutral bases. [Urea-M]2+ and [thiourea-M]2+ (M = Mg, Ca, Cu) complexes. Physical Chemistry Chemical Physics, 2008, 10, 3229.	1.3	39
2902	Thermodynamics and Kinetics of Intramolecular Water Assisted Proton Transfer in Na⁺-1-Methylcytosine Water Complexes. Journal of Physical Chemistry B, 2008, 112, 8624-8633.	1.2	18
2903	Intermolecular HH Vibrations of Dihydrogen Bonded Complexes H₃EH^{â˜}Â·Â·Â·HOR in the Low-Frequency Region: Theory and IR Spectra. Journal of Physical Chemistry A, 2008, 112, 8198-8204.	1.1	15
2904	Structure, Binding Energies, and IR-Spectral Fingerprinting of Formic Acid Dimers. Journal of Chemical Theory and Computation, 2008, 4, 533-541.	2.3	21
2905	Simple, Nitrogen-Rich, Energetic Salts of 5-Nitrotetrazole. Inorganic Chemistry, 2008, 47, 6014-6027.	1.9	134
2906	Parametrization, Molecular Dynamics Simulation, and Calculation of Electron Spin Resonance Spectra of a Nitroxide Spin Label on a Polyalanine Î±-Helix. Journal of Physical Chemistry B, 2008, 112, 5755-5767.	1.2	98

#	Article	IF	Citations
2907	Experimental and Computational Thermochemistry of 1,4-Benzodioxan and its 6-R Derivatives. Journal of Physical Chemistry A, 2008, 112, 7961-7968.	1.1	9
2908	Transition-State Analysis of the DNA Repair Enzyme MutY. Journal of the American Chemical Society, 2008, 130, 5789-5797.	6.6	87
2909	Consequences of Spin Contamination in Unrestricted Calculations on Open-Shell Species: Effect of Hartreeâ^'Fock and MÃ¸llerâ^'Plesset Contributions in Hybrid and Double-Hybrid Density Functional Theory Approaches. Journal of Physical Chemistry A, 2008, 112, 13225-13230.	1.1	137
2910	Characterizing High-Energy-Density Propellants for Space Propulsion Applications. Journal of Thermophysics and Heat Transfer, 2008, 22, 727-740.	0.9	10
2911	Sigma Stellation:â€‰ A Design Strategy for Electron Boxes. Journal of Physical Chemistry A, 2008, 112, 983-988.	1.1	29
2912	Experimental and theoretical investigation of a coordination polymer [Cu(pda)(2,2â€²-bpy)(H2O)] n Â· 2nH2O. Journal of Coordination Chemistry, 2008, 61, 2132-2141.	0.8	5
2913	Structural Characteristics of Perhydrogenated Boron Nitride Fullerenes. Journal of Physical Chemistry C, 2008, 112, 10032-10037.	1.5	21
2914	Comparative Study of the Photochemistry of the Azidopyridine 1-Oxides. Journal of Organic Chemistry, 2008, 73, 3441-3451.	1.7	16
2915	Pronounced non-Arrhenius behaviour of hydrogen-abstractions from toluene and derivatives by phthalimide-N-oxyl radicals: a theoretical study. Physical Chemistry Chemical Physics, 2008, 10, 1125.	1.3	30
2916	Ex and In Situ Confocal Raman Studies of Organic Thin Film and Its On-Working Transistors. Journal of Physical Chemistry C, 2008, 112, 19718-19726.	1.5	11
2917	Use of Effective Core Potential Calculations for the Conformational and Vibrational Study of Platinum(II) Anticancer Drugs. cis-Diamminedichloroplatinum(II) as a Case Study. Journal of Physical Chemistry A, 2008, 112, 3253-3259.	1.1	36
2918	Calculation of pK_a Values of Nucleobases and the Guanine Oxidation Products Guanidinohydantoin and Spiroiminodihydantoin using Density Functional Theory and a Polarizable Continuum Model. Journal of Physical Chemistry B, 2008, 112, 16860-16873.	1.2	179
2919	Protic ionic liquids based on the dimeric and oligomeric anions: [(AcO)xHxâ^'1]â^'. Physical Chemistry Chemical Physics, 2008, 10, 2972.	1.3	129
2920	Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM). Journal of Physical Chemistry A, 2008, 112, 13164-13171.	1.1	435
2921	Experimental and Theoretical Studies of the Redox Potentials of Cyclic Nitroxides. Journal of Organic Chemistry, 2008, 73, 6763-6771.	1.7	130
2922	Nitrogen Monoxide Interaction with Cu(I) Sites in Zeolites X and Y: Quantum Chemical Calculations and IR Studies. Journal of Physical Chemistry C, 2008, 112, 17998-18010.	1.5	30
2923	Computational Study of the Reaction of n-Bromopropane with OH Radicals and Cl Atoms. Advances in Quantum Chemistry, 2008, 55, 215-244.	0.4	1
2924	Donorâ^'Acceptor Dissociation Energies of Group 13â^'15 Donorâ^'Acceptor Complexes Containing Fluorinated Substituents: Approximate Lewis Acidities of (F₃C)₃M vs (F₅C₆)₃M and the Effects of Phosphine Steric Bulk. Journal of Chemical Theory and Computation, 2008, 4, 1681-1689.	2.3	29

#	Article	IF	Citations
2925	Selenoureaâ^'Ca²⁺Reactions in Gas Phase. Similarities and Dissimilarities with Urea and Thiourea. Journal of Physical Chemistry B, 2008, 112, 5479-5486.	1.2	26
2926	Gas-Phase Interaction of Calcium (Ca²⁺) with Seleno Derivatives of Uracil. Journal of Chemical Theory and Computation, 2008, 4, 1002-1011.	2.3	14
2927	Differential Tuning of the Electron Transfer Parameters in 1,3,5-Triarylpyrazolines: A Rational Design Approach for Optimizing the Contrast Ratio of Fluorescent Probes. Journal of the American Chemical Society, 2008, 130, 13023-13032.	6.6	70
2928	High Level ab Initio Exploration on the Conversion of Carbon Dioxide into Oxazolidinones: The Mechanism and Regioselectivity. Journal of Physical Chemistry A, 2008, 112, 6708-6714.	1.1	26
2929	In-Adamantane, a Small Inside-Out Molecule. Journal of Organic Chemistry, 2008, 73, 7906-7908.	1.7	6
2930	MFI Fingerprint: How Pentasil-Induced IR Bands Shift during Zeolite Nanogrowth. Journal of Physical Chemistry C, 2008, 112, 9186-9191.	1.5	59
2931	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m using the projector augmented wave method: Performance of hybrid and semilocal functionals. Physical Review B, 2008, 78, .	1.1	219
2932	Hydrogen-Bonding Dynamics in Aqueous Solutions of Amides and Acids: Monomer, Dimer, Trimer, and Polymer. Journal of Physical Chemistry B, 2008, 112, 13542-13551.	1.2	46
2933	Chiral Recognition between Î±-Hydroxylesters: A Double-Resonance IR/UV Study of the Complexes of Methyl Mandelate with Methyl Glycolate and Methyl Lactate. Journal of Physical Chemistry A, 2008, 112, 9731-9741.	1.1	14
2934	Tripodal N,N,O-ligands for metalloenzyme models and organometallics. Advances in Inorganic Chemistry, 2008, , 101-165.	0.4	29
2935	Direct Observation of Photoinduced Bent Nitrosyl Excited-State Complexes. Journal of Physical Chemistry A, 2008, 112, 8505-8514.	1.1	18
2936	DFT-UX3LYP Studies on the Coordination Chemistry of Ni²⁺. Part 1: Six Coordinate [Ni(NH₃)_n(H₂O)_{6â^'n}]²⁺Complexes. Journal of Physical Chemistry A, 2008, 112, 10657-10666.	1.1	61
2937	Photochemistry of N-Acetyl-, N-Trifluoroacetyl-, N- Mesyl-, and N-Tosyldibenzothiophene Sulfilimines. Journal of Organic Chemistry, 2008, 73, 4398-4414.	1.7	52
2938	Synthesis and evaluation of nitrostyrene derivative compounds, new snake venom phospholipase A2 inhibitors. Toxicon, 2008, 51, 1467-1478.	0.8	21
2939	Fourier Transform Infrared Studies in Hypergolic Ignition of Ionic Liquids. Journal of Physical Chemistry A, 2008, 112, 7816-7824.	1.1	123
2940	Exploration of Electrostatic Field Force in Surface-Enhanced Raman Scattering: An Experimental Investigation Aided by Density Functional Calculations. Journal of Physical Chemistry C, 2008, 112, 17862-17876.	1.5	31
2941	Ab Initio Evaluation of the Thermodynamic and Electrochemical Properties of Alkyl Halides and Radicals and Their Mechanistic Implications for Atom Transfer Radical Polymerization. Journal of the American Chemical Society, 2008, 130, 12762-12774.	6.6	274
2942	Raman and Infrared Fingerprint Spectroscopy of Peroxide-Based Explosives. Applied Spectroscopy, 2008, 62, 906-915.	1.2	85

#	Article	IF	Citations
2943	Modeling the effects of bond environment on equilibrium iron isotope fractionation in ferric aquo-chloro complexes. Geochimica Et Cosmochimica Acta, 2008, 72, 1939-1958.	1.6	97
2944	Formation and abundance of doubly-substituted methane isotopologues (13CH3D) in natural gas systems. Geochimica Et Cosmochimica Acta, 2008, 72, 5446-5456.	1.6	45
2945	The iron-isotope fractionation dictated by the carboxylic functional: An ab-initio investigation. Geochimica Et Cosmochimica Acta, 2008, 72, 5920-5934.	1.6	19
2946	Ab initio calculations for equilibrium fractionations in multiple sulfur isotope systems. Chemical Geology, 2008, 249, 357-376.	1.4	78
2947	Theoretical study of two pathways of double-bond isomerization of pentene catalyzed by zeolites. Computational Materials Science, 2008, 42, 179-185.	1.4	9
2948	Interaction of Ca2+ with uracil and its thio derivatives in the gas phase. Organic and Biomolecular Chemistry, 2008, 6, 3695.	1.5	40
2949	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	1.2	27
2950	Quantum chemical studies on the potentially important imidates. Computational and Theoretical Chemistry, 2008, 861, 62-67.	1.5	1
2951	Al(III) Hydration Revisited. An ab Initio Quantum Mechanical Charge Field Molecular Dynamics Study. Journal of Physical Chemistry B, 2008, 112, 11726-11733.	1.2	43
2952	Theoretical Studies of the Tautomers of Pyridinethiones. Journal of Physical Chemistry A, 2008, 112, 3231-3238.	1.1	9
2953	A substantial oxygen isotope effect at O2 in the OMP decarboxylase reaction: Mechanistic implications. Organic and Biomolecular Chemistry, 2008, 6, 4533.	1.5	8
2955	Femtosecond pulsed laser deposition and optical properties of diamond-like amorphous carbon films embedded with sp-bonded carbon chains. Diamond and Related Materials, 2008, 17, 1643-1646.	1.8	17
2956	Diels-Alder Addition of Dicyclopentadiene with Cyclopentadiene in Polar Solvents. Chemical Research in Chinese Universities, 2008, 24, 175-179.	1.3	10
2957	Assigning the NH Stretches of the Guanine Tautomers Using Adiabatic Separation:â€‰ CCSD(T) Benchmark Calculations. Journal of Physical Chemistry A, 2008, 112, 1854-1856.	1.1	11
2958	In situ ATRâ€FTIR Spectroscopy of Poly(ethylene terephthalate) Subjected to Highâ€Temperature Methanol. Macromolecular Symposia, 2008, 265, 195-204.	0.4	60
2959	Gas phase vibrational spectroscopy of mass-selected vanadium oxide anions. Physical Chemistry Chemical Physics, 2008, 10, 3992.	1.3	81
2960	Molecular mechanisms in the pyrolysis of unsaturated chlorinated hydrocarbons. New Journal of Chemistry, 2008, 32, 2245.	1.4	7
2961	A multi-technique approach to predicting the molecular structure of cuprizone in the gas phase and in the crystalline state. CrystEngComm, 2008, , .	1.3	2

#	Article	IF	Citations
2962	Gas phase synthesis, structure and unimolecular reactivity of silver iodide cluster cations, AgnIm+ (n) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.6	20
2963	On the thermal unimolecular decomposition of the cyclohexoxy radicalâ€"an experimental and theoretical study. Physical Chemistry Chemical Physics, 2008, 10, 320-329.	1.3	19
2964	Using elementary reactions to model growth processes of polyaromatic hydrocarbons under pyrolysis conditions of light feedstocks. Molecular Simulation, 2008, 34, 193-199.	0.9	11
2965	HCO formation in the thermal unimolecular decomposition of glyoxal: rotational and weak collision effects. Physical Chemistry Chemical Physics, 2008, 10, 6520.	1.3	20
2966	Mid-IRspectra of different conformers of phenylalanine in the gas phase. Physical Chemistry Chemical Physics, 2008, 10, 1248-1256.	1.3	53
2967	The contribution of tunnelling to the 1,5 H-shift isomerisation reaction of alkoxyl radicals. Physical Chemistry Chemical Physics, 2008, 10, 965-973.	1.3	13
2968	Thermodynamic properties of ionic liquidsâ€"a cluster approach. Physical Chemistry Chemical Physics, 2008, 10, 4333.	1.3	73
2969	Is the FeO₂^{â^'} Anion Bent or Linear?. Journal of Physical Chemistry A, 2008, 112, 13641-13649.	1.1	22
2970	Structures, Electron Affinities, and Harmonic Vibrational Frequencies of the Simplest Alkyl Peroxyl Radicals and Their Anions. Journal of Physical Chemistry A, 2008, 112, 6999-7014.	1.1	6
2971	Vibrational Spectra of Anhydrous and Monohydrated Caffeine and Theophylline Molecules and Crystals. Journal of Physical Chemistry A, 2008, 112, 10210-10219.	1.1	27
2972	Determination of the Barrier Height for Acetyl Radical Dissociation from Acetyl Chloride Photodissociation at 235 nm Using Velocity Map Imaging. Journal of Physical Chemistry B, 2008, 112, 16050-16058.	1.2	21
2973	Structure, Conformations, Vibrations, and Ideal-Gas Properties of 1-Alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Ionic Pairs and Constituent Ions. Journal of Physical Chemistry B, 2008, 112, 15708-15717.	1.2	63
2974	Bâ€"H Activation by frustrated Lewis pairs: borenium or boryl phosphonium cation?. Chemical Communications, 2008, , 4303.	2.2	158
2975	Isomer Energy Differences for the C₄H₃and C₄H₅Isomers Using Diffusion Monte Carlo. Journal of Physical Chemistry A, 2008, 112, 2065-2068.	1.1	5
2976	Infrared Spectra, Structure, and Bonding of the Group 6 and Ammonia M:NH₃, H₂Nâ^'MH, and Nâ‰¡MH₃ Reaction Products in Solid Argon. Organometallics, 2008, 27, 4885-4891.	1.1	23
2977	A Study of the Photochemistry of Diazo Meldrumâ€™s Acid by Ultrafast Time-Resolved Spectroscopies. Journal of Physical Chemistry A, 2008, 112, 10108-10112.	1.1	25
2978	High-Resolution Microwave Spectroscopic and ab initio Studies of Propanoic Acid and Its Hydrates. Journal of Physical Chemistry A, 2008, 112, 8208-8214.	1.1	38
2979	Infrared Spectra of Methylidynes Formed in Reactions of Re Atoms with Methane, Methyl Halides, Methylene Halides, and Ethane: Methylidyne Câ^'H Stretching Absorptions, Bond Lengths, and s Character. Inorganic Chemistry, 2008, 47, 1653-1662.	1.9	43

#	Article	IF	Citations
2980	A Computational Study of Chlorocarbene Additions to Cyclooctyne. Journal of Organic Chemistry, 2008, 73, 8537-8544.	1.7	4
2981	Hydration-Dependent Structural Deformation of Guanine in the Electronic Singlet Excited State. Journal of Physical Chemistry B, 2008, 112, 5139-5152.	1.2	42
2982	The Effect and Influence of cis-Ligands on the Electronic and Oxidizing Properties of Nonheme Oxoiron Biomimetics. A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12887-12895.	1.1	18
2983	Câ^'H Activation of Ethane by Group 4 Metal Atoms:â€‰ Observation and Characterization of the MHâ^'CH₂CH₃, MH₂â^'(CH₂)₂, and MH₃â^'CHCH₂ Complexes. Journal of Physical Chemistry A, 2008, 112, 1519-1525.	1.1	22
2984	Surprisingly Slow Reaction of Dimethylsilylene with Dimethylgermane:â€‰ Time-Resolved Kinetic Studies and Related Quantum Chemical Calculations. Journal of Physical Chemistry A, 2008, 112, 849-857.	1.1	13
2985	Carbeneâ^'Alkene Complexes between a Nucleophilic Carbene and Electron-Poor Alkenes. Journal of the American Chemical Society, 2008, 130, 14634-14639.	6.6	12
2986	Experimental and Computational Investigation of Gas-Phase Reaction of Chlorine with n-Propanol:â€‰ Observation of Chloropropanol Conformational Isomerization at Room Temperature. Journal of Physical Chemistry A, 2008, 112, 2773-2781.	1.1	8
2987	Methylidyne Complexes Prepared by Reactions of Laser-Ablated Os Atoms with Methane, Methyl Halides, and Ethane: Observation of the Câ€”H and Osâ€”H Stretching Absorptions. Organometallics, 2008, 27, 1786-1796.	1.1	41
2988	Comparative Quantum Mechanics/Molecular Mechanics (QM/MM) and Density Functional Theory Calculations on the Oxoâ^'Iron Species of Taurine/Î±-Ketoglutarate Dioxygenase. Journal of Physical Chemistry A, 2008, 112, 2464-2468.	1.1	86
2989	Reaction of Iminopropadienones with Aminesâ€”Formation of Zwitterionic Intermediates, Ketenes, and Ketenimines. Journal of Physical Chemistry A, 2008, 112, 9742-9750.	1.1	5
2990	From Fulleranes and Icosahedral Diamondoids to Polyicosahedral Nanowires: Structural, Electronic, and Mechanical Characteristics. Journal of Physical Chemistry C, 2008, 112, 11122-11129.	1.5	12
2991	Characterization of Reactive Intermediates Generated During Photolysis of 4-Acetoxy-4-aryl-2,5-cyclohexadienones: Oxenium Ions and Aryloxy Radicals. Journal of the American Chemical Society, 2008, 130, 16021-16030.	6.6	35
2992	Planar Tetracoordinate Carbons in Cyclic Semisaturated Hydrocarbons. Journal of Organic Chemistry, 2008, 73, 7037-7044.	1.7	35
2993	Determining the Transition-State Structure for Different S_N2 Reactions Using Experimental Nucleophile Carbon and Secondary Î±-Deuterium Kinetic Isotope Effects and Theory. Journal of Physical Chemistry A, 2008, 112, 10264-10273.	1.1	12
2994	Vanadium(V) Compounds with the Bis-(hydroxylamino)-1,3,5-triazine Ligand, H₂bihyat: Synthetic, Structural, and Physical Studies of [V₂^VO₃(bihyat)₂] and of the Enhanced Hydrolytic Stability Speciescis-[V^VO₂(bihyat)]^{â^'}. Inorganic Chemistry, 2008, 47, 11698-11710.	1.9	29
2995	Modeling the Microhydration of Protonated Alanine. Journal of Physical Chemistry B, 2008, 112, 9896-9902.	1.2	21
2996	Structural and Electronic Characteristics of Diamondoid Analogues of Group 14 Elements. Journal of Physical Chemistry C, 2008, 112, 16324-16330.	1.5	14
2997	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122

#	Article	IF	Citations
2998	Thermal Properties of the Gel Made by Low Molecular Weight Gelator 1,2-O-(1-ethylpropylidene)-Î±-d-glucofuranose with Toluene and Molecular Dynamics of Solvent. Langmuir, 2008, 24, 534-540.	1.6	30
2999	The Vibrational Spectrum of the Secondary Electron Acceptor, A₁, in Photosystem I. Journal of Physical Chemistry B, 2008, 112, 3844-3852.	1.2	7
3000	Reactivity of 13,13-Dibromo-2,4,9,11-tetraoxadispiro[5.0.5.1]tridecane toward Organolithiums: Remarkable Resistance to the DMS Rearrangement. Journal of Organic Chemistry, 2008, 73, 5732-5744.	1.7	7
3001	First-Principles Prediction of Rate Coefficients for Free-Radical Cyclization Reactions at Selenium. Journal of Physical Chemistry A, 2008, 112, 13622-13627.	1.1	26
3002	Synthesis and Characterization of Ester-Derivatized Tetrathiatriarylmethyl Radicals as Intracellular Oxygen Probes. Journal of Organic Chemistry, 2008, 73, 1490-1497.	1.7	62
3003	Microhydration of Protonated Glycine:â€‰ An ab initio Family Tree. Journal of Physical Chemistry B, 2008, 112, 2430-2438.	1.2	42
3004	G3//BMK and Its Application to Calculation of Bond Dissociation Enthalpies. Journal of Chemical Theory and Computation, 2008, 4, 1324-1331.	2.3	23
3005	Gas-Phase Mechanisms of Degradation of Hazardous Organophosphorus Compounds: Do They Follow a Common Pattern of Alkaline Hydrolysis Reaction As in Phosphotriesterase?. Journal of Physical Chemistry B, 2008, 112, 9982-9991.	1.2	31
3006	Asymmetric Synthesis of a Tertiary Arsine by Nucleophilic Addition to a Chiral Phosphine-Stabilized Arsenium Salt. Organometallics, 2008, 27, 5099-5107.	1.1	21
3007	Base-Induced Decomposition of Alkyl Hydroperoxides in the Gas Phase. Part 3. Kinetics and Dynamics in HO^{â˙} + CH₃OOH, C₂H₅OOH, and tert-C₄H₉OOH Reactions. Journal of Physical Chemistry A, 2008, 112, 9516-9525.	1.1	17
3008	Hydrothermal In Situ Synthesis and Characterization of Cu(II) Complexes. Inorganic Chemistry, 2008, 47, 1249-1251.	1.9	38
3009	Infrared Photodissociation Spectroscopy of Protonated Acetylene and Its Clusters. Journal of Physical Chemistry A, 2008, 112, 1897-1906.	1.1	70
3010	DFT Study on Chemical N₂ Fixation by Using a Cubane-Type RuIr₃S₄ Cluster: Energy Profile for Binding and Reduction of N₂ to Ammonia via Ruâ˜NâNH_x (x = 1â˜3) Intermediates with Unique Structures. Journal of the American Chemical Society, 2008, 130, 9037-9047.	6.6	49
3011	Proton Transfers in Aromatic and Antiaromatic Systems. How Aromatic or Antiaromatic Is the Transition State? An Ab Initio Study. Journal of the American Chemical Society, 2008, 130, 4934-4944.	6.6	17
3012	Time-Resolved Cavity Ringdown Measurements and Kinetic Modeling of the Pressure Dependences of the Recombination Reactions of SiH₂ with the Alkenes C₂H₄, C₃H₆, and t-C₄H₈. Journal of Physical Chemistry A, 2008, 112, 5636-5646.	1.1	9
3013	A Quantum Mechanical Strategy to Investigate the Structure of Liquids: The Cases of Acetonitrile, Formamide, and Their Mixture. Journal of Physical Chemistry B, 2008, 112, 6803-6813.	1.2	8
3014	Analytic Calculations of Vibrational Hyperpolarizabilities in the Atomic Orbital Basis. Journal of Physical Chemistry A, 2008, 112, 11942-11950.	1.1	30
3015	Ni⁺Reactions with Aminoacrylonitrile, A Species of Potential Astrochemical Relevance. Journal of Physical Chemistry A, 2008, 112, 10509-10515.	1.1	6

#	Article	IF	Citations
3016	A Density Functional Theory Study of the Structure and Vibrational Spectra of Î²-Carotene, Capsanthin, and Capsorubin. Journal of Physical Chemistry A, 2008, 112, 4815-4825.	1.1	34
3017	Theoretical and Experimental Studies of Tyrosyl Hydroperoxide Formation in the Presence of H-Bond Donors. Chemical Research in Toxicology, 2008, 21, 1923-1932.	1.7	10
3018	Infrared Spectra of Metallacyclopropane, Insertion, and Dihydrido Complex Products in Reactions of Laser-Ablated Group 6 Metal Atoms with Ethylene Molecules. Journal of Physical Chemistry A, 2008, 112, 12071-12080.	1.1	14
3019	Zeolite-Catalyzed Hydrogenation of Carbon Dioxide and Ethene. Journal of the American Chemical Society, 2008, 130, 9790-9799.	6.6	71
3020	Room-Temperature First-Order Phase Transition in a Charge-Disproportionated Molecular Conductor (MeEDO-TTF)₂PF₆. Chemistry of Materials, 2008, 20, 7551-7562.	3.2	25
3021	New Organic Sensitizer for Stable Dye-Sensitized Solar Cells with Solvent-Free Ionic Liquid Electrolytes. Journal of Physical Chemistry C, 2008, 112, 17478-17485.	1.5	73
3022	Mechanism and Kinetics for Ammonium Perchlorate Sublimation: A First-principles Study. Journal of Physical Chemistry C, 2008, 112, 14481-14485.	1.5	27
3023	The Phonon Spectrum of Phase-I Ammonia:â€‰ Reassignment of Lattice Mode Symmetries from Combined Molecular and Lattice Dynamics Calculations. Journal of Physical Chemistry A, 2008, 112, 1322-1329.	1.1	11
3024	Synthesis and Spin-Trapping Properties of a New Spirolactonyl Nitrone. Journal of Organic Chemistry, 2008, 73, 2533-2541.	1.7	26
3025	Infrared Spectra, Structure, and Bonding of the GeH3â€”CrH, HGeâ‰¡MoH3, and HGeâ‰¡WH3 Molecules in Solid Neon and Argon. Inorganic Chemistry, 2008, 47, 8159-8166.	1.9	5
3026	Refining the Active Site Structure of Ironâ€'Iron Hydrogenase Using Computational Infrared Spectroscopy. Inorganic Chemistry, 2008, 47, 2380-2388.	1.9	40
3027	Mechanism and Regioselectivity of the Cycloaddition of Thiones Derived from Meldrumâ€™s Acid, Malonates, or Other Dicarbonyls. Journal of Organic Chemistry, 2008, 73, 7457-7466.	1.7	10
3028	Contributions of the 8-Methyl Group to the Vibrational Normal Modes of Flavin Mononucleotide and Its 5-Methyl Semiquinone Radical. Journal of Physical Chemistry A, 2008, 112, 6179-6189.	1.1	20
3029	Polarized Raman Spectra of a Rubrene Single Crystal. Journal of Physical Chemistry C, 2008, 112, 17416-17422.	1.5	45
3030	Bond Dissociation Energies and Equilibrium Structures of Cu⁺(MeOH)_x, x = 1â€'6, in the Gas Phase:â€‰ Competition between Solvation of the Metal Ion and Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2008, 112, 388-401.	1.1	19
3031	Vibronic Coupling in Naphthalene Anion:â€‰ Vibronic Coupling Density Analysis for Totally Symmetric Vibrational Modes. Journal of Physical Chemistry A, 2008, 112, 758-767.	1.1	75
3032	Reactions of Laser-Ablated Iron Atoms with Halomethanes: Infrared Spectra, Density Functional Calculations, and Structures of Simple Iron Insertion and Methylidene Complexes. Organometallics, 2008, 27, 5241-5251.	1.1	41
3033	Electronic, Optical, and Vibrational Properties of Bridged Dithienylethylene-Based NLO Chromophores. Journal of Physical Chemistry C, 2008, 112, 3109-3120.	1.5	48

#	Article	IF	Citations
3034	Mechanism for Iron-Catalyzed Alkene Isomerization in Solution. Organometallics, 2008, 27, 4370-4379.	1.1	44
3035	Magnetic properties, infrared spectroscopy, thermal and theoretical studies of oxomolybdenum(V) complexes with 2,2â€²-bipyrimidine. Journal of Coordination Chemistry, 2008, 61, 3815-3828.	0.8	10
3036	Infrared Spectra of the WH4(H2)4Complex in Solid Hydrogen. Journal of the American Chemical Society, 2008, 130, 1972-1978.	6.6	31
3037	Vibrational Spectra of Triiodomesitylene: Combination of DFT Calculations and Experimental Studies. Effects of the Environment. Journal of Physical Chemistry A, 2008, 112, 11124-11141.	1.1	17
3038	Infrared Spectrum of the CH3â^'PtH Complex in Solid Argon Prepared in the Oxidative Câ^'H Insertion of Methane by Laser-Ablated Pt Atoms. Journal of Physical Chemistry A, 2008, 112, 12293-12295.	1.1	29
3039	Computational Study of the Aminolysis of Anhydrides: Effect of the Catalysis to the Reaction of Succinic Anhydride with Methylamine in Gas Phase and Nonpolar Solution. Journal of Physical Chemistry A, 2008, 112, 5224-5235.	1.1	21
3040	Infrared Spectra and Electronic Structures of Agostic Uranium Methylidene Molecules. Inorganic Chemistry, 2008, 47, 1435-1442.	1.9	53
3041	Hydrogenation of Molecular Cyclic Diborane(4) Compounds Featuring Bâ^'B Bonds and Olefinic or Aromatic Bridges: a Quantum Chemical Study. Inorganic Chemistry, 2008, 47, 7631-7637.	1.9	4
3042	A Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Isolated Vanadate Species Supported on Titania. Journal of Physical Chemistry C, 2008, 112, 13204-13214.	1.5	70
3043	Infrared Spectrum of the RuH₂(H₂)₄ Complex in Solid Hydrogen. Organometallics, 2008, 27, 4273-4276.	1.1	9
3044	Reactivity of Superoxide Radical Anion and Hydroperoxyl Radical with Î±-Phenyl-N-tert-butylnitrone (PBN) Derivatives. Journal of Physical Chemistry A, 2008, 112, 12498-12509.	1.1	35
3045	Reaction of Diphenyldiazomethane with Singlet Oxygen Studied by Time-Resolved IR Spectroscopy. Journal of Organic Chemistry, 2008, 73, 7118-7123.	1.7	11
3046	A Combined Spectroscopic and Theoretical Study of Dibutyltin Diacetate and Dilaurate in Supercritical CO2. Journal of Physical Chemistry A, 2008, 112, 8379-8386.	1.1	10
3047	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide (DMPO). 3. Effect of Mildly Acidic pH on the Thermodynamics and Kinetics of Adduct Formation. Journal of Physical Chemistry A, 2008, 112, 2447-2455.	1.1	30
3048	Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. Journal of Physical Chemistry A, 2008, 112, 12385-12392.	1.1	9
3049	Preparation and Characterization of Simple Dihalomethylidene Platinum Dihalide Complexes in Reactions of Laser-Ablated Pt Atoms with Tetrahalomethanes. Journal of the American Chemical Society, 2008, 130, 15836-15841.	6.6	42
3050	Exploring Structure and Dynamics of the Diaquotriamminezinc(II) Complex by QM/MM MD Simulation. Journal of Physical Chemistry B, 2008, 112, 5788-5794.	1.2	10
3051	Specific Hydration Effects on Oxoâ^'Thio Triazepine Derivatives. Journal of Physical Chemistry A, 2008, 112, 1791-1797.	1.1	12

#	Article	IF	Citations
3052	Molecular Recognition at Methyl Methacrylate/n-Butyl Acrylate (MMA/nBA) Monomer Unit Boundaries of Phospholipids at p-MMA/nBA Copolymer Surfaces. Langmuir, 2008, 24, 10382-10389.	1.6	9
3053	Hydrothermal Reaction of Cu(II)/Pyrazine-2,3,5-tricarboxylic acid and Characterization of the Copper(II) Complexes. Inorganic Chemistry, 2008, 47, 5225-5233.	1.9	47
3054	A Combined Theoretical and Experimental Study of Simple Terminal Group 6 Nitride and Phosphide Nâ‰¡MX3 and Pâ‰¡MX3 Molecules. Journal of Physical Chemistry A, 2008, 112, 8030-8037.	1.1	27
3055	Infrared Multiple Photon Dissociation Spectra of Proton- and Sodium Ion-Bound Glycine Dimers in the Nâ^'H and Oâ^'H Stretching Region. Journal of Physical Chemistry A, 2008, 112, 10220-10225.	1.1	52
3056	Lithium monoxide anion: A ground-state triplet with the strongest base to date. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7647-7651.	3.3	36
3057	Azido-derivatized compounds as IR probes of local electrostatic environment: Theoretical studies. Journal of Chemical Physics, 2008, 129, 174512.	1.2	72
3058	Ab initio Studies on the Carcinogenic Mechanism of the Derivatives of 3,5-Dimethyl-Nitrosopiperazine. , 2008, , .		0
3059	High-Resolution Spectroscopy of Methyl 4-Hydroxycinnamate and Its Hydrogen-Bonded Water Complex. Journal of Physical Chemistry B, 2008, 112, 4427-4434.	1.2	37
3060	REACTION THERMODYNAMICS IN CHEMICAL VAPOR DEPOSITION OF BORON CARBIDES WITH BCl₃â€“C₃H₆ (PROPENE)-H₂ PRECURSORS. Journal of Theoretical and Computational Chemistry, 2008, 07, 1269-1312.	1.8	12
3062	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. Journal of Chemical Physics, 2008, 129, 184110.	1.2	74
3063	Nitrile and thiocyanate IR probes: Quantum chemistry calculation studies and multivariate least-square fitting analysis. Journal of Chemical Physics, 2008, 128, 134506.	1.2	168
3064	Density functional localized orbital corrections for transition metals. Journal of Chemical Physics, 2008, 129, 164108.	1.2	42
3065	Nitrile and thiocyanate IR probes: Molecular dynamics simulation studies. Journal of Chemical Physics, 2008, 128, 154504.	1.2	124
3066	Computational Quantum Chemistry: A New Approach to Atmospheric Nucleation. Advances in Quantum Chemistry, 2008, , 449-478.	0.4	39
3067	Adsorption Behavior of CH2 and CH3 on Metal Clusters Cun (n= 16). Chinese Journal of Chemical Physics, 2008, 21, 445-450.	0.6	3
3068	Zinc cysteine active sites of metalloproteins: A density functional theory and x-ray absorption fine structure study. Journal of Chemical Physics, 2008, 128, 115104.	1.2	10
3069	Ab initiospectroscopy and photoinduced cooling of thetrans-stilbene molecule. Journal of Chemical Physics, 2008, 128, 164303.	1.2	75
3070	Substituent Effect on Infrared Spectra and Thermodynamic Properties of Polynitroamino Substituted Cyclopentane and Cyclohexane. Chinese Journal of Chemical Physics, 2008, 21, 526-534.	0.6	1

#	Article	IF	Citations
3071	Molecular structure and vibrational spectra of 4-nitrobenzylchloride byab initioHartreeâ€“Fock and density functional methods. Molecular Simulation, 2008, 34, 619-630.	0.9	0
3072	High-symmetry low-energy structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:mrow></mml:math>and related fullerenes and nanotubes. Physical Review B, 2008, 77, .	1.1	18
3073	Theoretical Study of Heterocyclic Nitro Compounds for Use as Novel Explosives and Propellants. Journal of the Chinese Chemical Society, 2008, 55, 1272-1276.	0.8	1
3074	Synthesis and Chemical Transformation of 2-iodomethyl-1-(phenylmethyl)-1,5,6,7-tetrahydroindol-4-ones. Journal of Chemical Research, 2008, 2008, 227-231.	0.6	3
3075	1- and 3-Nitreno-2-naphthylcarbenes. A Combined Experimental and Computational Study. Bulletin of the Chemical Society of Japan, 2008, 81, 1629-1637.	2.0	4
3076	Synthesis and Photolysis of Biphenylenetetracarboxylic Dianhydride in Low-temperature Neon Matrixes. Chemistry Letters, 2008, 37, 334-335.	0.7	2
3077	Interpretation of experimental IR spectra of (z)-4-(2- (acryloyloxy)ethoxy)-4-oxobut-2-enoic acid and its polymers. E-Polymers, 2008, 8, .	1.3	0
3078	Infrared and Raman Study of the Charge-Ordered State in the Vicinity of the Superconducting State in the Organic Conductor Î²-(meso-DMBEDT-TTF)₂PF₆. Journal of the Physical Society of Japan, 2008, 77, 024714.	0.7	21
3079	Selenomaltol â€" Synthesis, Spectroscopy and Theoretical Calculations. Heterocycles, 2008, 75, 1931.	0.4	9
3080	An Exploration of Mechanisms for the Transformation of 8-Oxoguanine to Guanidinohydantoin and Spiroiminodihydantoin by Density Functional Theory. Journal of the American Chemical Society, 2008, 130, 5245-5256.	6.6	85
3081	Addition Reactions of Alkyl and Carboxyl Radicals to Vinylidene Fluoride. Journal of Physical Chemistry A, 2008, 112, 4483-4489.	1.1	7
3082	Cellulosic ethanol: progress towards a simulation model of lignocellulosic biomass. Journal of Physics: Conference Series, 2008, 125, 012055.	0.3	4
3085	THE INFRARED SPECTRUM OF PROTONATED NAPHTHALENE AND ITS RELEVANCE FOR THE UNIDENTIFIED INFRARED BANDS. Astrophysical Journal, 2009, 702, 301-306.	1.6	137
3086	In situreal-time monitoring of biomolecular interactions by using surface infrared spectroscopy. Journal of Applied Physics, 2009, 105, 102039.	1.1	16
3087	A Theoretical Study on the Mechanism and Kinetic of the Reaction between Ozone and Benzene. Ozone: Science and Engineering, 2009, 31, 393-401.	1.4	14
3088	DFT Study of deNO_x Reactions in the Gas Phase: Mimicking the Reaction Mechanism over BaNaY Zeolites. Journal of Physical Chemistry A, 2009, 113, 6730-6739.	1.1	3
3089	Synthesis, Bioactivity and SAR study of Nâ€²-(5-substituted-1,3,4-thiadiazol-2-yl)-N-cyclopropylformyl-thioureas as ketol-acid reductoisomerase Inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 545-552.	2.5	16
3090	Synthesis, spectral, thermal, and structural studies of copper(II)-squarate coordination polymer with 2-hydroxyethylpyridine, {[Cu(Î¼-sq)(etpy)2] Â· H2O} n. Journal of Coordination Chemistry, 2009, 62, 2438-2448.	0.8	5

#	Article	IF	Citations
3091	Prediction of Caged Polyaza Polynitroamine (Tetracyclo-HMX) as Energetic Compound. Journal of Energetic Materials, 2009, 27, 133-143.	1.0	3
3092	Computational studies on cyclic [n]paraphenyleneacetylenes using homodesmotic reactions. Molecular Physics, 2009, 107, 2149-2158.	0.8	14
3093	TS-1 from First Principles. Journal of Physical Chemistry A, 2009, 113, 15006-15015.	1.1	51
3094	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
3095	Anion-Additive Interactions Studied by Ab Initio Calculations and Raman Spectroscopy. Journal of the Electrochemical Society, 2009, 156, A305.	1.3	4
3096	Amide I Raman optical activity of polypeptides: Fragment approximation. Journal of Chemical Physics, 2009, 130, 014503.	1.2	21
3097	Theoretical investigation of the water/corundum (0001) interface. Journal of Chemical Physics, 2009, 130, 064702.	1.2	15
3098	Modeling Dinitrogen Activation by Lithium: A Mechanistic Investigation of the Cleavage of N₂ by Stepwise Insertion into Small Lithium Clusters. Journal of the American Chemical Society, 2009, 131, 13045-13053.	6.6	44
3099	Infrared Spectroscopy and Structures of Cobalt Carbonyl Cations, Co(CO)_n⁺ (n = 1â˜9). Journal of Physical Chemistry A, 2009, 113, 4701-4708.	1.1	50
3100	Proton momentum distribution and anomalous scattering intensities in a pseudo-spherical ammonium ion: a neutron Compton scattering study of (NH4)2PdCl6and (NH4)2TeCl6. Journal of Physics Condensed Matter, 2009, 21, 075502.	0.7	2
3101	Advantages and Drawbacks of Quantum Mechanical Static and Dynamic Approaches to Modelling Infrared Spectra. Chinese Journal of Chemical Physics, 2009, 22, 123-128.	0.6	2
3102	Molecular orientation and electronic structure of 11,11,12,12-tetracyanonaphtho-2,6-quinodimethane vacuum-deposited on metal substrates: Charge transfer, complexation, and potassium doping. Journal of Applied Physics, 2009, 105, 023703.	1.1	11
3103	Accurate calculation of vibrational frequencies using explicitly correlated coupled-cluster theory. Journal of Chemical Physics, 2009, 130, 054105.	1.2	173
3104	Infrared spectroscopic and theoretical studies on the formation of Au2NOâ˜ and AunNO (n=2â€“5) in solid argon. Journal of Chemical Physics, 2009, 130, 134511.	1.2	13
3105	Optical spectra obtained from amorphous films of rubrene: Evidence for predominance of twisted isomer. Journal of Chemical Physics, 2009, 130, 214507.	1.2	40
3106	Toward Understanding of Hydrogen Storage in Single-Walled Carbon Nanotubes by Investigations of Chemisorption Mechanism. , 2009, , 297-313.		7
3107	Uncertainties in scaling factors forab initiovibrational zero-point energies. Journal of Chemical Physics, 2009, 130, 114102.	1.2	74
3108	Photolysis of Indan-1,2-dione Derivatives in Oxygen-Doped Argon Matrix at Low Temperature. Bulletin of the Chemical Society of Japan, 2009, 82, 475-481.	2.0	7

#	Article	IF	Citations
3111	Ambipolar Organic Fieldâ€Effect Transistors from Crossâ€Conjugated Aromatic Quaterthiophenes; Comparisons with Quinoidal Parent Materials. Advanced Functional Materials, 2009, 19, 386-394.	7.8	71
3112	Palladiumâ€Catalyzed Cyclopropanation of Unsaturated Endoperoxides. A New Peroxideâ€Preserving Reaction. Advanced Synthesis and Catalysis, 2009, 351, 999-1004.	2.1	15
3113	Aluminium Speciation in 1â€Butylâ€1â€Methylpyrrolidinium Bis(trifluoromethylsulfonyl)amide/AlCl₃ Mixtures. Chemistry - A European Journal, 2009, 15, 3435-3447.	1.7	69
3114	Linker Conjugation Effects in Rhenium(I) Bifunctional Holeâ€Transport/Emitter Molecules. Chemistry - A European Journal, 2009, 15, 3682-3690.	1.7	39
3115	Thiopheneâ€“Diazine Molecular Semiconductors: Synthesis, Structural, Electrochemical, Optical, and Electronic Structural Properties; Implementation in Organic Fieldâ€Effect Transistors. Chemistry - A European Journal, 2009, 15, 5023-5039.	1.7	82
3116	Oxidation of Endâ€Capped Pentathienoacenes and Characterization of Their Radical Cations. Chemistry - A European Journal, 2009, 15, 12346-12361.	1.7	17
3117	A Novel Multistep Mechanism for the Stereocontrolled Ring Opening of Hindered Sulfamidates: Mild, Green, and Efficient Reactivity with Alcohols. Chemistry - A European Journal, 2009, 15, 9810-9823.	1.7	23
3118	Oligoâ€and Polyselenophenes: A Theoretical Study. Chemistry - A European Journal, 2009, 15, 8613-8624.	1.7	134
3119	Theoretical Calculations on the Tetramethyldisilene Rearrangement: A New Approach to an Old Mechanistic Problem. Chemistry - A European Journal, 2009, 15, 8526-8532.	1.7	8
3120	Sparing the orthoâ€position in nucleophilic aromatic substitutionâ€specific displacement of the 4â€SePh group in 2,4â€bis(phenylseleno)nitrobenzene. Heteroatom Chemistry, 2009, 20, 101-108.	0.4	9
3121	Structures and vibrational spectroscopic parameters of selenoxopropanedinitrile and selenoxosilanedicarbonitrile: Theoretical study based on density functional theory method. Heteroatom Chemistry, 2009, 20, 208-217.	0.4	2
3122	New aluminumâ€based ionic liquids: Synthesis, characterization, and theoretical study. Heteroatom Chemistry, 2009, 20, 398-404.	0.4	3
3123	Theoretical Studies on the Infrared Vibrational Spectra, Thermodynamic Properties and Nuclear Magnetic Resonance Spectra for Polynitroâ€1,3â€bishomopentaprismanes. Chinese Journal of Chemistry, 2009, 27, 455-468.	2.6	3
3124	A Theoretical Study on the Vibrational Spectra and Thermodynamic Properties for the Derivatives of HNS. Chinese Journal of Chemistry, 2009, 27, 687-696.	2.6	6
3125	Theoretical Studies on the Structures, Stabilities, Vibrational Spectra, and Thermodynamic Properties of Polynitromethylbenzenes. Chinese Journal of Chemistry, 2009, 27, 1668-1674.	2.6	5
3126	Theoretical Studies on the Structures, Thermodynamic Properties, Detonation Performance, and Pyrolysis Mechanisms for Six Dinitrate Esters. Chinese Journal of Chemistry, 2009, 27, 1871-1878.	2.6	3
3127	A Vibrational Raman Optical Activity Study of 1,1â€²â€Binaphthyl Derivatives. ChemPhysChem, 2009, 10, 2017-2025.	1.0	10
3128	Electronic Studies on Oligothienylenevinylenes: Understanding the Nature of Their Ground and Excited Electronic States. ChemPhysChem, 2009, 10, 1901-1910.	1.0	6

#	Article	IF	Citations
3129	Theoretical Simulation of Vibrational Sumâ€Frequency Generation Spectra from Density Functional Theory: Application to pâ€Nitrothiophenol and 2,4â€Dinitroaniline. ChemPhysChem, 2009, 10, 2132-2142.	1.0	35
3130	FT Raman and DFT Study on a Series of Allâ€anti Oligothienoacenes Endâ€Capped with Triisopropylsilyl Groups. ChemPhysChem, 2009, 10, 3069-3076.	1.0	11
3131	Quantumâ€chemical treatment of the linoleic acid molecule and two of its conjugated isomers. European Journal of Lipid Science and Technology, 2009, 111, 1035-1041.	1.0	2
3132	Controlling Selectivity for Cycloadditions of Nitrones and Alkenes Tethered by Benzimidazoles: Combining Experiment and Theory. European Journal of Organic Chemistry, 2009, 2009, 1578-1584.	1.2	10
3133	Computational and Matrix Isolation Studies of Tetraâ€tertâ€butylethane. European Journal of Organic Chemistry, 2009, 2009, 4340-4345.	1.2	4
3134	A molecular mechanics force field for lignin. Journal of Computational Chemistry, 2009, 30, 457-467.	1.5	89
3135	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with leastâ€square calibration. Journal of Computational Chemistry, 2009, 30, 1007-1015.	1.5	6
3136	Stability of carbonâ€centered radicals: Effect of functional groups on the energetics of addition of molecular oxygen. Journal of Computational Chemistry, 2009, 30, 1016-1026.	1.5	117
3137	Vibrational Raman optical activity of Ï€â€conjugated helical systems: Hexahelicene and heterohelicenes. Journal of Computational Chemistry, 2009, 30, 1261-1278.	1.5	34
3138	Predicting PH vibrations of gas phase molecules and surfaceâ€adsorbed species using bond lengthâ€frequency correlations. Journal of Computational Chemistry, 2009, 30, 1872-1881.	1.5	4
3139	CHARMM general force field: A force field for drugâ€like molecules compatible with the CHARMM allâ€atom additive biological force fields. Journal of Computational Chemistry, 2010, 31, 671-690.	1.5	4,718
3140	Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the H₂O â†' H₂O, CH₃OH â†' H₂O, and H₂O â†' CH₃OH dimers. Journal of Computational Chemistry, 2010, 31, 963-972.	1.5	17
3141	Quantum mechanical studies on model Î±â€pleated sheets. Journal of Computational Chemistry, 2010, 31, 1216-1223.	1.5	10
3142	Electronic structure and reactivity of guanylthiourea: A quantum chemical study. Journal of Computational Chemistry, 2010, 31, 1259-1267.	1.5	18
3143	Metal ion attachment to the matrix mesoâ€tetrakis(pentafluorophenyl)porphyrin, related matrices and analytes: an experimental and theoretical study. Journal of Mass Spectrometry, 2009, 44, 1556-1564.	0.7	19
3144	The reaction of spiro[indolineâ€naphthopyrans] with nitrogen oxides. Not a case of biradical double trapping. Magnetic Resonance in Chemistry, 2010, 48, 25-37.	1.1	1
3145	Antioxidant phenolic esters with potential anticancer activity: solution equilibria studied by Raman spectroscopy. Journal of Raman Spectroscopy, 2009, 40, 80-85.	1.2	17
3146	Effect of hydrogen bonding in the vibrational spectra of transâ€cinnamic acid. Journal of Raman Spectroscopy, 2009, 40, 394-400.	1.2	32

#	Article	IF	Citations
3147	Analysis of alizarin by surfaceâ€enhanced and FTâ€Raman spectroscopy. Journal of Raman Spectroscopy, 2009, 40, 436-441.	1.2	44
3148	FTâ€Raman and FTâ€IR spectral and quantum chemical studies on some flavonoid derivatives: Baicalein and Naringenin. Journal of Raman Spectroscopy, 2009, 40, 562-570.	1.2	62
3149	Experimental and theoretical Raman and surfaceâ€enhanced Raman scattering study of cysteine. Journal of Raman Spectroscopy, 2009, 40, 632-638.	1.2	90
3150	Spectroscopic and thermal studies on the inclusion of transâ€cinnamic acid and a number of its hydroxylâ€derivatives with Î±, Î² and Î³â€cyclodextrins molecules. Journal of Raman Spectroscopy, 2009, 40, 687-695.	1.2	7
3151	Fourierâ€transform infrared and Raman spectra, vibrational assignment and density functional theory calculations of 1,4,5â€triazanaphthalene. Journal of Raman Spectroscopy, 2009, 40, 1183-1187.	1.2	3
3152	Inclusion compounds of phenol derivatives with cyclodextrins: a combined spectroscopic and thermal analysis. Journal of Raman Spectroscopy, 2009, 40, 1624-1633.	1.2	4
3153	Molecular structure, NMR and vibrational spectral analysis of 2,4â€difluorophenol by ab initio HF and density functional theory. Journal of Raman Spectroscopy, 2009, 40, 1657-1663.	1.2	26
3154	First order molecular hyperpolarizabilities and intramolecular charge transfer from the vibrational spectra of NLO material: ethylâ€3â€(3, 4â€dihydroxyphenyl)â€2â€propenoate. Journal of Raman Spectroscopy, 2009, 40, 1822-1830.	1.2	14
3155	Hydrogen bonding in nitrofurantoin polymorphs: a computationâ€assisted spectroscopic study. Journal of Raman Spectroscopy, 2009, 40, 1956-1965.	1.2	22
3156	Experimental and theoretical investigation of the apomorphine Raman spectrum. Journal of Raman Spectroscopy, 2009, 40, 2074-2079.	1.2	5
3157	Raman and SERS study of metoclopramide at different pH values. Journal of Raman Spectroscopy, 2010, 41, 248-255.	1.2	4
3158	Computational prediction of vibrational spectra of normal and modified DNA nucleobases. Journal of Raman Spectroscopy, 2009, 40, 1726-1748.	1.2	30
3159	Theoretical study of cyclohexane hydroxylation by three possible isomers of [FeIV(O)(R-TPEN)]2+: does the pentadentate ligand wrapping around the metal center differently lead to the different stability and reactivity?. Journal of Biological Inorganic Chemistry, 2009, 14, 533-545.	1.1	11
3160	The effect of ring size on vibrational spectroscopy and hydrogen bonding properties for the complexes between small ring carbonyl compounds with HF and HCl: Theoretical analysis. Journal of Molecular Modeling, 2009, 15, 247-256.	0.8	0
3161	Accurate micro- and macro- gas phase basicities of hydroxyl-radical-modified pyrimidines estimated by advanced quantum chemistry methods. Journal of Molecular Modeling, 2009, 15, 711-722.	0.8	2
3162	Theoretical investigation of tautomerism in N-hydroxy amidines. Journal of Molecular Modeling, 2009, 15, 807-816.	0.8	31
3163	Theoretical study of the geometrical and electronic structures and thermochemistry of spherophanes. Journal of Molecular Modeling, 2009, 15, 1067-1078.	0.8	1
3164	Synthesis, spectroscopic and structural elucidation of sympathomimetic amine, tyraminium dihydrogenphosphate. Amino Acids, 2009, 36, 185-193.	1.2	14

#	Article	IF	Citations
3165	Density functional theory study of the near edge X-ray absorption fine structure and infrared spectroscopy of acetylene and benzene on group IV semiconductor surfaces. Surface Science, 2009, 603, 158-164.	0.8	11
3166	Ethanol adsorption on MgO surface with and without defects from a theoretical point of view. Surface Science, 2009, 603, 1093-1098.	0.8	34
3167	Carbocation rearrangements in aspernomine biosynthesis. Tetrahedron Letters, 2009, 50, 1578-1581.	0.7	15
3168	A computational study of the chemistry of substituted 3-nitrenopyridine 1-oxides. Computational and Theoretical Chemistry, 2009, 894, 93-102.	1.5	11
3169	Structural stabilities of metalated histidines in gas phase and existence of gaseous zwitterionic histidine conformers. Computational and Theoretical Chemistry, 2009, 895, 65-71.	1.5	20
3170	Theoretical studies of zinc phthalocyanine monomer, dimer and trimer forms. Computational and Theoretical Chemistry, 2009, 899, 71-78.	1.5	35
3171	Ab initio studies of the thermal decomposition pathways of 1-bromo-3,3,3-trifluoropropene. Computational and Theoretical Chemistry, 2009, 899, 98-110.	1.5	10
3172	DFT study of electronic properties, structure and spectra of aryl diazonium cations. Computational and Theoretical Chemistry, 2009, 904, 14-20.	1.5	20
3173	Experimental and density functional studies on 4-(3,4-dihydroxybenzylideneamino)antipyrine, and 4-(2,3,4-trihydroxybenzylideneamino)antipyrine. Computational and Theoretical Chemistry, 2009, 904, 74-82.	1.5	292
3174	Density functional study of the infrared spectrum of glucose and glucose monohydrates in the OH stretch region. Computational and Theoretical Chemistry, 2009, 905, 59-69.	1.5	22
3175	The role of isomerism and medium effects on stability of anions of formo- and thioformohydroxamic acid. Computational and Theoretical Chemistry, 2009, 911, 30-39.	1.5	7
3176	Characterizing high-energy-density propellants for space propulsion applications. Acta Astronautica, 2009, 65, 967-986.	1.7	25
3177	Geometry and Raman spectra of P.R. 255 and its furo-furanone analogue. Chemical Physics, 2009, 359, 45-52.	0.9	6
3178	Theoretical and spectroscopic studies of 5-fluoro-isatin-3-(N-benzylthiosemicarbazone) and its zinc(II) complex. Journal of Molecular Structure, 2009, 917, 63-70.	1.8	146
3179	Conformational analysis, tautomerization, IR, Raman, and NMR studies of 3-phenylazo-2,4-pentanedione. Journal of Molecular Structure, 2009, 920, 301-309.	1.8	12
3180	Experimental and theoretical investigation of 5-para-nitro-benzylidene-thiazolidine-2-thione-4-one molecule. Journal of Molecular Structure, 2009, 924-926, 361-370.	1.8	6
3181	Spectroscopic and theoretical study of 1,2,4-triazole-3-one based salicylaldimine complexes and evaluation of superoxide-scavenging properties. Journal of Molecular Structure, 2009, 922, 1-10.	1.8	37
3182	Theoretical and experimental vibrational spectroscopic study of 3-piperidino-propylamine. Journal of Molecular Structure, 2009, 923, 120-126.	1.8	19

#	Article	IF	Citations
3183	Experimental and density functional studies on 4-(2,3-dichlorobenzylideneamino)antipyrine and 4-(2,5-dichlorobenzylideneamino)antipyrine. Journal of Molecular Structure, 2009, 929, 10-21.	1.8	36
3184	Infrared spectroscopy and ab initio computation in conformer determination of keto ester and diketo triphenylphosphonium ylides. Journal of Molecular Structure, 2009, 936, 132-136.	1.8	7
3185	Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin. Journal of Chemical Thermodynamics, 2009, 41, 308-314.	1.0	25
3186	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. Topics in Catalysis, 2009, 52, 444-455.	1.3	11
3187	Thermodynamics of the gas-phase reactions in chemical vapor deposition of silicon carbide with methyltrichlorosilane precursor. Theoretical Chemistry Accounts, 2009, 122, 1-22.	0.5	32
3188	A theoretical study of the thermodynamics and kinetics of small organosulfur compounds. Theoretical Chemistry Accounts, 2009, 123, 391-412.	0.5	32
3189	Effects of microsolvation and aqueous solvation on the tautomers of histidine: a computational study on energy, structure and IR spectrum. Theoretical Chemistry Accounts, 2009, 124, 37-47.	0.5	27
3190	Zwitterionic structures of strained cis-pyramidalized disilenes: fact or artifact. Theoretical Chemistry Accounts, 2009, 124, 421-430.	0.5	8
3191	Thermophysical properties of the Î±â€“Î²â€“Î³ polymorphs of Mg2SiO4: a computational study. Physics and Chemistry of Minerals, 2009, 36, 87-106.	0.3	44
3192	A computational study of stereospecifity in the thermal elimination reaction of menthyl benzoate in the gas phase. Journal of Physical Organic Chemistry, 2009, 22, 971-977.	0.9	142
3193	A DFT/TDâ€ÐFT study for the ground and excited states of peramine and some pyrrolopyrazinone compounds. Journal of Physical Organic Chemistry, 2009, 22, 1058-1064.	0.9	3
3194	Gas chromatography/timeâ€ofâ€flight mass spectrometry of triacetone triperoxide based on femtosecond laser ionization. Rapid Communications in Mass Spectrometry, 2009, 23, 3101-3106.	0.7	12
3195	Theoretical analysis of vibrational spectra and scalingâ€factor of 2â€arylâ€1,3,4â€oxadiazole derivatives. International Journal of Quantum Chemistry, 2009, 109, 328-341.	1.0	30
3196	Substituent effect on Nï£¿H bond dissociation enthalpies of amines and amides: A theoretical study. International Journal of Quantum Chemistry, 2009, 109, 559-568.	1.0	9
3197	Evaluation of recent scaling free methods to predict phenol and phenoxyl radical vibrational propertiesâ€"Guidelines for more complex models of lignin or protein moieties. International Journal of Quantum Chemistry, 2009, 109, 1531-1546.	1.0	3
3198	Exact mathematical treatment of the modifications of finiteâ€dimensional quantum systems. International Journal of Quantum Chemistry, 2009, 109, 2831-2859.	1.0	1
3199	Comparative vibrational spectroscopic study of 1,3-diacetylbenzene and 2,6-diacetylpyridine aided with density functional calculation. Vibrational Spectroscopy, 2009, 49, 84-95.	1.2	6
3200	Spectroelectrochemical studies of self assembled monolayers of biphenyl ethynyl thiols on gold electrodes. Vibrational Spectroscopy, 2009, 49, 162-173.	1.2	4

#	Article	IF	Citations
3201	Molecular and vibrational structure of the extracellular bacterial signal compound N-butyryl-homoserine lactone (C4-HSL). Vibrational Spectroscopy, 2009, 49, 237-241.	1.2	8
3202	Conformational analysis and vibrational spectroscopic investigation of 3-phenylpropylamine. Vibrational Spectroscopy, 2009, 50, 277-284.	1.2	15
3203	Unimolecular dissociation of aniline molecular ion: A theoretical study. International Journal of Mass Spectrometry, 2009, 279, 25-31.	0.7	31
3204	Radical cation/radical reactions: A Fourier transform ion cyclotron resonance study of allyl radical reacting with aromatic radical cations. International Journal of Mass Spectrometry, 2009, 287, 8-15.	0.7	11
3205	Inductive effects on cationâ€“Ï€ interactions: Structures and bond dissociation energies of alkali metal cationâ€“halobenzene complexes. International Journal of Mass Spectrometry, 2009, 283, 35-47.	0.7	23
3206	2-Nitrophenyl aryl sulfides undergo both intramolecular and electrospray-induced intermolecular oxidation of sulfur: An experimental and theoretical case study. International Journal of Mass Spectrometry, 2009, 283, 222-228.	0.7	7
3207	Dissociation of fluorotoluene molecular ions: A theoretical study. International Journal of Mass Spectrometry, 2009, 286, 104-111.	0.7	7
3208	Condensation reaction of C4H4+ with pyridine. International Journal of Mass Spectrometry, 2009, 288, 22-35.	0.7	2
3209	Structures and properties of 1,7-disubstituted perylene tetracarboxylic diimides: The substitutional effect study based on density functional theory calculations. Journal of Molecular Structure, 2009, 917, 133-141.	1.8	27
3210	Raman spectroscopic and DFT theoretical study of 4-(2-pyridylazo)resorcinol and its complexes with zinc(II) and copper(II). Journal of Molecular Structure, 2009, 919, 94-99.	1.8	18
3211	Spectroscopic and DFT study of 3-quinolyl-Î±-aminophosphonates. Journal of Molecular Structure, 2009, 924-926, 66-72.	1.8	17
3212	Exact treatment of the vibrational isotope effect in the harmonic approximation: Out-of-plane vibrations of planar molecules. Journal of Molecular Structure, 2009, 924-926, 477-492.	1.8	3
3213	Conformer determination of stabilized triphenyl phosphonium acyl ylides by infrared spectroscopy. Journal of Molecular Structure, 2009, 921, 6-12.	1.8	5
3214	Relationship between molecular structure and Raman spectra of quinolines. Journal of Molecular Structure, 2009, 924-926, 301-308.	1.8	42
3215	Vibrational and electronic structure of PTCDI and melamineâ€“PTCDI complexes. Journal of Molecular Structure, 2009, 924-926, 47-53.	1.8	27
3216	Raman spectroscopy applied to reveal polycrystalline grain structures and carrier transport properties of organic semiconductor films: Application to pentacene-based organic transistors. Organic Electronics, 2009, 10, 289-298.	1.4	33
3217	Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives. Tetrahedron, 2009, 65, 232-239.	1.0	17
3218	Stepwise insertion of carbenes into Câ€“H bonds: the case of foiled carbenes. Tetrahedron, 2009, 65, 765-770.	1.0	8

#	Article	IF	Citations
3219	Electron affinities of a homologous series of tertiary alkyl radicals and their Câ€“H bond dissociation energies (BDEs). Tetrahedron, 2009, 65, 1655-1659.	1.0	2
3220	Scaling factors for carbon NMR chemical shifts obtained from DFT B3LYP calculations. Computational and Theoretical Chemistry, 2009, 893, 1-5.	1.5	82
3221	Change of tautomeric equilibria, intramolecular interactions and Ï€-electron delocalization when going from phenol to uracil. Computational and Theoretical Chemistry, 2009, 894, 103-111.	1.5	16
3222	A density functional study of substituted pyrazole derivatives. Computational and Theoretical Chemistry, 2009, 896, 96-102.	1.5	32
3223	Theoretical studies on the structures, thermodynamic properties, detonation properties, and pyrolysis mechanisms of four trinitrate esters. Computational and Theoretical Chemistry, 2009, 900, 90-95.	1.5	22
3224	Theoretical study on the thermolysis of methyl-3-hydroxypropanoate in m-xylene solution. Computational and Theoretical Chemistry, 2009, 902, 41-48.	1.5	6
3225	Effect of electron-withdrawing group on the [3,3]-sigmatropic rearrangements of 1,5-enynes, 1,5-diynes and 1,2-diene-5-ynes: A theoretical study. Computational and Theoretical Chemistry, 2009, 904, 69-73.	1.5	8
3226	Inter- and intra-molecular OH stretching modes of bicarbonate in aqueous solution. Computational and Theoretical Chemistry, 2009, 913, 236-239.	1.5	9
3227	DFT computational studies of hydrogen bonding-based diastereomeric complexes â€“ Limitations and applications to enantiodifferentiation. Computational and Theoretical Chemistry, 2009, 913, 247-253.	1.5	3
3228	DFT RX3LYP and RPBEPBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands. Computational and Theoretical Chemistry, 2009, 915, 20-32.	1.5	12
3229	The S1â†S0 0â€“0 transition energies of polychlorinated dibenzofurans (PCDFs) revisited: CIS(D) and MP2 calculations with correction for correlation energies. Computational and Theoretical Chemistry, 2009, 915, 79-85.	1.5	4
3230	Computational study to assign structure, tautomerism, E/Z and s-cis/s-trans isomerism, Ï€-delocalization, partial aromaticity, and the ring size of 1,3-thiazolidin-4-ones and 1,3-thiazin-4-ones formed from thiosemicarbazides. Computational and Theoretical Chemistry, 2009, 916, 105-118.	1.5	13
3231	Computational study of simple and water-assisted tautomerism of hydroxamic acids. Computational and Theoretical Chemistry, 2009, 916, 172-179.	1.5	26
3232	Correlations between MO eigenvectors and enthalpies of formation for simple organic substances. Thermochimica Acta, 2009, 495, 14-21.	1.2	0
3233	Raman and DFT study of static, dynamic interactions and isotope effect in pyridazine+H2O/D2O systems. Vibrational Spectroscopy, 2009, 49, 242-250.	1.2	5
3234	Spectroscopic and theoretical study on peramine and some pyrrolopyrazinone compounds. Vibrational Spectroscopy, 2009, 49, 265-273.	1.2	7
3235	Adsorption change of cyclohexyl acetylene on gold nanoparticle surfaces. Vibrational Spectroscopy, 2009, 51, 193-198.	1.2	8
3236	Theoretical studies on polynitro-1,3-bishomopentaprismanes as potential high energy density compounds. Journal of Hazardous Materials, 2009, 166, 931-938.	6.5	40

#	Article	IF	Citations
3237	Determination of the absolute configuration of two estrogenic nonylphenols in solution by chiroptical methods. Journal of Molecular Structure, 2009, 918, 14-18.	1.8	6
3238	Orientations of water molecule and hydronium ion in 1-methylquinolinium-3-carboxy chloride monohydrate studied by X-ray diffraction, DFT calculations, NMR, FTIR and Raman spectra. Journal of Molecular Structure, 2009, 918, 39-54.	1.8	7
3239	The adsorption behavior of two hydroxyl-terminated Schiff bases on the silver surface and the correlated study of SERS effect. Journal of Molecular Structure, 2009, 919, 7-11.	1.8	3
3240	A theoretical IR spectroscopic study based on DFT calculations for free mn-15S2O3 maleonitrile-dithiacrown ether compound. Journal of Molecular Structure, 2009, 919, 128-139.	1.8	2
3241	An effective scaling frequency factor method for scaling of harmonic vibrational frequencies: Application to toluene, styrene and its 4-methyl derivative. Journal of Molecular Structure, 2009, 924-926, 493-503.	1.8	16
3242	Spectroscopic and theoretical study of amlodipine besylate. Journal of Molecular Structure, 2009, 924-926, 385-392.	1.8	23
3243	Vibrational spectra and molecular structure of 3-(piperidine-1-yl-methyl)-1,3-benzoxazol-2(3H)-one molecule by density functional theory and Hartreeâ€“Fock calculations. Journal of Molecular Structure, 2009, 923, 141-152.	1.8	26
3244	5-Benzyl-4-[3-(1H-imidazol-1-yl)propyl]- 2H-1,2,4-triazol-3(4H)-ones: Synthesis, spectroscopic characterization, crystal structure and a comparison of theoretical and experimental IR results by DFT calculations. Journal of Molecular Structure, 2009, 936, 46-55.	1.8	20
3245	Tautomerism, normal coordinate analysis, vibrational assignments, calculated IR, Raman and NMR spectra of adenine. Journal of Molecular Structure, 2009, 938, 263-276.	1.8	57
3246	Ab initio investigation of the hydration of deprotonated amino acids. Journal of the American Society for Mass Spectrometry, 2009, 20, 632-638.	1.2	20
3247	Gas-phase nazarov cyclization of protonated 2-methoxy and 2-hydroxychalcone: An example of intramolecular proton-transport catalysis. Journal of the American Society for Mass Spectrometry, 2009, 20, 805-818.	1.2	26
3248	A reevaluation of computed proton affinities for the common Î±-amino acids. Journal of the American Society for Mass Spectrometry, 2009, 20, 2116-2123.	1.2	66
3249	Thermochemical study of some methoxytetralones. Journal of Chemical Thermodynamics, 2009, 41, 69-73.	1.0	5
3250	Energetics of flavone and flavanone. Journal of Chemical Thermodynamics, 2009, 41, 1408-1412.	1.0	9
3251	Determination of local effects for chloroaluminate ionic liquids on Dielsâ€“Alder reactions. Journal of Molecular Graphics and Modelling, 2009, 28, 95-101.	1.3	22
3252	Synthesis and structure of ferrocenylmethylphosphines, their borane adducts, and some related derivatives. Journal of Organometallic Chemistry, 2009, 694, 2279-2289.	0.8	27
3253	Exploring the oxidative decompositions of methyl esters: Methyl butanoate and methyl pentanoate as model compounds for biodiesel. Proceedings of the Combustion Institute, 2009, 32, 263-270.	2.4	56
3254	Theoretical study of the vibrational spectra of the hydrogen-bonded systems between pyridine-3-carboxamide (nicotinamide) and DMSO. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 71, 1720-1727.	2.0	13

#	Article	IF	Citations
3255	Spectroscopic, quantum chemical DFT/HF study and synthesis of [2.2.1] hept-2â€²-en-2â€²-amino-N-azatricyclo [3.2.1.02,4] octane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 71, 1749-1755.	2.0	35
3256	Experimental, anticancer activity and density functional theory study on the vibrational spectra of 2-(4-fluorobenzylideneamino) propanoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 26-31.	2.0	3
3257	Experimental and CIS, TD-DFT, ab initio calculations of visible spectra and the vibrational frequencies of sulfonyl azide-azoic dyes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 369-377.	2.0	128
3258	Fourier transform infrared and FT-Raman spectra, assignment, ab initio, DFT and normal co-ordinate analysis of 2-chloro-4-methylaniline and 2-chloro-6-methylaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 436-444.	2.0	99
3259	Experimental and density functional theory and ab initio Hartree-Fock study on the vibrational spectra of 5-chloro-6-(4-chlorobenzoyl)-2-benzothiazolinone molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 801-810.	2.0	17
3260	Infrared optical constants, dielectric constants, molar polarizabilities, transition moments, dipole moment derivatives and Raman spectrum of liquid cyclohexane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 947-953.	2.0	25
3261	The spectroscopic (FTIR, FT-IR gas phase and FT-Raman), first order hyperpolarizabilities, NMR analysis of 2,4-dichloroaniline by ab initio HF and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 11-19.	2.0	74
3262	Molecular structure and vibrational and chemical shift assignments of 3-(2-Hydroxyphenyl)-4-phenyl-1H-1,2,4-triazole-5-(4H)-thione by DFT and ab initio HF calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 212-217.	2.0	43
3263	DFT simulations and vibrational analysis of FT-IR and FT-Raman spectra of 2,4-diamino-6-hydroxypyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 642-649.	2.0	23
3264	Infrared spectra prediction and potential energy surface studies of methylarsine and methylstibine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 730-737.	2.0	6
3265	Experimental and theoretical studies on 4-(2,4-dichlorobenzylideneamino)antipyrine and 4-(2,6-dichlorobenzylideneamino)antipyrine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 772-781.	2.0	28
3266	Experimental and theoretical studies on vibrational spectra of 4-(2-furanylmethyleneamino)antipyrine, 4-benzylideneaminoantipyrine and 4-cinnamilideneaminoantipyrine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 892-901.	2.0	50
3267	An exploration of conformational search of leucine molecule and their vibrational spectra in gas phase using ab initio methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 73, 865-870.	2.0	22
3268	Molecular structure, IR spectra of 2-mercaptobenzothiazole and 2-mercaptobenzoxazole by density functional theory and ab initio Hartreeâ€“Fock calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 168-173.	2.0	27
3269	Revised vibrational band assignments for the experimental IR and Raman spectra of 2,3,4-trifluorobenzonitrile based on ab initio, DFT and normal coordinate calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 200-204.	2.0	6
3270	NBO analysis and vibrational spectra of 2,6-bis(p-methyl benzylidene cyclohexanone) using density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 349-356.	2.0	49
3271	Synthesis, structural, vibrational and quantum chemical investigations of N-(2-methylphenyl)-2,2-dichloroacetamide and N-(4-methylphenyl)-2,2-dichloroacetamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 607-616.	2.0	16
3272	Structural, vibrational and DFT studies on 2-chloro-1H-isoindole-1,3(2H)-dione and 2-methyl-1H-isoindole-1,3(2H)-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 642-649.	2.0	46

#	Article	IF	Citations
3273	A theoretical study on the vibrational spectra and thermodynamic properties for the nitro derivatives of phenols. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 569-574.	2.0	22
3274	The spectroscopic FT-IR gas phase, FT-IR, FT-Raman, polarizabilities analysis of Naphthoic acid by density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 704-713.	2.0	48
3275	Experimental FTIR, FT-IR (gas phase), FT-Raman and NMR spectra, hyperpolarizability studies and DFT calculations of 3,5-dimethylpyrazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 788-797.	2.0	84
3276	Vibrational spectra, ab initio/DFT electronic structure calculations, and normal coordinate analysis of 2-bromo-5-fluorobenzaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 74, 1260-1267.	2.0	32
3277	Ultrafast time-resolved absorption spectroscopy of geometric isomers of carotenoids. Chemical Physics, 2009, 357, 4-16.	0.9	54
3278	Cyanoacetylenic complexes as pre-reactional species leading to the HC7N synthesis. Part II: Experimental and theoretical identifications of the HC5N:C2H2 complex. Chemical Physics, 2009, 358, 13-20.	0.9	7
3279	Cyanoacetylenic complexes as pre-reactional species leading to the HC7N synthesis. Part I: Experimental and theoretical identification of the HC3N:C4H2 complexes. Chemical Physics, 2009, 358, 7-12.	0.9	6
3280	Calculations of intermode coupling constants and simulations of amide I, II, and III vibrational spectra of dipeptides. Chemical Physics, 2009, 361, 168-175.	0.9	27
3281	The solidâ€“liquid phase diagrams of binary mixtures of consecutive, even saturated fatty acids. Chemistry and Physics of Lipids, 2009, 160, 85-97.	1.5	75
3282	Theoretical study of cocaine and ecgonine methyl ester in gas phase and in aqueous solution. Chemical Physics Letters, 2009, 467, 249-254.	1.2	9
3283	Investigation of crystalline 2-pyridone using terahertz spectroscopy and solid-state density functional theory. Chemical Physics Letters, 2009, 478, 166-171.	1.2	7
3284	Infrared spectroscopy of protonated ethylene: The nature of proton binding in the non-classical structure. Chemical Physics Letters, 2009, 480, 17-20.	1.2	36
3285	The photophysics of alloxazine: a quantum chemical investigation in vacuum and solution. Photochemical and Photobiological Sciences, 2009, 8, 1655-1666.	1.6	37
3286	Quantum chemical study on the catalytic mechanism of Na/K on NO-char heterogeneous reactions during the coal reburning process. Journal of Zhejiang University: Science A, 2009, 10, 423-433.	1.3	6
3287	How Aromaticity Affects the Chemical and Physicochemical Properties of Heterocycles: A Computational Approach. Topics in Heterocyclic Chemistry, 2009, , 155-202.	0.2	16
3288	Alkyl Radicals as Hydrogen Bond Acceptors: Computational Evidence. Journal of the American Chemical Society, 2009, 131, 8627-8635.	6.6	49
3289	Looking for High Energy Density Compounds among 1,3-Bishomopentaprismane Derivatives with CN, NC, and ONO2 Groups. Journal of Physical Chemistry A, 2009, 113, 2607-2614.	1.1	37
3290	Quantum chemical study of valence isomerization of bis(5-thioxopenta-1,3-dien-1-yl) sulfide in the ground and excited states. Russian Journal of General Chemistry, 2009, 79, 972-979.	0.3	1

#	Article	IF	Citations
3291	Quantum-chemical investigation of the formation of 1,3-diiodoacetone at the photoinitiated disproportionation of 1-iodoacetone. Russian Journal of Organic Chemistry, 2009, 45, 1610-1615.	0.3	0
3292	Standardless structural-group analysis of supramolecular systems. Journal of Analytical Chemistry, 2009, 64, 1000-1006.	0.4	4
3293	Formation and Calculations of the Simple Terminal Triplet Pnictinidene Molecules NÃ·MF₃, PÃ·MF₃, and AsÃ·MF₃ (M = Ti, Zr, Hf). Inorganic Chemistry, 2009, 48, 6297-6302.	1.9	14
3294	Infrared Spectra of Platinum Insertion and Methylidene Complexes Prepared in Oxidative Câ^'H(X) Reactions of Laser-Ablated Pt Atoms with Methane, Ethane, and Halomethanes. Organometallics, 2009, 28, 1358-1368.	1.1	59
3295	Energetics of Hydroxytetralones: A Calorimetric and Computational Thermochemical Study. Journal of Chemical & Engineering Data, 2009, 54, 2189-2194.	1.0	4
3296	1-Pyridine- and 1-Quinuclidine-1-boraadamantane as Models for Derivatives of 1-Borabicyclo[2.2.2]octane. Experimental and Theoretical Evaluation of the Bâ^'N Fragment as a Polar Isosteric Substitution for the Câ^'C Group in Liquid Crystal Compounds. Journal of Organic Chemistry, 2009, 74, 1709-1720.	1.7	20
3297	From Classical Adducts to Frustrated Lewis Pairs: Steric Effects in the Interactions of Pyridines and B(C₆F₅)₃. Inorganic Chemistry, 2009, 48, 10466-10474.	1.9	122
3298	Aggregation Models of Potential Cyclical Trimethylsulfonium Dicyanamide Ionic Liquid Clusters. Journal of Physical Chemistry B, 2009, 113, 2031-2041.	1.2	16
3299	Combustion Pathways of the Alkylated Heteroaromatics: Bond Dissociation Enthalpies and Alkyl Group Fragmentations. Journal of Physical Chemistry A, 2009, 113, 12370-12379.	1.1	13
3300	Hydration Modes of an Amphiphilic Molecule: NMR, FTIR, and Theoretical Study of the Interactions in the Waterâ^'Lutidine System. Journal of Physical Chemistry B, 2009, 113, 11950-11958.	1.2	10
3301	Density Functional Theory Calculation of Bonding and Charge Parameters for Molecular Dynamics Studies on [FeFe] Hydrogenases. Journal of Chemical Theory and Computation, 2009, 5, 1137-1145.	2.3	76
3302	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide. 5. Thermodynamics and Kinetics of Unimolecular Decomposition. Journal of Physical Chemistry A, 2009, 113, 6398-6403.	1.1	30
3303	Vanadium Oxides Supported on a Thin Silica Film Grown on Mo(112): Insights from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 8336-8342.	1.5	17
3304	Does Tetrahydrofuran Ring Open upon Ionization and Dissociation? A TPES and TPEPICO Investigation. Journal of Physical Chemistry A, 2009, 113, 10923-10932.	1.1	14
3305	A Second Metal Center Enhances the Reactivity of an Organomagnesate: Comparison of the Gas-Phase Reactions of Water with [RCCMgCl2]â^' and [RCCMg2Cl4]â^' (R = H, Ph). Organometallics, 2009, 28, 5002-5011.	1.1	29
3306	A Reactive Molecular Dynamics Study of the Thermal Decomposition of Perfluorodimethyl Ether. Journal of Physical Chemistry B, 2009, 113, 13670-13677.	1.2	15
3307	Investigation of Gaussian4 Theory for Transition Metal Thermochemistry. Journal of Physical Chemistry A, 2009, 113, 5170-5175.	1.1	65
3308	Theoretical Study of Mechanism of 2,3-Dihydro-1,5-benzodiazepin-2-ones Hydrazinolysis. Journal of Physical Chemistry A, 2009, 113, 1475-1480.	1.1	6

#	Article	IF	Citations
3309	Ion-Pair Binding Energies of Ionic Liquids: Can DFT Compete with Ab Initio-Based Methods?. Journal of Physical Chemistry A, 2009, 113, 7064-7072.	1.1	163
3310	Study of the S₁ Excited State of para-Methoxy-3-phenyl-3-methyl Diazirine by Ultrafast Time Resolved UVâ^'Vis and IR Spectroscopies and Theory. Journal of the American Chemical Society, 2009, 131, 13784-13790.	6.6	33
3311	Gas-Phase Protonation Thermochemistry of Glutamic Acid. Journal of Physical Chemistry A, 2009, 113, 6666-6676.	1.1	27
3312	DENSITY FUNCTIONAL THEORY STUDY OF STRUCTURE AND ELECTRIC PROPERTIES OF POLY(VINYLIDENE) Tj ETQq1 1 0.784314 rgBT /C	0.8	6
3313	Ab Initio Study of the Geometry, Stability, and Aromaticity of the Cyclic S2N3+ Cation Isomers and Their Isoelectronic Analogues. Inorganic Chemistry, 2009, 48, 6773-6780.	1.9	15
3314	Attractionâ^'Repulsion Mechanism for Carbon Monoxide Adsorption on Platinum and Platinumâ^'Ruthenium Alloys. Journal of Physical Chemistry C, 2009, 113, 18730-18739.	1.5	47
3315	Experimental and Theoretical Investigation of Simple Terminal Group 6 Arsenide Asâ‰¡MF3 Molecules. Journal of Physical Chemistry A, 2009, 113, 6064-6069.	1.1	6
3316	Infrared spectra, structure and bonding in the LiO₂, LiO₂Li, LiO and Li₂O molecules in solid neon. Molecular Physics, 2009, 107, 739-748.	0.8	49
3317	A Synergy between Experiment and Theory for the Formation of Pyridine and Pyrrole Derivatives from Selected Butadienes and Organolithium Reagents: Mechanism, Solvent, and Substituent Effect. Organometallics, 2009, 28, 5848-5856.	1.1	7
3318	Adsorbed CO on Group 10 Metal Fragments: A DFT Study. Journal of Chemical Information and Modeling, 2009, 49, 1223-1233.	2.5	6
3319	CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures. Journal of Physical Chemistry A, 2009, 113, 3555-3559.	1.1	188
3320	Matrix Infrared Spectra of the Câ^'H Insertion and Dihydrido Cyclic Products from Reactions of Group 3 Metal Atoms with Ethylene. Journal of Physical Chemistry A, 2009, 113, 6677-6688.	1.1	7
3321	Hydrolysis and Photolysis of 4-Acetoxy-4-(benzothiazol-2-yl)-2,5-cyclohexadien-1-one, a Model Anti-Tumor Quinol Ester. Journal of Organic Chemistry, 2009, 74, 4463-4471.	1.7	13
3322	Theoretical Insights into the Hydrated (10.4) Calcite Surface: Structure, Energetics, and Bonding Relationships. Langmuir, 2009, 25, 6813-6824.	1.6	60
3323	Infrared Spectra and Density Functional Calculations of the SUO2 Molecule. Inorganic Chemistry, 2009, 48, 6888-6895.	1.9	23
3324	Peroxo-Type Intermediates in Class I Ribonucleotide Reductase and Related Binuclear Non-Heme Iron Enzymes. Journal of the American Chemical Society, 2009, 131, 12155-12171.	6.6	41
3325	Mechanistic Aspects of the Formation of Guanidinohydantoin from Spiroiminodihydantoin under Acidic Conditions. Chemical Research in Toxicology, 2009, 22, 526-535.	1.7	27
3326	Sulfur versus Oxygen Reactivity of Organic Molecules at the Ge(100)-2Ã—1 Surface. Journal of the American Chemical Society, 2009, 131, 7005-7015.	6.6	33

#	Article	IF	Citations
3327	Exploring 1,2-Hydrogen Shift in Silicon Nanoparticles: Reaction Kinetics from Quantum Chemical Calculations and Derivation of Transition State Group Additivity Database. Journal of Physical Chemistry A, 2009, 113, 10933-10946.	1.1	34
3328	Acryloyl Chloride and Acryloyl Isocyanate (CH₂â•CHC(O)X, X = Cl, NCO): A HeI Photoelectron Spectroscopy and Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3108-3115.	1.1	6
3329	Rate Constants for OH with Selected Large Alkanes: Shock-Tube Measurements and an Improved Group Scheme. Journal of Physical Chemistry A, 2009, 113, 5047-5060.	1.1	111
3330	A Density Functional Study of the Interaction of NCO with Small Copper Clusters. Journal of Physical Chemistry A, 2009, 113, 1075-1085.	1.1	16
3331	Theoretical Calculation of Separation Factors for Boron Isotopic Exchange between BF3 and BF3Â·C6H5OCH3. Journal of Physical Chemistry A, 2009, 113, 7267-7274.	1.1	6
3332	Methyl t-Butyl Ether and Methyl Trimethylsilyl Ether Ions Dissociate near Their Ionization Thresholds: A TPES, TPEPICO, RRKM, and G3 Investigation. Journal of Physical Chemistry A, 2009, 113, 5823-5831.	1.1	7
3333	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes. Organometallics, 2009, 28, 5623-5632.	1.1	31
3334	Coordination of (Glycyl)_nglycine (n= 1â“3) to Co⁺and Co²⁺. Journal of Physical Chemistry A, 2009, 113, 8883-8892.	1.1	9
3335	Raman Study of Chromophore States in Photochromic Fluorescent Proteins. Journal of the American Chemical Society, 2009, 131, 96-103.	6.6	41
3336	Matrix Infrared Spectra of Dihydrido Cyclic and Trihydrido Ethynyl Products from Reactions of Th and U Atoms with Ethylene Molecules. Journal of Physical Chemistry A, 2009, 113, 5073-5081.	1.1	13
3337	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Palladium Atoms with Halomethanes. Organometallics, 2009, 28, 6871-6879.	1.1	19
3338	Revisiting the Hydration of Pb(II): A QMCF MD Approach. Journal of Physical Chemistry B, 2009, 113, 13007-13013.	1.2	38
3339	Experimental and Theoretical Investigation into the Formation and Reactivity of M(Cp)(CO)₂(CO₂) (M = Mn or Re) in Liquid and Supercritical CO₂ and the Effect of Different CO₂ Coordination Modes on Reaction Rates with CO, H₂, and N₂. Organometallics, 2009, 28, 3113-3122.	1.1	13
3340	Infrared Spectra and Theoretical Calculations for Fe, Ru, and Os Metal Hydrides and Dihydrogen Complexes. Journal of Physical Chemistry A, 2009, 113, 551-563.	1.1	26
3341	Kinetics and Mechanism for Formation of Enols in Reaction of Hydroxide Radical with Propene. Journal of Physical Chemistry A, 2009, 113, 2372-2382.	1.1	46
3342	Toward Detecting the Formation of a Single Helical Turn by 2D IR Cross Peaks between the Amide-I and -II Modes. Journal of Physical Chemistry B, 2009, 113, 11775-11786.	1.2	33
3343	Ozone Oxidation of Single Walled Carbon Nanotubes from Density Functional Theory. Journal of Physical Chemistry C, 2009, 113, 17636-17642.	1.5	45
3344	Computational Studies of Pericyclic Reactions between Aminoalanes and Ethyne, Ethene, and Dienes. A Reactive Aminoalane That Should Prefer [2 + 2] and [4 + 2] Cyclizations to Dimerization. Organometallics, 2009, 28, 787-794.	1.1	5

#	Article	IF	Citations
3345	Vibrational Modes of the Vinyl and Deuterated Vinyl Radicals. Journal of Physical Chemistry A, 2009, 113, 8857-8870.	1.1	23
3346	Understanding the solid-state forms of fenofibrate â€“ A spectroscopic and computational study. European Journal of Pharmaceutics and Biopharmaceutics, 2009, 71, 100-108.	2.0	85
3347	Theoretical prediction for several important equilibrium Ge isotope fractionation factors and geological implications. Earth and Planetary Science Letters, 2009, 287, 1-11.	1.8	72
3348	Isotopic fractionations associated with phosphoric acid digestion of carbonate minerals: Insights from first-principles theoretical modeling and clumped isotope measurements. Geochimica Et Cosmochimica Acta, 2009, 73, 7203-7225.	1.6	224
3349	Hydration in solution is critical for stable oxygen isotope fractionation between carbonate ion and water. Geochimica Et Cosmochimica Acta, 2009, 73, 5283-5291.	1.6	40
3350	Equilibrium 2H/1H fractionations in organic molecules: I. Experimental calibration of ab initio calculations. Geochimica Et Cosmochimica Acta, 2009, 73, 7060-7075.	1.6	38
3351	Vibrational properties of two fullereneâ€“thiophene-based dyads. Synthetic Metals, 2009, 159, 2539-2543.	2.1	13
3352	Raman crystallography of RNA. Methods, 2009, 49, 101-111.	1.9	30
3353	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	0.8	96
3354	Stereospecificity of Dielsâ€“Alder Reactions Validated Using Ab Initio Calculations: Synthesis of Novel Coumarin and Phenanthridine Derivatives. Synthetic Communications, 2009, 39, 2954-2972.	1.1	14
3355	Predicting Raman Spectra Using Density Functional Theory. Applied Spectroscopy, 2009, 63, 733-741.	1.2	29
3356	Computed Rate Coefficients and Product Yields for c-C₅H₅ + CH₃ â†' Products. Journal of Physical Chemistry A, 2009, 113, 8871-8882.	1.1	72
3357	Molecular structure, vibrational spectra and HOMO, LUMO analysis of 4-piperidone by density functional theory andab initioHartreeâ€“Fock calculations. Molecular Simulation, 2009, 35, 705-713.	0.9	18
3358	IR Spectroscopy and Theory of Cu+(H2O)Ar2 and Cu+(D2O)Ar2 in the Oâ^'H (Oâ^'D) Stretching Region: Fundamentals and Combination Bands. Journal of Physical Chemistry A, 2009, 113, 4849-4854.	1.1	55
3359	Periodic Trends and Index of Boron Lewis Acidity. Journal of Physical Chemistry A, 2009, 113, 5985-5992.	1.1	79
3360	A Comparative Ab Initio and DFT Study of Polyaniline Leucoemeraldine Base and Its Oligomers. Journal of Physical Chemistry B, 2009, 113, 14629-14639.	1.2	33
3361	A spectroscopic and DFT study of thiophene-substituted metalloporphyrins as dye-sensitized solar cell dyes. Physical Chemistry Chemical Physics, 2009, 11, 5598.	1.3	71
3362	Multidimensional Exploration of Valleyâ^'Ridge Inflection Points on Potential-Energy Surfaces. Journal of the American Chemical Society, 2009, 131, 2530-2540.	6.6	56

#	Article	IF	Citations
3363	Transient Complex Formation in CO₂â^'Hexafluorobenzene Mixtures: a Combined Raman and ab Initio Investigation. Journal of Physical Chemistry A, 2009, 113, 184-192.	1.1	19
3364	Spectroscopic investigation of the species involved in the rhodium-catalyzed oxidative carbonylation of toluene to toluic acid. Physical Chemistry Chemical Physics, 2009, 11, 9903.	1.3	13
3365	Combining Metal Stable Isotope Fractionation Theory with Experiments. Elements, 2009, 5, 369-374.	0.5	47
3366	Synthesis and characterization of two new halo complexes of iodine: (C4H9)4N[I2Br]â^'and (C4H9)4N[I2Cl]â^'and theoretical calculations of their structures. Main Group Chemistry, 2009, 8, 299-306.	0.4	3
3367	Ab Initio Thermochemistry with High-Level Isodesmic Corrections: Validation of the ATOMIC Protocol for a Large Set of Compounds with First-Row Atoms (H, C, N, O, F). Journal of Physical Chemistry A, 2009, 113, 11517-11534.	1.1	30
3368	Photochromic optical memory based on non-destructive IR read-out. Photochemical and Photobiological Sciences, 2009, 8, 1590-1594.	1.6	3
3369	Meta-Substituted Thienyl Benzenes: A Comparative Synthetic, Structural and Computational Study. Journal of Organic Chemistry, 2009, 74, 530-544.	1.7	14
3370	Synthesis and properties of 5-nitrotetrazole derivatives as new energetic materials. Journal of Materials Chemistry, 2009, 19, 2240.	6.7	76
3371	Photophysics of phenalenone: quantum-mechanical investigation of singletâ€"triplet intersystem crossing. Physical Chemistry Chemical Physics, 2009, 11, 1688.	1.3	31
3372	CHARMM Additive All-Atom Force Field for Acyclic Polyalcohols, Acyclic Carbohydrates, and Inositol. Journal of Chemical Theory and Computation, 2009, 5, 1315-1327.	2.3	150
3373	Alkali and transition metal (Ag, Cu) salts of bridged 5-nitrotetrazole derivatives for energetic applications. Dalton Transactions, 2009, , 1825.	1.6	51
3374	Formation of carbyne complexes in reactions of laser-ablated Os atoms with halomethanes: characterization by Câ€"H(X) and Osâ€"H(X) stretching absorptions and computed structures. Dalton Transactions, 2009, , 5858-5866.	1.6	22
3375	Vibrations of Silica Supported Vanadia: Variation with Particle Size and Local Surface Structure. Journal of Physical Chemistry C, 2009, 113, 12454-12464.	1.5	34
3376	Surface-enhanced Raman scattering of 5-fluorouracil adsorbed on silver nanostructures. Physical Chemistry Chemical Physics, 2009, 11, 7437.	1.3	23
3377	Inclusion Mechanism of Steroid Drugs into Î²-Cyclodextrins. Insights from Free Energy Calculations. Journal of Physical Chemistry B, 2009, 113, 7836-7843.	1.2	56
3378	Energetics of Coumarin and Chromone. Journal of Physical Chemistry B, 2009, 113, 11216-11221.	1.2	38
3379	Beryllium(II): The Strongest Structure-Forming Ion in Water? A QMCF MD Simulation Study. Journal of Physical Chemistry B, 2009, 113, 9289-9295.	1.2	39
3380	Infrared Spectra and Density Functional Theory Calculations of Group 10 Transition Metal Sulfide Molecules and Complexes. Journal of Physical Chemistry A, 2009, 113, 3336-3343.	1.1	21

#	Article	IF	Citations
3381	Density Functional Theory Study of the Stability and Vibrational Spectra of the Î²-Carotene Isomers. Journal of Physical Chemistry A, 2009, 113, 9899-9907.	1.1	24
3382	Charge Transport Parameters and Structural and Electronic Properties of Octathio[8]circulene and Its Plate-like Derivatives. Journal of Physical Chemistry A, 2009, 113, 255-262.	1.1	35
3383	Intramolecular and Intermolecular Hydrogen Bond Formation by Some Ortho-Substituted Phenols: Some Surprising Results from an Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2009, 113, 6275-6288.	1.1	47
3384	Consequences of Acid Strength for Isomerization and Elimination Catalysis on Solid Acids. Journal of the American Chemical Society, 2009, 131, 6554-6565.	6.6	138
3385	Synthesis and Reactivity of [closo-1-CB₉H₉-1-N₂]: Functional Group Interconversion at the Carbon Vertex of the {closo-1-CB₉} Cluster. Inorganic Chemistry, 2009, 48, 7313-7329.	1.9	21
3386	Experimental IR study andab initiomodelling of ethylene adsorption in a MFI-type host zeolite. Molecular Physics, 2009, 107, 2081-2093.	0.8	6
3387	Infrared Spectra and Density Functional Calculations for SMO₂ Molecules (M = Cr, Mo,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.1	12
3388	Fluoxetine and Norfluoxetine Revisited: New Insights into the Electrochemical and Spectroscopic Properties. Journal of Physical Chemistry A, 2009, 113, 9934-9944.	1.1	23
3389	Heat-Set Poly(ethylacrylic acid) Nanoparticles: Combined Light Scattering, Calorimetric, and FTIR Study. Macromolecules, 2009, 42, 7439-7446.	2.2	13
3390	The Quinones of Benzocyclobutadiene: A Computational Study. Journal of Physical Chemistry A, 2009, 113, 9485-9500.	1.1	9
3391	Fluorine substituent effects on dihydrogen bonding of transition metal hydrides. Physical Chemistry Chemical Physics, 2009, 11, 7231.	1.3	10
3392	Interaction of Water Highly Diluted in 1-Alkyl-3-methyl Imidazolium Ionic Liquids with the PF6â^' and BF4â^' Anions. Journal of Physical Chemistry A, 2009, 113, 2873-2889.	1.1	113
3393	Toward an Understanding of the Unexpected Regioselective Hetero-Dielsâ^'Alder Reactions of Asymmetric Tetrazines with Electron-Rich Ethylenes: A DFT Study. Journal of Organic Chemistry, 2009, 74, 2726-2735.	1.7	92
3394	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2996-3009.	2.3	21
3395	Molecular dynamics study of zinc binding to cysteines in a peptide mimic of the alcohol dehydrogenase structural zinc site. Physical Chemistry Chemical Physics, 2009, 11, 975-983.	1.3	54
3396	Gas-Phase Facial Diastereoselectivity of Equatorial and Axial 4-Chloro-adamant-2-yl Cations. Journal of Organic Chemistry, 2009, 74, 5135-5144.	1.7	6
3397	DFT Investigation of Intermediate Steps in the Hydrolysis of Î±-Al₂O₃(0001). Journal of Physical Chemistry C, 2009, 113, 2149-2158.	1.5	81
3398	Experimental and density functional studies on 4-(4-cyanobenzylideneamino)antipyrine. Molecular Physics, 2009, 107, 223-235.	0.8	113

#	Article	IF	Citations
3399	Vibrational analysis of glycine radical: a comparative ab initio static and dynamic study. Physical Chemistry Chemical Physics, 2009, 11, 4375.	1.3	31
3400	Singlet oxygen quenching and radical scavenging capacities of structurally-related flavonoids present in Zuccagnia punctata Cav.. Free Radical Research, 2009, 43, 553-564.	1.5	42
3401	An integrated experimental and theoretical investigation on Cu(hfa)2Â·TMEDA: structure, bonding and reactivity. Physical Chemistry Chemical Physics, 2009, 11, 5998.	1.3	43
3402	Substituent effect on the interaction of aromatic primary amines and diamines with supercritical CO2 from infrared spectroscopy and quantum calculations. Physical Chemistry Chemical Physics, 2009, 11, 5052.	1.3	17
3403	Infrared spectra and density functional calculations of triplet pnictinidene NÃ·ThF3, PÃ·ThF3 and AsÃ·ThF3 molecules. Dalton Transactions, 2009, , 9260.	1.6	19
3404	Quantum mechanical study and vibrational spectra of indazolium-3-carboxylate and its decarboxylation product, the N-heterocyclic carbene indazol-3-ylidene. Physical Chemistry Chemical Physics, 2009, 11, 341-348.	1.3	5
3405	Photoinduced linkage isomerism of {RuNO}6 complexes with bioligands and related chelators. Dalton Transactions, 2009, , 1034.	1.6	23
3406	Detection and kinetics of the single-crystal to single-crystal complete transformation of a thiiranium ion into thietanium ion. Physical Chemistry Chemical Physics, 2009, 11, 7181.	1.3	7
3407	The ab initio assigning of the vibrational probing modes of tryptophan: linear shifting of approximate anharmonic frequencies vs. multiplicative scaling of harmonic frequencies. Physical Chemistry Chemical Physics, 2009, 11, 3921.	1.3	10
3408	The unusual reactivity of benzene and monosubstituted benzenes towards tetracyanoethylene oxide: a theoretical study. New Journal of Chemistry, 2009, 33, 471-478.	1.4	2
3409	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(i) oxidation state. Physical Chemistry Chemical Physics, 2009, 11, 10219.	1.3	28
3410	Molecular and electronic structures of acryloyl isothiocyanate, CH2CHC(O)NCS: a joint experimental and theoretical study. New Journal of Chemistry, 2009, 33, 2155.	1.4	4
3411	A Potential Mechanism for Cu²⁺Reduction, Î²-Cleavage, and Î²-Sheet Initiation Within The N-Terminal Domain of the Prion Protein: Insights from Density Functional Theory and Molecular Dynamics Calculations. Journal of Toxicology and Environmental Health - Part A: Current Issues, 2009, 72, 1040-1059.	1.1	17
3412	A theoretical study of the rearrangement processes of energized CCCB and CCCAl. Physical Chemistry Chemical Physics, 2009, 11, 7553.	1.3	10
3413	The effect of water on infrared spectra of DNA. Journal of Physics Condensed Matter, 2009, 21, 064242.	0.7	10
3414	Computational study of substituted 2,2â€²-bi-1H-imidazole as high energetic materials. Computational and Theoretical Chemistry, 2009, 907, 29-34.	1.5	6
3415	Asâ‰¡UF3 Molecule with a Weak Triple Bond to Uranium. Inorganic Chemistry, 2009, 48, 6594-6598.	1.9	23
3416	Mechanism of Hydrogen Peroxide Production by Copper-Bound Amyloid Beta Peptide: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 1202-1209.	1.2	64

#	Article	IF	Citations
3417	Structures and Properties of Closed Ladderanes C₂₄H₂₄, Laddersilanes Si₂₄H₂₄, and Their Nitrogen-Containing Isoelectronic Equivalents: A G3(MP2) Investigation. Journal of Physical Chemistry A, 2009, 113, 3413-3419.	1.1	5
3418	Kinetic and thermodynamic control in the stereoselective formation of trans- and cis-2-ferrocenyl-3-pivaloyl-4-alkyl-1,3-oxazolidin-5-ones. Organic and Biomolecular Chemistry, 2009, 7, 518-526.	1.5	8
3419	NMR and molecular modeling of the dimeric self-association of the enantiomers of 1,1â€²-bi-2-naphthol and 1-phenyl-2,2,2-trifluoroethanol in the solution state and their relevance to enantiomer self-disproportionation on achiral-phase chromatography (ESDAC). Organic and Biomolecular Chemistry, 2009, 7, 537-542.	1.5	48
3420	Structure and molecular dynamics of crystalline and liquid anthracene and naphthalene: Possible transient rotator phase of naphthalene. Journal of Chemical Physics, 2009, 130, 124501.	1.2	9
3421	Molecular Design of 1,2,4,5-Tetrazine-Based High-Energy Density Materials. Journal of Physical Chemistry A, 2009, 113, 9404-9412.	1.1	180
3422	Tautomerism and Regioselectivity of Acylation of 4-Hydroxy-2-mercaptopyridine-N-oxide and 2,4-Dimercaptopyridine-N-oxide: A Computational Study. Phosphorus, Sulfur and Silicon and the Related Elements, 2009, 184, 1296-1306.	0.8	3
3423	CHARMM Additive All-Atom Force Field for Glycosidic Linkages between Hexopyranoses. Journal of Chemical Theory and Computation, 2009, 5, 2353-2370.	2.3	578
3424	Mononuclear Platinum(II) Complexes Incorporating Î²²-Carboxylate Ligands: Synthesis, Structure, and Reactivity. Inorganic Chemistry, 2009, 48, 6972-6978.	1.9	13
3425	Intersystem Crossings of the Triplet and Singlet States in Cobalt and Copper Mononitrosyls. Journal of Physical Chemistry A, 2009, 113, 11266-11272.	1.1	7
3426	Experimental and Theoretical Investigation Into Hydrogen Storage via Spillover in IRMOF-8. Journal of Physical Chemistry C, 2009, 113, 3222-3231.	1.5	68
3427	IR Spectroscopy andab initiocalculations of imidazophenazine and its derivatives in a low-temperature argon matrix. Low Temperature Physics, 2009, 35, 491-502.	0.2	2
3428	Photolysis of 1,2-Naphthoquinone in Oxygen-Doped Argon Matrix at Low Temperature. Bulletin of the Chemical Society of Japan, 2009, 82, 737-742.	2.0	2
3429	Extension of Density Functional Theory to Nuclear Orbital plus Molecular Orbital Theory: Self-Consistent Field Calculations with the Colleâ€“Salvetti Electronâ€“Nucleus Correlation Functional. Bulletin of the Chemical Society of Japan, 2009, 82, 1133-1139.	2.0	22
3431	From Molecular Vibrations to Bonding, Chemical Reactions, and Reaction Mechanism. Current Organic Chemistry, 2010, 14, 1524-1560.	0.9	139
3432	A Computational Study of the Radical Ring-Opening Polymerization of Diphosphetanes. Australian Journal of Chemistry, 2010, 63, 1189.	0.5	4
3433	Adventures of Quantum Chemistry in the Realm of Inorganic Chemistry. , 2010, , 83-127.		0
3434	Effect of Nematic Conformation on the Stability of Segmented Main-Chain Liquid Crystals. Kobunshi Ronbunshu, 2010, 67, 254-262.	0.2	1
3435	Synthesis, Structures, and Reactivity of Kinetically Stabilized Anthryldiphosphene Derivatives. Bulletin of the Chemical Society of Japan, 2010, 83, 456-478.	2.0	18

#	Article	IF	Citations
3436	Stereochemistry of seven-membered heterocycles: XLVII. Synthesis, NMR, XRD, and theoretical investigation of monosulfoxides of (Z)-4,7-dihydro-1Î»4,3-dithiepine series. Russian Journal of Organic Chemistry, 2010, 46, 246-251.	0.3	1
3437	Heterocumulenes reactions with organometallic reagents: XV. Quantum-chemical investigatiom of skeleton rearrangements of 2-methyl-6-methoxy-3H-azepine originating from valence tautomerism. Russian Journal of Organic Chemistry, 2010, 46, 722-739.	0.3	3
3438	Reactions of heterocumulenes with organometallic reagents: XVI. Quantum-chemical study on the mechanisms of formation of homo- and heteroannular azacycloheptadienes in reactions of 2-aza-1,3,5-trienes with potassium tert-butoxide. Russian Journal of Organic Chemistry, 2010, 46, 1848-1857.	0.3	1
3439	Vibrational spectroscopic and conformational studies of 1-(4-pyridyl)piperazine. Chemical Papers, 2010, 64, .	1.0	3
3440	A theoretical and spectroscopic study of Î³-crystalline and amorphous indometacin. Journal of Pharmacy and Pharmacology, 2010, 59, 261-269.	1.2	68
3441	Simulation of Hopping Transport Based on Charge Carrier Localization Times Derived for a Two-Level System. Journal of Physical Chemistry C, 2010, 114, 20424-20430.	1.5	11
3442	Density Functional Theory Study of Several Nitrotriazole Derivatives. Journal of Energetic Materials, 2010, 28, 251-272.	1.0	13
3443	Importance of selenium in antioxidant behavior of ebselen: A theoretical study. Computational and Theoretical Chemistry, 2010, 939, 118-123.	1.5	2
3444	Linear Free-Energy Relationships for the Alkyl Radical Affinities of Nitroxides: A Theoretical Study. Macromolecules, 2010, 43, 3728-3743.	2.2	47
3445	Side Reactions of Nitroxide-Mediated Polymerization: Nâ˜O versus Oâ˜C Cleavage of Alkoxyamines. Journal of Physical Chemistry A, 2010, 114, 10458-10466.	1.1	57
3446	A Quantum Mechanical Study of Methacrylate Free-Radical Polymerizations. Journal of Physical Chemistry A, 2010, 114, 10988-10996.	1.1	6
3447	Development of Detailed Kinetic Models for the Thermal Conversion of Biomass via First Principle Methods and Rate Estimation Rules. ACS Symposium Series, 2010, , 201-243.	0.5	23
3448	Synthesis and Properties of N₇O⁺. Inorganic Chemistry, 2010, 49, 1245-1251.	1.9	15
3449	A universal approach for continuum solvent pK a calculations: are we there yet?. Theoretical Chemistry Accounts, 2010, 125, 3-21.	0.5	408
3450	Computational methods for analysis of an unsaturated carbocycle: heptafulvene. Theoretical Chemistry Accounts, 2010, 126, 55-73.	0.5	8
3451	The sodium cation-bound dimer of theophylline: IRMPD spectroscopy of a highly symmetric electrostatically bound species. International Journal of Mass Spectrometry, 2010, 297, 76-84.	0.7	19
3452	Understanding excited-state structure in metal polypyridyl complexes using resonance Raman excitation profiles, time-resolved resonance Raman spectroscopy and density functional theory. Coordination Chemistry Reviews, 2010, 254, 2505-2518.	9.5	72
3453	Molecular first order hyperpolarizability and vibrational spectral investigation of Warfarin sodium. Chemical Physics, 2010, 378, 88-102.	0.9	11

#	Article	IF	Citations
3454	Molecular structure and vibrational bands and chemical shift assignments of 4-allyl-5-(2-hydroxyphenyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione by DFT and ab initio HF calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 189-198.	2.0	80
3455	Molecular structure, vibrational spectra and DFT molecular orbital calculations (TD-DFT and NMR) of the antiproliferative drug Methotrexate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 264-275.	2.0	55
3456	Vibrational spectroscopic study and NBO analysis on bis(4-amino-5-mercapto-1,2,4-triazol-3-yl) methane using DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 877-884.	2.0	48
3457	Vibrational spectroscopic analysis of 2-chlorotoluene and 2-bromotoluene: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 1005-1013.	2.0	48
3458	Theoretical investigation of double-bond isomerization of 1-hexene to trans-2-hexene on H-ZSM-5 zeolite. Computational and Theoretical Chemistry, 2010, 940, 135-139.	1.5	4
3459	Crystal structure landscapes from combined vibrational spectroscopy and ab initio calculations: 4-(Dimethylamino)benzaldehyde. Computational and Theoretical Chemistry, 2010, 946, 65-69.	1.5	12
3460	Static and dynamic reaction pathways involved in the reaction of Oâ˙ and CH3F. Computational and Theoretical Chemistry, 2010, 947, 1-8.	1.5	6
3461	DFT study on energetic tetrazolo-[1,5-b]-1,2,4,5-tetrazine and 1,2,4-triazolo-[4,3-b]-1,2,4,5-tetrazine derivatives. Journal of Hazardous Materials, 2010, 179, 581-590.	6.5	115
3462	Simultaneous quantitative analysis of mebendazole polymorphs Aâ€“C in powder mixtures by DRIFTS spectroscopy and ANN modeling. Journal of Pharmaceutical and Biomedical Analysis, 2010, 51, 512-520.	1.4	37
3463	Theoretical and experimental vibrational spectroscopic study of 4-(1-Pyrrolidinyl)piperidine. Journal of Molecular Structure, 2010, 966, 1-7.	1.8	49
3464	Monitoring the Î±â†'Î² solidâ€“solid phase transition of RDX with Raman spectroscopy: A theoretical and experimental study. Journal of Molecular Structure, 2010, 970, 51-58.	1.8	57
3465	Molecular structure and vibrational and chemical shift assignments of 3,5-bis-(4-methylbenzoyl)-2,6-bis(4-methylphenyl)-4H-pyran-4-one: A combined experimental and theoretical analysis. Journal of Molecular Structure, 2010, 975, 234-241.	1.8	2
3466	Optical properties and ab initio study on the hybrid organicâ€“inorganic material [(CH3)2NH2]3[Bil6]. Journal of Molecular Structure, 2010, 977, 72-77.	1.8	45
3467	An experimental and theoretical approach to molecular structure of 4-benzoyl-5-phenyl-1-p-methoxyphenyl-1H-pyrazole-3-carboxylic acid methanol solvate. Journal of Molecular Structure, 2010, 980, 1-6.	1.8	21
3468	Ab initio Hartreeâ€“Fock and density functional theory investigations on the conformational stability, molecular structure and vibrational spectra of 3-(2-(4-methylpiperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one. Journal of Molecular Structure, 2010, 980, 230-244.	1.8	29
3469	Experimental and theoretical study of 4-cyanobenzaldehyde isonicotinoyl-hydrazone monohydrate. Journal of Molecular Structure, 2010, 984, 389-395.	1.8	6
3470	Steric hindrance effect of the equatorial ligand on Fe(IV)O and Ru(IV)O complexes: a density functional study. Journal of Biological Inorganic Chemistry, 2010, 15, 351-359.	1.1	18
3471	Hydrogen bonding interactions in PNÂ·Â·Â·HX complexes: DFT and ab initio studies of structure, properties and topology. Journal of Molecular Modeling, 2010, 16, 965-974.	0.8	13

#	Article	IF	Citations
3472	Ab initio studies on the reactivity of the CF3OCH2O radical: Thermal decomposition vs. reaction with O2. Journal of Molecular Modeling, 2010, 16, 1473-1480.	0.8	21
3473	Formation of the silylene-bridged complex Fe2(CO)6(Î¼2-SiCl2)3 from cis-Fe(CO)4(SiCl3)2: an experimental and computational study. Monatshefte FÃ¼r Chemie, 2010, 141, 671-675.	0.9	7
3474	Quantum chemical investigation of nitrotyrosine (3-nitro-l-tyrosine) and 8-nitroguanine. Amino Acids, 2010, 38, 319-327.	1.2	3
3475	NIR-FT Raman, FT-IR and surface-enhanced Raman scattering and DFT based theoretical studies on the adsorption behaviour of (S)-phenylsuccinic acid on silver nanoparticles. Journal of Chemical Sciences, 2010, 122, 511-519.	0.7	23
3476	Molecular structure, vibrational spectroscopic studies and natural bond orbital analysis of 7-amino-4-trifluoromethyl coumarin. Pramana - Journal of Physics, 2010, 74, 845-850.	0.9	10
3477	A quantum chemical study of the interaction of monomethyl mercury cation with G, H, S, and Y amino acids. Journal of Structural Chemistry, 2010, 51, 1034-1044.	0.3	0
3478	Quantum chemical calculations of vibrational spectra of para-ethylbenzenesulfonic acid. Journal of Applied Spectroscopy, 2010, 77, 189-193.	0.3	5
3479	Analysis of vibrational, structural, and electronic properties of rivastigmine by density functional theory. Journal of Applied Spectroscopy, 2010, 77, 468-478.	0.3	1
3480	Thermochemistry of chromone- and coumarin-3-carboxylic acid. Journal of Thermal Analysis and Calorimetry, 2010, 100, 519-526.	2.0	10
3481	Ab initio HF and DFT calculations on an organic non-linear optical material. Structural Chemistry, 2010, 21, 213-219.	1.0	78
3482	The Role of Oxazolidinones in l-Proline-Assisted Aldol-Type Reactions. Topics in Catalysis, 2010, 53, 1031-1038.	1.3	4
3483	An experimental and theoretical investigation of the structure and reactivity of bilayered VOx/TiOx/SiO2 catalysts for methanol oxidation. Journal of Catalysis, 2010, 270, 163-171.	3.1	37
3484	Markovnikov Regiocontrol in Hydroboration of Alkene by Trifluoromethyl Substituent. Chinese Journal of Chemistry, 2001, 19, 296-298.	2.6	1
3485	Vibrational and Thermodynamic Properties of 2,2â€²,4,4â€²,6,6â€²â€Hexanitroazobenzene and Its Derivatives: A Density Functional Theory Study. Chinese Journal of Chemistry, 2010, 28, 149-158.	2.6	2
3486	A Theoretical Study on the Vibrational Spectra and Thermodynamic Properties for the Derivatives of 2,5â€Dipicrylâ€1,3,4â€oxadiazole with N₃, ONO₂, and NNO₂ Groups. Chinese Journal of Chemistry, 2010, 28, 1345-1354.	2.6	5
3487	A Theoretical Study on the Vibrational Spectra and Thermodynamic Properties for the Derivatives of 2,5â€Dipicrylâ€1,3,4â€oxadiazole with â€“NO₂, â€“NH₂, â€“OH and â€“CH₃ Groups. Chinese Journal of Chemistry, 2010, 28, 1538-1546.	2.6	1
3488	Theoretical Studies on Energetic Property and Stability of Pyrazine and Pyridine Derivatives. Chinese Journal of Chemistry, 2010, 28, 2364-2370.	2.6	5
3489	Kinetics of Substituted Silylene Addition and Elimination in Silicon Nanocluster Growth Captured by Group Additivity. ChemPhysChem, 2010, 11, 1978-1994.	1.0	31

#	Article	IF	Citations
3490	SERS of Î²â€Thioglucose Adsorbed on Nanostructured Silver Electrodes. ChemPhysChem, 2010, 11, 1460-1467.	1.0	12
3491	Molecular Wires in Singleâ€Molecule Junctions: Charge Transport and Vibrational Excitations. ChemPhysChem, 2010, 11, 2256-2260.	1.0	77
3492	Atmospheric Lifetimes and Global Warming Potentials of CF 3 CH 2 CH 2 OH and CF 3 (CH 2) 2 CH 2 OH. ChemPhysChem, 2010, 11, 4079-4087.	1.0	24
3493	What is the minimum number of water molecules required to dissolve a potassium chloride molecule?. Journal of Computational Chemistry, 2010, 31, 2948-2954.	1.5	6
3494	DFT Study on Tautomerism of Dihydroâ€2Hâ€1,5â€benzodiazepinâ€2â€ones and Dihydroâ€2Hâ€1,5â€benzodiazepineâ€2â€thiones. European Journal of Organic Chemistry, 2010, 2010, 280-291.	1.2	19
3495	Computational Study of Câ€“H Insertion Reactions with Ethyl Bromodiazoacetate. European Journal of Organic Chemistry, 2010, 2010, 4355-4359.	1.2	11
3498	Quinoidal Oligothiophenes: Towards Biradical Groundâ€State Species. Chemistry - A European Journal, 2010, 16, 470-484.	1.7	74
3499	Neutral and Oxidized Triisopropylsilyl Endâ€Capped Oligothienoacenes: A Combined Electrochemical, Spectroscopic, and Theoretical Study. Chemistry - A European Journal, 2010, 16, 5481-5491.	1.7	25
3500	Boraneâ€“Lewis Base Complexes as Homolytic Hydrogen Atom Donors. Chemistry - A European Journal, 2010, 16, 6861-6865.	1.7	75
3503	Calculations and Matrix Infrared Spectra of Terminal Borylene Complexes FBï£¾MF₂. Angewandte Chemie - International Edition, 2010, 49, 157-160.	7.2	37
3504	Tracking Flavin Conformations in Protein Crystal Structures with Raman Spectroscopy and QM/MM Calculations. Angewandte Chemie - International Edition, 2010, 49, 2324-2327.	7.2	71
3505	Molecular structure, vibrational spectroscopic, firstâ€order hyperpolarizability and HOMO, LUMO studies of 3â€hydroxyâ€2â€naphthoic acid hydrazide. Journal of Raman Spectroscopy, 2010, 41, 53-62.	1.2	69
3506	Surfaceâ€enhanced Raman scattering and density functional theory studies of bis(4â€aminophenyl)sulfone. Journal of Raman Spectroscopy, 2010, 41, 160-166.	1.2	9
3507	Experimental and theoretical studies on corals. I. Toward understanding the origin of color in precious red corals from Raman and IR spectroscopies and DFT calculations. Journal of Raman Spectroscopy, 2010, 41, 651-658.	1.2	34
3508	Concentration and pH dependent SERS spectra of sulfanilic acid sodium salt on colloidal silver particles. Journal of Raman Spectroscopy, 2010, 41, 944-951.	1.2	33
3509	Crystal â†' nematic phase transition in the liquid crystalline system 1â€isothiocyanatoâ€4â€(transâ€4â€propylcyclohexyl) benzene (3CHBT) probed by temperatureâ€dependent microâ€Raman study and DFT calculations. Journal of Raman Spectroscopy, 2010, 41, 1067-1075.	1.2	10
3510	Density functional theory calculation and vibrational spectral analysis of 4â€hydroxyâ€3â€(3â€oxoâ€1â€phenylbutyl)â€2Hâ€1â€benzopyranâ€2â€one. Journal of Raman Spectroscopy, 2010, 41, 1076-1084.	1.2	24
3511	XRD studies, vibrational spectra, and molecular structure of 1Hâ€imidazo [4,5â€b]pyridine based on DFT quantum chemical calculations. Journal of Raman Spectroscopy, 2010, 41, 1021-1029.	1.2	16

#	Article	IF	Citations
3512	Molecular structure, spectroscopic (FTIR, FTIR gas phase, FTâ€Raman) firstâ€order hyperpolarizability and HOMOâ€“LUMO analysis of 4â€methoxyâ€2â€methyl benzoic acid. Journal of Raman Spectroscopy, 2010, 41, 1369-1378.	1.2	68
3513	Collisionâ€induced dissociation mass spectra of glucosinolate anions. Journal of Mass Spectrometry, 2010, 45, 272-283.	0.7	34
3514	FTâ€IR, Raman, RRS measurements and DFT calculation for doxorubicin. Microscopy Research and Technique, 2010, 73, 991-995.	1.2	95
3515	Computational studies on the reactions of 3â€butenyl and 3â€butenylperoxy radicals. International Journal of Chemical Kinetics, 2010, 42, 273-288.	1.0	49
3516	Thermochemical properties for nâ€propyl, isoâ€propyl, and tertâ€butyl nitroalkanes, alkyl nitrites, and their carbonâ€centered radicals. International Journal of Chemical Kinetics, 2010, 42, 181-199.	1.0	7
3517	Experimental and theoretical study on molecular structure and FT-IR, Raman, NMR spectra of 4,4â€²-dibromodiphenyl ether. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 429-434.	2.0	27
3518	FT-IR, FT-Raman, ab initio and DFT structural and vibrational frequency analysis of 6-aminopenicillanic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 183-190.	2.0	14
3519	Ab initio study on the formation of triiodide CT complex from the reaction of iodine with 2,3-diaminopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 198-202.	2.0	22
3520	Vibrational spectroscopic study of o-, m- and p-hydroxybenzylideneaminoantipyrines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 203-211.	2.0	29
3521	Experimental and theoretical studies on o-, m- and p-chlorobenzylideneaminoantipyrines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1115-1124.	2.0	362
3522	Molecular structure, vibrational spectra and nonlinear optical properties of orthoarsenic acidâ€“tris-(hydroxymethyl)-aminomethane DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1315-1320.	2.0	21
3523	DFT (LSDA, B3LYP and B3PW91) comparative vibrational spectroscopic analysis of Î±-acetonaphthone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 12-21.	2.0	58
3524	Vibrational spectra, normal modes, ab initio and DFT calculations for 6-Chloro- and 7-Chloro-4-bromomethylcoumarins. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 351-358.	2.0	29
3525	Anharmonic vibrational analysis of 3,4-diaminopyridine and 3-aminopyridine by density functional theory calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 502-512.	2.0	26
3526	DFT computations and spectroscopic analysis of a pesticide: Chlorothalonil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 36-44.	2.0	62
3527	Vibrational spectroscopic investigation and DFT studies on 2,2â€²,4,4â€²-tetrabromodiphenyl ether. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 572-578.	2.0	15
3528	Ab initio/DFT electronic structure calculations, spectroscopic studies and normal coordinate analysis of 2-chloro-5-bromopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 918-926.	2.0	20
3529	Vibrational and ab initio studies of 3-acetyl-6-bromocoumarin and 3-acetyl-6-methylcoumarin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 77, 1039-1047.	2.0	7

#	Article	IF	Citations
3530	Role of hydration and water coordination in micellization of Pluronic block copolymers. Journal of Colloid and Interface Science, 2010, 352, 415-423.	5.0	27
3531	Enthalpies of formation of Î²-alanine, sarcosine, and 4-aminobutanoic acid from quantum chemical calculations. Journal of Chemical Thermodynamics, 2010, 42, 1056-1062.	1.0	6
3532	Energetics of the isomers: 3- and 4-hydroxycoumarin. Journal of Chemical Thermodynamics, 2010, 42, 1372-1378.	1.0	11
3533	NMR spectral enantioresolution of spirobrassinin and 1-methoxyspirobrassinin enantiomers using (S)-(â˘)-ethyl lactate and modeling of spirobrassinin self-association for rationalization of its self-induced diastereomeric anisochromism (SIDA) and enantiomer self-disproportionation on achiral-phase chromatography (ESDAC) phenomena. Journal of Fluorine Chemistry, 2010, 131, 467-476.	0.9	37
3534	Computational study of imidazole derivative as high energetic materials. Journal of Hazardous Materials, 2010, 183, 622-631.	6.5	69
3535	Common basis for the mechanism of metallo and non-metallo KDO8P synthases. Journal of Inorganic Biochemistry, 2010, 104, 1267-1275.	1.5	5
3536	Ab initio Hartreeâ€“Fock and density functional theory investigations on the conformational stability, molecular structure and vibrational spectra of 7-acetoxy-6-(2,3-dibromopropyl)-4,8-dimethylcoumarin molecule. Journal of Molecular Structure, 2010, 964, 134-151.	1.8	209
3537	Structure of 1H-2-oxo-2,3-dihydroimidazo[1,2-a]pyridinium perchlorate studied by X-ray diffraction, DFT calculations and by FTIR and NMR spectroscopy. Journal of Molecular Structure, 2010, 976, 119-128.	1.8	14
3538	The experimental and theoretical study of crystal structure, IR, 1H NMR and UVâ€“vis of 2-styryl-Î²-naphthathiazole dye. Journal of Molecular Structure, 2010, 977, 39-44.	1.8	4
3539	Structure of 3-aminopyridine betaine hydrochloride studied by X-ray diffraction, DFT calculations, FTIR and NMR spectroscopy. Journal of Molecular Structure, 2010, 979, 12-21.	1.8	8
3540	Synthesis, crystal structure, and physical property of radical cation salt of 2-(thiopyran-4-ylidene)-4,5-ethylenedithio-1,3-dithiole (TP-EDTT): (TP-EDTT)2SbF6. Physica B: Condensed Matter, 2010, 405, S49-S54.	1.3	3
3541	Quantum-chemical, spectroscopic and X-ray diffraction studies on nickel complex of 2-hydroxyacetophenone thiosemicarbazone with triphenylphospine. Polyhedron, 2010, 29, 2393-2403.	1.0	43
3542	Evaluation of dispersion-corrected density functional theory (B3LYP-DCP) for compounds of biochemical interest. Journal of Molecular Graphics and Modelling, 2010, 29, 178-187.	1.3	19
3543	Synthesis and characterization of iron and ruthenium complexes bearing Pâ€“N ligands based on 8-hydroxyquinoline. Inorganica Chimica Acta, 2010, 363, 3674-3679.	1.2	11
3544	Terahertz spectroscopic investigations of caffeine and 3-acetylmorphine. Optik, 2010, 121, 1712-1716.	1.4	12
3545	Charge disproportionation in a semiconducting Î¸-type salt of BTM-TTP. Physica B: Condensed Matter, 2010, 405, S198-S201.	1.3	0
3546	Coordination chemistry of nickel(II) nitrate with superbasic guanidines as studied by electrospray mass spectrometry. International Journal of Mass Spectrometry, 2010, 290, 22-31.	0.7	9
3547	Dissociation of the phenylphosphine molecular ion: A theoretical study. International Journal of Mass Spectrometry, 2010, 294, 40-46.	0.7	11

#	Article	IF	Citations
3548	Infrared spectroscopic characterization of the oxidative dehydrogenation of propane by V4O10+. International Journal of Mass Spectrometry, 2010, 297, 102-106.	0.7	29
3549	Confirmation of NH species in the framework of nitrogen-incorporated ZSM-5 zeolite by experimental and theoretical studies. Microporous and Mesoporous Materials, 2010, 127, 25-31.	2.2	20
3550	Interaction of water diluted in 1-butyl-3-methyl imidazolium ionic liquids by vibrational spectroscopy modeling. Journal of Molecular Liquids, 2010, 153, 57-66.	2.3	51
3551	Molecular structure and vibrational spectroscopic analysis of an antiplatelet drug; clopidogrel hydrogen sulphate (form 2) â€“ A combined experimental and quantum chemical approach. Journal of Molecular Structure, 2010, 964, 88-96.	1.8	19
3552	Structure of propanoic acid dimers as studied by means of MIR and FIR spectroscopy. Journal of Molecular Structure, 2010, 976, 263-269.	1.8	6
3553	Spectroscopic studies, molecular structure and hydrogen bonding in hydrates of Gemini betaines. Journal of Molecular Structure, 2010, 973, 163-172.	1.8	12
3554	Vibrational spectroscopic investigation and conformational analysis of 1-cyclohexylpiperazine. Journal of Molecular Structure, 2010, 975, 85-92.	1.8	15
3555	Hydrogen bonding and molecular association in 2-(quinuclidinium)-butyric acid bromide hydrate studied by X-ray diffraction, DFT calculations, FTIR and NMR spectroscopy, and potentiometric titration. Journal of Molecular Structure, 2010, 975, 357-366.	1.8	8
3556	The hydrogen bonding network in the dimer of syn-N-phenyl-Nâ€²-sulfinylhydrazine, PhNHNSO. Journal of Molecular Structure, 2010, 979, 101-107.	1.8	7
3557	FT-IR, FT-Raman, NMR spectral analysis and theoretical NBO, HOMOâ€“LUMO analysis of bis(4-amino-5-mercapto-1,2,4-triazol-3-yl)ethane by ab initio HF and DFT methods. Journal of Molecular Structure, 2010, 981, 59-70.	1.8	35
3558	Spectroscopic and theoretical study on inclusion complexation of beta-cyclodextrin with permethrin. Journal of Molecular Structure, 2010, 981, 194-203.	1.8	63
3559	A simple, mild, and regioselective method for the benzylation of carbohydrate derivatives promoted by silver carbonate. Carbohydrate Research, 2010, 345, 559-564.	1.1	34
3560	Investigation of the Effect of Functional Group Substitutions on the Gas-Phase Electron Affinities and Ionization Energies of Room-Temperature Ionic Liquids Ions using Density Functional Theory. Electrochimica Acta, 2010, 55, 3804-3811.	2.6	64
3561	Thiourea catalyzed aminolysis of epoxides under solvent free conditions. Electronic control of regioselective ring opening. Tetrahedron, 2010, 66, 3042-3049.	1.0	32
3562	The 1,3-dipolar cycloaddition of 1H-pyridinium-3-olate and 1-methylpyridinium-3-olate with methyl acrylate: a density functional theory study. Tetrahedron, 2010, 66, 9187-9193.	1.0	17
3563	Enantiodifferentiation of phytoalexin spirobrassinin derivatives using the chiral solvating agent (R)-(+)-1,1â€²-bi-2-naphthol in conjunction with molecular modeling. Tetrahedron: Asymmetry, 2010, 21, 647-658.	1.8	38
3564	Computational comparison of Rh2(esp)2 and Rh2(O2CH)4 as catalysts in a carbenoid reaction. Tetrahedron Letters, 2010, 51, 5298-5301.	0.7	14
3565	In search of aromatic seven-membered rings. Computational and Theoretical Chemistry, 2010, 943, 23-31.	1.5	22

#	Article	IF	Citations
3566	FT-IR and FT-Raman spectra, ab initio and density functional computations of the vibrational spectra, molecular geometry, atomic charges and some molecular properties of the biomolecule 5-iodouracil. Computational and Theoretical Chemistry, 2010, 940, 29-44.	1.5	21
3567	Molecular structure and vibrational study on 2,3-dihydro-1H-indene and its derivative 1H-indene-1,3(2H)-dione by density functional theory calculations. Computational and Theoretical Chemistry, 2010, 940, 82-86.	1.5	74
3568	Experimental and computational study of the energetics of methoxycoumarins. Computational and Theoretical Chemistry, 2010, 946, 13-19.	1.5	8
3569	Ultrafine copper phthalocyanine complex and its molecular structure in solvents. Computational and Theoretical Chemistry, 2010, 954, 2-6.	1.5	1
3570	Importance of CH tautomers in the tautomeric mixture of uric acid. Computational and Theoretical Chemistry, 2010, 947, 83-91.	1.5	12
3571	Quantum-chemical study on the antioxidation mechanisms of trans-resveratrol reactions with free radicals in the gas phase, water and ethanol environment. Computational and Theoretical Chemistry, 2010, 951, 37-48.	1.5	34
3572	The spectroscopic, NMR analysis of 1-(2,6-Dichloro-4-nitrophenyl)-5-amino-4-cyanopyrazole by ab initio HF and density functional methods. Computational and Theoretical Chemistry, 2010, 957, 15-20.	1.5	1
3573	Electronic structure, non-linear properties and vibrational analysis of Acenaphthene and its carbonyl derivative Acenaphthenequinone by density functional theory. Computational and Theoretical Chemistry, 2010, 958, 33-40.	1.5	17
3574	Structure and normal vibrations in xanthine and its methyl derivatives from first principle calculations. Computational and Theoretical Chemistry, 2010, 960, 86-92.	1.5	7
3575	Comprehensive ab initio study on the conformations of L-Threonine and L-allo-Threonine and related species in gas phase. Computational and Theoretical Chemistry, 2010, 962, 23-32.	1.5	19
3576	Intramolecular dihydrogen bond: A new perspective in Lewis acid catalyzed nucleophilic epoxide ring opening reaction. Computational and Theoretical Chemistry, 2010, 962, 97-100.	1.5	6
3577	Epitaxial and polycrystalline growth of AlN by high temperature CVD: Experimental results and simulation. Surface and Coatings Technology, 2010, 205, 1294-1301.	2.2	29
3578	Chemisorption of isocyanate (NCO) on the Pd(100) surface at different coverages. Surface Science, 2010, 604, 442-450.	0.8	10
3579	Reaction of tert-butyl isocyanate and tert-butyl isothiocyanate at the Ge(100) â˜ 2 Ã— 1 Surface. Surface Science, 2010, 604, 1791-1799.	0.8	11
3580	Study of the interaction between cardiolipin bilayers and methylene blue in polymer-based Layer-by-Layer and Langmuir films applied as membrane mimetic systems. Vibrational Spectroscopy, 2010, 54, 93-102.	1.2	33
3581	An experimental and theoretical vibrational spectroscopic study on niflumic acid, a non-steroidal anti-inflammatory drug. Vibrational Spectroscopy, 2010, 53, 239-247.	1.2	11
3582	Intramolecular charge transfer and hydrogen bonding interactions of nonlinear optical material N-benzoyl glycine: Vibrational spectral study. Vibrational Spectroscopy, 2010, 54, 72-80.	1.2	49
3583	Determination of enthalpy of formation of methyl and ethyl esters of fatty acids. Chemistry and Physics of Lipids, 2010, 163, 172-181.	1.5	33

#	Article	IF	Citations
3584	An ab initio and DFT study of structure and vibrational spectra of Î³ form of Oleic acid: Comparison to experimental data. Chemistry and Physics of Lipids, 2010, 163, 207-217.	1.5	34
3585	Molecular dynamics simulation of self-assembly structure for AOK based reverse micelle in supercritical CO2. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2010, 367, 148-154.	2.3	18
3586	FTIR and UV/vis as methods for evaluation of oxidative degradation of model paper: DFT approach for carbonyl vibrations. Carbohydrate Polymers, 2010, 82, 370-375.	5.1	73
3587	Infrared spectroscopic detection of the methylgermyl (H2GeCH3) radical and its perdeuterated counterpart in low temperature matrices. Chemical Physics Letters, 2010, 492, 226-234.	1.2	8
3588	Solvent effects on blue shifted improper hydrogen bond of Câ€“Hâ‹¯O in deoxycytidine isomers. Chemical Physics Letters, 2010, 500, 327-333.	1.2	14
3589	Quantitative structureâ€“antioxidant activity relationship of trans-resveratrol oligomers, trans-4,4â€²-dihydroxystilbene dimer, trans-resveratrol-3-O-glucuronide, glucosides: Trans-piceid, cis-piceid, trans-astringin and trans-resveratrol-4â€²-O-Î²-D-glucopyranoside. European Journal of Medicinal Chemistry, 2010, 45, 2366-2380.	2.6	91
3590	Low Energy Monopropellants Based on the Guanylurea Cation. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 163-175.	0.6	21
3591	[(BeCl2)2(18-Krone-6)] und sein Hydrolyseprodukt [{Be3(Î¼-OH)3(H2O)6}-(18-Krone-6)]Cl3Â·3H2O: Kristallstrukturen und DFT-Rechnungen. [(BeCl2)2(18-Crown-6)] and its Product of Hydrolysis [{Be3(Î¼-OH)3(H2O)6}-(18-Crown-6)]Cl3Â·3H2O: Crystal Structures and DFT C. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 2364-2371.	0.6	23
3592	Lowâ€band gap copolymers containing thienothiadiazole units: Synthesis, optical, and electrochemical properties. Journal of Polymer Science Part A, 2010, 48, 2743-2756.	2.5	31
3593	Deposition of Functional Organic Thin Films by Pulsed Plasma Polymerization: A Joint Theoretical and Experimental Study. Plasma Processes and Polymers, 2010, 7, 172-181.	1.6	55
3594	Substituent Effects on Thermodynamic and Detonation Properties of Polynitrobenzenes. Propellants, Explosives, Pyrotechnics, 2010, 35, 567-571.	1.0	2
3595	A theoretical density functional study of association of Zn²⁺ with oxazolidine and its thio derivatives in the gas phase. Journal of Physical Organic Chemistry, 2010, 23, 751-758.	0.9	3
3596	Theoretical and experimental studies on stability of the Câ€ON bond in new ketone functionalized Nâ€alkoxyamines. Journal of Physical Organic Chemistry, 2010, 23, 1146-1154.	0.9	8
3597	Theoretical study of substituent effects on gasâ€phase stabilities of benzylic anions. Journal of Physical Organic Chemistry, 2010, 23, 1057-1065.	0.9	13
3598	Baseâ€dependent selectivity of an S_NAr reaction. Journal of Physical Organic Chemistry, 2011, 24, 751-763.	0.9	2
3599	Timeâ€independent and timeâ€dependent methods for the calculation of the vibrational spectra: H₂CN as example. International Journal of Quantum Chemistry, 2010, 110, 578-585.	1.0	3
3600	Theoretical studies on heats of formation, detonation properties, and bond dissociation energies of monofurazan derivatives. International Journal of Quantum Chemistry, 2010, 110, 1549-1558.	1.0	20
3601	Theoretical study of morphine and heroin: Conformational study in gas phase and aqueous solution and electron distribution analysis. International Journal of Quantum Chemistry, 2010, 110, 2472-2482.	1.0	3

#	Article	IF	Citations
3602	Simulation of a tetramer form of 5-iodouracil: The vibrational spectra and molecular structure in the isolated and in the solid state by using DFT calculations. Vibrational Spectroscopy, 2010, 52, 108-121.	1.2	15
3604	Structural analysis of the antimalarial drug halofantrine by means of Raman spectroscopy and density functional theory calculations. Journal of Biomedical Optics, 2010, 15, 041516.	1.4	47
3605	Effect of 2, 5- substituents on the stability of cyclic nitrone superoxide spin adducts: A density functional theory approach. Free Radical Research, 2010, 44, 751-778.	1.5	3
3606	Density functional theory, restricted Hartreeâ€“Fock simulations and vibrational spectroscopic studies of nicorandil. Molecular Simulation, 2010, 36, 425-433.	0.9	27
3607	Finite temperature infrared spectroscopy of polycyclic aromatic hydrocarbon molecules: Path-integral molecular dynamics. Journal of Chemical Physics, 2010, 132, 124308.	1.2	24
3608	Calibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functional. Journal of Chemical Physics, 2010, 133, 114109.	1.2	32
3609	An ab initio study of model triazene-based anticancer agents. Canadian Journal of Chemistry, 2010, 88, 709-715.	0.6	4
3610	On photoinduced volume change in amorphous selenium: Quantum chemical calculation and Raman spectroscopy. Journal of Applied Physics, 2010, 107, .	1.1	36
3611	Density functional calculation of the infrared spectrum of surface hydroxyl groups on goethite (Â-FeOOH). American Mineralogist, 2010, 95, 414-417.	0.9	34
3612	Anisotropy in structural and physical properties in tetrathiafulvalene derivatives-based zone-cast layers as seen by Raman spectroscopy, UV-visible spectroscopy, and field effect measurements. Journal of Applied Physics, 2010, 108, 014504.	1.1	18
3613	Vibrational properties of ferroelectricÎ²-vinylidene fluoride polymers and oligomers. Physical Review B, 2010, 81, .	1.1	30
3614	VIBRATIONAL SPECTROSCOPIC INVESTIGATION AND CONFORMATIONAL ANALYSIS OF 1-PENTYLAMINE: A COMPARATIVE DENSITY FUNCTIONAL STUDY. Journal of Theoretical and Computational Chemistry, 2010, 09, 667-685.	1.8	27
3615	Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water â€“ a computational study. Atmospheric Chemistry and Physics, 2010, 10, 4961-4974.	1.9	245
3616	Nuclear momentum distribution in solid and liquid HF from ab initio calculation. Journal of Chemical Physics, 2010, 133, 144505.	1.2	19
3617	Theoretical Study on Destruction Mechanism of 2,3,7,8-TCDD by O3 and NO3. Chinese Journal of Chemical Physics, 2010, 23, 303-309.	0.6	8
3618	Calculations of vibrationally resonant sum- and difference-frequency-generation spectra of chiral molecules in solutions: Three-wave-mixing vibrational optical activity. Journal of Chemical Physics, 2010, 132, 074506.	1.2	10
3619	Mechanistic Investigation on the Reaction of Oâ¯ with CH3CN Using Density Functional Theory. Chinese Journal of Chemical Physics, 2010, 23, 643-648.	0.6	1
3620	Trace Detection of Triphenylene by Surface Enhanced Raman Spectroscopy Using Functionalized Silver Nanoparticles with Bis-Acridinium Lucigenine. Langmuir, 2010, 26, 6977-6981.	1.6	20

#	Article	IF	Citations
3621	Adsorption Behavior of Bifunctional Molecules on Ge(100)-2 Ã— 1: Comparison of Mercaptoethanol and Mercaptamine. Journal of Physical Chemistry C, 2010, 114, 22230-22236.	1.5	13
3622	Scaling of Computed Cyano-Stretching Frequencies and IR Intensities of Nitriles, Their Anions, and Radicals. Journal of Physical Chemistry A, 2010, 114, 5149-5161.	1.1	14
3623	A comparison of methods for measuring relative radical stabilities of carbon-centred radicals. Physical Chemistry Chemical Physics, 2010, 12, 9597.	1.3	97
3624	First Principles Prediction of The Propagation Rate Coefficients of Acrylic and Vinyl Esters: Are We There Yet?. Macromolecules, 2010, 43, 553-560.	2.2	66
3625	Thermochemical Properties of exo-Tricyclo[5.2.1.0^{2,6}]decane (JP-10 Jet Fuel) and Derived Tricyclodecyl Radicals. Journal of Physical Chemistry A, 2010, 114, 9545-9553.	1.1	42
3626	A study into the effect of subtle structural details and disorder on the terahertz spectrum of crystalline benzoic acid. Physical Chemistry Chemical Physics, 2010, 12, 5329.	1.3	78
3627	Ultrafast Multisequential Photochemistry of 5-Diazo Meldrumâ€™s Acid. Journal of the American Chemical Society, 2010, 132, 15213-15222.	6.6	31
3628	Fast Reactivity of a Cyclic Nitroneâ^'Calix[4]pyrrole Conjugate with Superoxide Radical Anion: Theoretical and Experimental Studies. Journal of the American Chemical Society, 2010, 132, 17157-17173.	6.6	50
3629	Effect of Watsonâ^'Crick and Hoogsteen Base Pairing on the Conformational Stability of C8-Phenoxyl-2â€²-deoxyguanosine Adducts. Journal of Physical Chemistry B, 2010, 114, 12995-13004.	1.2	17
3630	Multireference Configuration Interaction Study of the Vibronic Transitions and Photodissociation of Vinyl Bromide and Vinyl Chloride Radical Cations in the Second Excited State. Journal of Physical Chemistry A, 2010, 114, 7937-7944.	1.1	2
3631	Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory. Journal of Organic Chemistry, 2010, 75, 4964-4974.	1.7	19
3632	New Insights into the Relationship between Ion-Pair Binding Energy and Thermodynamic and Transport Properties of Ionic Liquids. Journal of Physical Chemistry C, 2010, 114, 20472-20478.	1.5	81
3633	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887.	2.3	1,183
3634	A Calorimetric and Computational Study of Aminomethoxybenzoic Acids. Journal of Physical Chemistry B, 2010, 114, 11570-11575.	1.2	7
3635	Raman and SERS spectroscopy of cucurbit[n]urils. Physical Chemistry Chemical Physics, 2010, 12, 10429.	1.3	71
3636	Theoretical spectroscopy of floppy peptides at room temperature. A DFTMD perspective: gas and aqueous phase. Physical Chemistry Chemical Physics, 2010, 12, 3336.	1.3	158
3637	Anionic Amino Acid [closo-1-CB9H8-1-COO-10-NH3]â^' and Dinitrogen Acid [closo-1-CB9H8-1-COOH-10-N2] as Key Precursors to Advanced Materials: Synthesis and Reactivity. Inorganic Chemistry, 2010, 49, 1166-1179.	1.9	46
3638	Induced Optical Activity in Boronic-Acid-Protected Silver Nanoclusters by Complexation with Chiral Fructose. Journal of Physical Chemistry C, 2010, 114, 15909-15915.	1.5	37

#	Article	IF	Citations
3639	Quantum chemical treatment of Î²-sitosterol molecule. Pharmaceutical Biology, 2010, 48, 637-642.	1.3	7
3640	Ab Initio Chemical Kinetics of Methyl Formate Decomposition: The Simplest Model Biodiesel. Journal of Physical Chemistry A, 2010, 114, 5478-5484.	1.1	50
3641	Prediction of Refractive Index of Polymers Using Artificial Neural Networks. Journal of Chemical & Engineering Data, 2010, 55, 5388-5393.	1.0	10
3642	Reaction of Phenyl Isocyanate and Phenyl Isothiocyanate with the Ge(100)-2 Ã— 1 Surface. Journal of Physical Chemistry C, 2010, 114, 14193-14201.	1.5	17
3643	Nucleophilic Cycloaromatization of Ynamide-Terminated Enediynes. Journal of Organic Chemistry, 2010, 75, 5953-5962.	1.7	39
3644	Theoretical Study on Activation and Protonation of Dinitrogen on Cubane-Type MIr₃S₄ Clusters (M = V, Cr, Mn, Fe, Co, Ni, Cu, Mo, Ru, and W). Inorganic Chemistry, 2010, 49, 2464-2470.	1.9	13
3645	Experimental and Computational Studies on the Structural and Thermodynamic Properties of Two Sulfur Heterocyclic Keto Compounds. Journal of Chemical & Engineering Data, 2010, 55, 5009-5017.	1.0	22
3646	Energetics and Structural Elucidation of Mechanisms for Gas Phase H/D Exchange of Protonated Peptides. Journal of Physical Chemistry A, 2010, 114, 11953-11963.	1.1	9
3647	Deposition of Ultrathin Polythiourea Films by Molecular Layer Deposition. Chemistry of Materials, 2010, 22, 5563-5569.	3.2	71
3648	Scaling Factors and Uncertainties for ab Initio Anharmonic Vibrational Frequencies. Journal of Chemical Theory and Computation, 2010, 6, 2822-2828.	2.3	64
3649	Cooperative Cation Migrations upon CO Addition in CuI- and Alkali-Exchanged Faujasite: A DFT Study. Journal of Physical Chemistry C, 2010, 114, 17802-17811.	1.5	25
3650	Trends in the frequencies of Î½(AsO_xH_{xâ€“1}) [x = 2â€“4] in selected As(V)-containing compounds investigated using quantum chemical calculations. Canadian Journal of Chemistry, 2010, 88, 65-77.	0.6	15
3651	Infrared Spectra of Simple Methylidyne, Methylidene, and Insertion Complexes Generated in Reactions of Laser-Ablated Rhodium Atoms with Halomethanes and Ethane. Organometallics, 2010, 29, 2211-2222.	1.1	30
3652	Entropic Contributions to the Atomic-Scale Charge-Carrier/Surface Interactions That Govern Macroscopic Surface Conductance. Journal of Physical Chemistry C, 2010, 114, 3991-3997.	1.5	5
3653	Computational Chemical Studies on Thermochemistry and Ring Strains in Cyclic [n]Metaphenyleneacetylenes, Butadiyne-Bridged [4_n]Metacyclophynes, and Butadiyne-Bridged [4_n]Paracyclophynes. Journal of Organic Chemistry, 2010, 75, 5797-5809.	1.7	17
3654	Type II Isopentenyl Diphosphate Isomerase: Probing the Mechanism with Alkyne/Allene Diphosphate Substrate Analogues. Biochemistry, 2010, 49, 6228-6233.	1.2	21
3655	Heats of Formation of C₆H₅^{â€¢}, C₆H₅⁺, and C₆H₅NO by Threshold Photoelectron Photoion Coincidence and Active Thermochemical Tables Analysis. Journal of Physical Chemistry A, 2010, 114, 13134-13145.	1.1	87
3656	Reactions of Laser-Ablated Nb and Ta Atoms with N₂: Experimental and Theoretical Study of M(NN)_x (M = Nb, Ta; x = 1â˜4) in Solid Neon. Journal of Physical Chemistry A, 2010, 114, 6837-6842.	1.1	10

#	Article	IF	Citations
3657	Analysis of Measured and Calculated Raman Spectra of Indole, 3-Methylindole, and Tryptophan on the Basis of Observed and Predicted Isotope Shifts. Journal of Physical Chemistry A, 2010, 114, 10897-10905.	1.1	29
3658	Mechanistic Study on the Gold-Catalyzed Câ^'S Bond Formation of Î±-Thioallenes To Form 2,5-Dihydrothiophenes. Journal of Organic Chemistry, 2010, 75, 8516-8521.	1.7	35
3659	Finite-Temperature IR Spectroscopy of Polyatomic Molecules: A Theoretical Assessment of Scaling Factors. Journal of Physical Chemistry A, 2010, 114, 3139-3146.	1.1	26
3660	Concerted Wolff Rearrangement in Two Simple Acyclic Diazocarbonyl Compounds. Journal of Physical Chemistry A, 2010, 114, 13065-13068.	1.1	22
3661	Retinylisoflavonoid as a Novel Membrane Antioxidant. Journal of Physical Chemistry B, 2010, 114, 13904-13910.	1.2	8
3662	Transition State Analysis of Thymidine Hydrolysis by Human Thymidine Phosphorylase. Journal of the American Chemical Society, 2010, 132, 13425-13433.	6.6	25
3663	An Ab Initio Study of the Ground and Excited State Chemistry of Phenyldiazirine and Phenyldiazomethane. Journal of Physical Chemistry A, 2010, 114, 5902-5912.	1.1	23
3664	Amide-I and -II Vibrations of the Cyclic Î²-Sheet Model Peptide Gramicidin S in the Gas Phase. Journal of the American Chemical Society, 2010, 132, 2085-2093.	6.6	62
3665	Assessing an Impulsive Model for Rotational Energy Partitioning to Acetyl Radicals from the Photodissociation of Acetyl Chloride at 235 nm. Journal of Physical Chemistry A, 2010, 114, 13005-13010.	1.1	20
3666	Infrared Spectra of CH₂â•Zr(H)NC, CH₃â^'ZrNC, and Î·₂-Zr(NC)-CH₃ Produced by Reactions of Laser-Ablated Zr Atoms with Acetonitrile. Journal of Physical Chemistry A, 2010, 114, 891-897.	1.1	28
3667	Prediction of Prop-2-enoate Polymer and Styrene Polymer Glass Transition Using Artificial Neural Networks. Journal of Chemical & Engineering Data, 2010, 55, 5340-5346.	1.0	3
3668	Formation of Organic Nanoscale Laminates and Blends by Molecular Layer Deposition. ACS Nano, 2010, 4, 331-341.	7.3	105
3669	Infrared Spectra of CX₂â•CoX₂ and CX₃â^'CoX Complexes from Reactions of Laser-Ablated Cobalt Atoms with Halomethanes. Journal of Physical Chemistry A, 2010, 114, 8056-8068.	1.1	18
3670	Influence of Molecular Oxide Cages on Metal Carbonyls. Journal of Physical Chemistry A, 2010, 114, 987-993.	1.1	2
3671	Microhydration of the Selenite Dianion: A Theoretical Study of Structures, Hydration Energies, and Electronic Stabilities of SeO₃^{2â^'}(H₂O)_n (n = 0â^'6, 9) Clusters. Journal of Physical Chemistry A, 2010, 114, 8948-8960.	1.1	8
3672	Proton and Hydride Affinities in Excited States: Magnitude Reversals in Proton and Hydride Affinities between the Lowest Singlet and Triplet States of Annulenyl and Benzannulenyl Anions and Cations. Journal of Organic Chemistry, 2010, 75, 2189-2196.	1.7	8
3673	Stereoelectronic Effects in Î±-Carbanions of Conformationally Constrained Sulfides, Sulfoxides, and Sulfones. Journal of Physical Chemistry A, 2010, 114, 8480-8487.	1.1	29
3674	Conformational and vibrational study of cis-diamminedichloropalladium(ii). Physical Chemistry Chemical Physics, 2010, 12, 14309.	1.3	14

#	Article	IF	Citations
3675	Determination of Structure and Dynamics of the Solvated Bisulfide (HS^{â^'}) Ion by ab Initio QMCF Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 12883-12887.	1.2	11
3676	Thermal Decomposition of NCN3as a High-Temperature NCN Radical Source: Singletâ^'Triplet Relaxation and Absorption Cross Section of NCN(3Î£)â€. Journal of Physical Chemistry A, 2010, 114, 12963-12971.	1.1	25
3677	SEIRA and SERS Effects in Cyclopentabithiophenethiol-Capped Gold Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 12900-12904.	1.5	11
3678	Reaction of Chlorosulfonyl Isocyanate with Fluorosubstituted Alkenes: Evidence of a Concerted Pathway. Journal of Organic Chemistry, 2010, 75, 7913-7916.	1.7	12
3679	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide. 6. Redox Properties. Journal of Physical Chemistry A, 2010, 114, 1153-1160.	1.1	25
3680	Kinetics and Thermodynamics of the Monomerâ^'Dimer Equilibria of Dialkoxydibutylstannanes. Organometallics, 2010, 29, 6384-6392.	1.1	16
3681	IR Fingerprints of U(VI) Nitrate Monoamides Complexes: A Joint Experimental and Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 10878-10884.	1.1	12
3682	Infrared Spectra of CH₂â•M(H)NC, CH₃â^'MNC, and Î·²-M(NC)â^'CH₃ Produced by Reactions of Laser-Ablated Group 5 Metal Atoms with Acetonitrile. Journal of Physical Chemistry A, 2010, 114, 5997-6006.	1.1	32
3683	Elucidating the Association of Water in Wet 1-Octanol from Normal to High Temperature by Near- and Mid-Infrared Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 9085-9093.	1.2	5
3684	How an Enzyme Might Accelerate an Intramolecular Dielsâ^'Alder Reaction: Theozymes for the Formation of Salvileucalin B. Organic Letters, 2010, 12, 1164-1167.	2.4	19
3685	Quantum Chemical Scaling and Its Importance: The Infrared and Raman Spectra of 5-Bromouracil. Spectroscopy Letters, 2010, 43, 51-59.	0.5	20
3686	Effects of Nucleophile, Oxidative Damage, and Nucleobase Orientation on the Glycosidic Bond Cleavage in Deoxyguanosine. Journal of Physical Chemistry B, 2010, 114, 2319-2326.	1.2	27
3687	Aggregation Behavior of a Conjugated C₃-Symmetric Molecule: A Description Based on Chiro-Optical Experimental and Theoretical Spectroscopies. Journal of Physical Chemistry B, 2010, 114, 5710-5717.	1.2	7
3688	Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures. Journal of Physical Chemistry A, 2010, 114, 2864-2873.	1.1	35
3689	Infrared Spectroscopy of Hydrated Bicarbonate Anion Clusters: HCO₃^{â^'}(H₂O)_{1â^'10}. Journal of the American Chemical Society, 2010, 132, 849-856.	6.6	146
3690	Cascade [1,3]-Sigmatropic Rearrangements of Ketene O,O-Acetals: Kinetic and DFT Level Mechanistic Studies. Journal of Organic Chemistry, 2010, 75, 1898-1910.	1.7	6
3691	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. Journal of Physical Chemistry C, 2010, 114, 20801-20808.	1.5	329
3692	A new value for the stable oxygen isotope fractionation between dissolved sulfate ion and water. Geochimica Et Cosmochimica Acta, 2010, 74, 818-828.	1.6	97

#	Article	IF	Citations
3693	On the proper use of the Bigeleisenâ€“Mayer equation and corrections to it in the calculation of isotopic fractionation equilibrium constants. Geochimica Et Cosmochimica Acta, 2010, 74, 6965-6983.	1.6	81
3694	Density functional theory study of the structure and electric properties of poly(vinylidene cyanide) Tj ETQq1 1 0.784314 rgBT /Overlo	2.1	4
3695	Hydrogen hyperfine splitting constants for phenoxyl radicals by DFT methods: regression analysis unravels hydrogen bonding effects. Organic and Biomolecular Chemistry, 2010, 8, 3136.	1.5	15
3696	Computational Study of Cyclopropanation Reactions with Halodiazoacetates. Journal of Organic Chemistry, 2010, 75, 2309-2320.	1.7	40
3697	Comparative Analysis of Surface-Enhanced Raman Spectroscopy of Daidzein and Formononetin. Journal of Physical Chemistry B, 2010, 114, 7104-7111.	1.2	10
3698	First-Principles Prediction of the pK_as of Anti-inflammatory Oxicams. Journal of Physical Chemistry A, 2010, 114, 11992-12003.	1.1	44
3699	The Stability of Aryl Carbanions Derived from PyridineN-Oxide: The Role of Resonance in Stabilizing Aryl Anions. Journal of the American Chemical Society, 2010, 132, 390-395.	6.6	13
3700	CHARMM Additive All-Atom Force Field for Glycosidic Linkages in Carbohydrates Involving Furanoses. Journal of Physical Chemistry B, 2010, 114, 12981-12994.	1.2	170
3701	Clarifying the Mechanism of the Denisov Cycle: How do Hindered Amine Light Stabilizers Protect Polymer Coatings from Photo-oxidative Degradation?. Macromolecules, 2010, 43, 4573-4583.	2.2	88
3702	Dissecting a Dyotropic Rearrangement. Journal of Organic Chemistry, 2010, 75, 1693-1700.	1.7	23
3703	Effect of Transition State Aromaticity and Antiaromaticity on Intrinsic Barriers of Proton Transfers in Aromatic and Antiaromatic Heterocyclic Systems; An ab Initio Study. Journal of Organic Chemistry, 2010, 75, 8422-8434.	1.7	10
3704	IR and UVâ€“visible spectroscopic studies of the adsorption of 3-fluorobenzoic acid on Au(111), Au(100) and Au(110) electrodes in neutral solution. Electrochimica Acta, 2010, 55, 8901-8907.	2.6	0
3705	Infrared Spectra and Quantum Chemical Calculations of the Uranium Carbide Molecules UC and CUC with Triple Bonds. Journal of the American Chemical Society, 2010, 132, 8484-8488.	6.6	55
3706	Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones. Organic and Biomolecular Chemistry, 2010, 8, 4884.	1.5	56
3707	Preparation of Trifluoromethylated Dihydrocoumarins, Indanones, and Arylpropanoic Acids by Tandem Superacidic Activation of 2-(Trifluoromethyl)acrylic Acid with Arenes. Journal of Organic Chemistry, 2010, 75, 2219-2226.	1.7	42
3708	Kinetic and Mechanistic Study onp-Quinodimethane Formation in the Sulfinyl Precursor Route for the Polymerization of Poly(p-phenylenevinylene) (PPV). Macromolecules, 2010, 43, 7424-7433.	2.2	26
3709	Infrared vibrational spectra as a structural probe of gaseous ions formed by caffeine and theophylline. Physical Chemistry Chemical Physics, 2010, 12, 3431.	1.3	22
3710	Structure of Donor Molecule 9,9-Bis(Methoxymethyl)-Fluorene in Ziegler-Natta Catalyst by Infrared Spectroscopy and Quantum Chemical Calculation. Journal of Physical Chemistry C, 2010, 114, 11475-11484.	1.5	43

#	Article	IF	Citations
3711	2-Pyridylnitrene and 3-Pyridazylcarbene and Their Relationship via Ring-Expansion, Ring-Opening, Ring-Contraction, and Fragmentation. Journal of Organic Chemistry, 2010, 75, 1600-1611.	1.7	35
3712	Time-resolved IR Studies on the Mechanism for the Functionalization of Primary Câ^'H Bonds by Photoactivated Cp*W(CO)₃(Bpin). Journal of the American Chemical Society, 2010, 132, 1848-1859.	6.6	41
3713	Computational Tests of Quantum Chemical Models for Structures, Vibrational Frequencies, and Heats of Formation of Molecules with Phosphorus and Sulfur Atoms. Journal of Physical Chemistry A, 2010, 114, 8142-8155.	1.1	12
3714	Reaction free energies in organic solvents: comparing different quantum mechanical methods. Molecular Simulation, 2010, 36, 1197-1207.	0.9	4
3715	Kinetically Controlled Photoinduced Electron Transfer Switching in Cu(I)-Responsive Fluorescent Probes. Journal of the American Chemical Society, 2010, 132, 737-747.	6.6	70
3716	Computational Studies of the Isomerization and Hydration Reactions of Acetaldehyde Oxide and Methyl Vinyl Carbonyl Oxide. Journal of Physical Chemistry A, 2010, 114, 9192-9204.	1.1	117
3717	Origins of Stereoselectivity in the Î±-Alkylation of Chiral Hydrazones. Journal of Organic Chemistry, 2010, 75, 8578-8584.	1.7	30
3718	Hydrogen donors in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> by infrared spectroscopy and first-principles calculations. Physical Review B, 2010, 82, .	1.1	50
3719	Sereneâ€"Ca²⁺versus sereneâ€"Cu²⁺complexes â€" AÂtheoretical perspective. Canadian Journal of Chemistry, 2010, 88, 759-768.	0.6	11
3720	Noncovalent Binding between Fullerenes and Protonated Porphyrins in the Gas Phase. Journal of Physical Chemistry A, 2010, 114, 11376-11385.	1.1	17
3721	The stability of [Zn(NH3)4]2+ in water: A quantum mechanical/molecular mechanical molecular dynamics study. Physical Chemistry Chemical Physics, 2010, 12, 9713.	1.3	28
3723	Facile Synthesis, Pure DFT Calculations, and PM3 Semiempirical MO Method Validation of Regiospecificity of Novel 1,4-Dihydropyrido[2,3-d]pyrimidine Derivatives. Synthetic Communications, 2010, 40, 2788-2805.	1.1	16
3724	Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics: Reaction Mechanism and Energetics. Journal of Physical Chemistry A, 2010, 114, 1996-2000.	1.1	29
3725	Ethanolysis of N-substituted norbornane epoxyimides: Discovery of diverse pathways depending on substituent's character. Organic and Biomolecular Chemistry, 2010, 8, 2142-57.	1.5	9
3726	Charge Transfer Interaction and Terahertz Studies of a Nonlinear Optical Material <scp>l</scp>-Glutamine Picrate: A DFT Study. Journal of Physical Chemistry A, 2010, 114, 13055-13064.	1.1	26
3727	Rules and trends of metal cation driven hydride-transfer mechanisms in metal amidoboranes. Physical Chemistry Chemical Physics, 2010, 12, 5446.	1.3	67
3728	Paracyclophanes as model compounds for strongly interacting Ï€-systems. Part 1. Pseudo-ortho-dihydroxy[2.2]paracyclophane. Physical Chemistry Chemical Physics, 2010, 12, 9339.	1.3	26
3729	Matrix infrared spectra and electronic structure calculations of the first actinide borylene: FBî€ThF2. Chemical Communications, 2010, 46, 1646.	2.2	26

#	Article	IF	Citations
3730	Infrared spectra of XCî€,IrX3 and CX2î€ŀrX2 prepared by reactions of laser-ablated iridium atoms with halomethanes. Dalton Transactions, 2010, 39, 5478.	1.6	23
3731	CO-promoted N2 adsorption on copper atoms. Physical Chemistry Chemical Physics, 2010, 12, 7077.	1.3	11
3732	Ultrafast time-resolved transient infrared and resonance Raman spectroscopic study of the photo-deprotection and rearrangement reactions of p-hydroxyphenacyl caged phosphates. Faraday Discussions, 0, 145, 171-183.	1.6	10
3733	Syntheses and molecular structures of some tricobaltcarbonylclusters containing 2,4,6-trimethyl-1,3,5-trithiane. Dalton Transactions, 2010, 39, 1222-1234.	1.6	11
3734	Kinetic correlations for H2 addition and elimination reaction mechanisms during silicon hydride pyrolysis. Physical Chemistry Chemical Physics, 2010, 12, 12676.	1.3	33
3735	Rate coefficients for cycloalkyl + O reactions and product branching in the decomposition of chemically activated cycloalkoxy radicals: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2010, 12, 8953.	1.3	11
3736	Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. Physical Chemistry Chemical Physics, 2010, 12, 5375.	1.3	29
3737	Theoretical and experimental investigation of the structural and spectroscopic properties of coumarin 343 fluoroionophores. Physical Chemistry Chemical Physics, 2010, 12, 14172.	1.3	23
3738	Vibrational signatures of metal-chelated monosaccharide epimers: gas-phase infrared spectroscopy of Rb+-tagged glucuronic and iduronic acid. Physical Chemistry Chemical Physics, 2010, 12, 3474.	1.3	41
3739	Comparative Theoretical Studies of Energetic Substituted Carbon- and Nitrogen-Bridged Difurazans. Journal of Physical Chemistry A, 2010, 114, 603-612.	1.1	76
3740	Infrared Spectra of a Species of Potential Prebiotic and Astrochemical Interest: Cyanoethenethiol (NCâˆ'CHâ•CHâˆ'SH). Journal of Physical Chemistry A, 2010, 114, 9583-9588.	1.1	8
3741	Electronic Properties of N(5)-Ethyl Flavinium Ion. Journal of Physical Chemistry A, 2010, 114, 12138-12147.	1.1	26
3742	Computational Investigation of the Reaction Mechanisms of Nitroxyl and Thiols. Journal of Organic Chemistry, 2010, 75, 4014-4024.	1.7	31
3743	Structure and Dynamics of the Chromate Ion in Aqueous Solution. An ab Initio QMCF-MD Simulation. Inorganic Chemistry, 2010, 49, 7964-7968.	1.9	16
3744	Assignment of the Vibrational Spectra of Enzyme-Bound Tryptophan Tryptophyl Quinones Using a Combined QM/MM Approach. Journal of Physical Chemistry A, 2010, 114, 1212-1217.	1.1	7
3745	Synthesis and Computational Study of Phosphorus Ionic Liquids. Phosphorus, Sulfur and Silicon and the Related Elements, 2010, 185, 2464-2471.	0.8	2
3746	Concerning the conformational preferences of the 2-cyano derivatives of oxane, thiane, and selenane. Canadian Journal of Chemistry, 2010, 88, 831-838.	0.6	5
3747	FT-IR, FT-Raman and UVâ€"vis spectra and quantum chemical investigation of trimetazidine. Molecular Simulation, 2010, 36, 969-977.	0.9	3

#	Article	IF	Citations
3748	The electronic structures of diruthenium complexes containing an oligo(phenylene ethynylene) bridging ligand, and some related molecular structures. Dalton Transactions, 2010, 39, 11605.	1.6	20
3749	Electron capture activation of the disulfide bond. The role of the asymmetry and electronegativity. Physical Chemistry Chemical Physics, 2010, 12, 1042-1050.	1.3	17
3750	High temperature Raman spectroscopic study of the micro-structure of a caesium triborate crystal and its liquid. CrystEngComm, 2011, 13, 3030.	1.3	13
3751	Structural Determinant of Chemical Reactivity and Potential Health Effects of Quinones from Natural Products. Chemical Research in Toxicology, 2011, 24, 1527-1539.	1.7	19
3752	Paracyclophanes as model compounds for strongly interacting Ï€-systems. Part 2: mono-hydroxy[2.2]paracyclophane. Physical Chemistry Chemical Physics, 2011, 13, 11076.	1.3	21
3753	Interfacial Ring Orientation in Polythiophene Field-Effect Transistors on Functionalized Dielectrics. Journal of Physical Chemistry C, 2011, 115, 16027-16036.	1.5	49
3754	Effect of Solvation on Ion Binding to Imidazole and Methylimidazole. Journal of Physical Chemistry A, 2011, 115, 1971-1984.	1.1	32
3755	Simultaneous Bridge-Localized and Mixed-Valence Character in Diruthenium Radical Cations Featuring Diethynylaromatic Bridging Ligands. Journal of the American Chemical Society, 2011, 133, 18433-18446.	6.6	138
3756	Excited-state Nâ€“Hâ‹¯S hydrogen bond between indole and dimethyl sulfide: time-dependent density functional theory study. Physical Chemistry Chemical Physics, 2011, 13, 15299.	1.3	29
3757	Density functional theory andab initiostudies of vibrational spectra of 2-bis (2-chloroethyl) aminoperhydro-1,3,2-oxazaphosphorinane-2-oxide. Molecular Simulation, 2011, 37, 1276-1288.	0.9	9
3758	Measurement of the interaction of aqueous copper(II) with a model amyloid-Î² protein fragmentÂâ€” Interference from buffers. Canadian Journal of Chemistry, 2011, 89, 1429-1444.	0.6	8
3759	Spectroscopic and computational study of Î²-ethynylphenylene substituted zinc and free-base porphyrins. Physical Chemistry Chemical Physics, 2011, 13, 1597-1605.	1.3	38
3760	A novel hydrazide type organocatalyst for enantioselective Dielsâ€“Alder reactions. Organic and Biomolecular Chemistry, 2011, 9, 3033.	1.5	13
3761	Ï€-Complexed polyfluoroarenes: a reactivity, bonding and spectroscopic study of (Î·6-C6F6)Cr(Î·6-C6H6) and related molecules. New Journal of Chemistry, 2011, 35, 2066.	1.4	5
3762	An indole-linked C8-deoxyguanosine nucleoside acts as a fluorescent reporter of Watsonâ€“Crick versus Hoogsteen base pairing. Organic and Biomolecular Chemistry, 2011, 9, 1565.	1.5	17
3763	Infrared spectra of CH3â€“MH, CH3â€“M, and CH3â€“MHâ‹¯ prepared via methane activation by laser-ablated Au, Ag, and Cu atoms. Dalton Transactions, 2011, 40, 11115.	1.6	35
3764	Structure and unimolecular chemistry of protonated sulfur betaines, (CH3)2S+(CH2)nCO2H (n = 1 and) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	3
3765	Oxidation of 4-substituted TEMPO derivatives reveals modifications at the 1- and 4-positions. Organic and Biomolecular Chemistry, 2011, 9, 4936.	1.5	47

#	Article	IF	Citations
3766	Experimental and theoretical investigations into the counter-intuitive shift in the antisymmetric Î½(Siâ€“O) vibrational modes upon deuteration of solvated silicic acid (H₄SiO₄). Physical Chemistry Chemical Physics, 2011, 13, 2314-2322.	1.3	27
3767	Structure and dynamics of the Zr⁴⁺ion in water. Physical Chemistry Chemical Physics, 2011, 13, 224-229.	1.3	29
3768	Effects of Side-Chain Orientation on the Backbone Conformation of the Dehydrophenylalanine Residue. Theoretical and X-ray Study. Journal of Physical Chemistry B, 2011, 115, 4295-4306.	1.2	15
3769	Reactions of Ions with Ionic Liquid Vapors by Selected-Ion Flow Tube Mass Spectrometry. Journal of Physical Chemistry Letters, 2011, 2, 874-879.	2.1	9
3770	Analysis of 5-Hydroxyisoflavones by Surface-Enhanced Raman Spectroscopy: Genistein and Methoxy Derivatives. Journal of Physical Chemistry B, 2011, 115, 13943-13954.	1.2	11
3771	Deep UV Resonance Raman Spectroscopy of Î²-Sheet Amyloid Fibrils: A QM/MM Simulation. Journal of Physical Chemistry B, 2011, 115, 13955-13962.	1.2	14
3772	Effective Fragment Potential Study of the Influence of Hydration on the Vibrational Spectrum of Glucose. Journal of Physical Chemistry A, 2011, 115, 12373-12379.	1.1	10
3773	Solid-State Tautomerism in 2-Carboxyindan-1,3-dione. Journal of Physical Chemistry A, 2011, 115, 2026-2034.	1.1	4
3774	Molecular Orientation of Asphaltenes and PAH Model Compounds in Langmuirâ^'Blodgett Films Using Sum Frequency Generation Spectroscopy. Langmuir, 2011, 27, 6049-6058.	1.6	116
3775	Theoretical Study of Isomerization and Dissociation Transition States of C3H5O Radical Isomers: Ab Initio Characterization of the Critical Points and Statistical Transition-State Theory Modeling of the Dynamics. Journal of Physical Chemistry A, 2011, 115, 1701-1712.	1.1	15
3776	Complete Family of Mono-, Bi-, and Trinuclear Re^I(CO)₃Cl Complexes of the Bridging Polypyridyl Ligand 2,3,8,9,14,15-Hexamethyl-5,6,11,12,17,18-hexaazatrinapthalene: Syn/Anti Isomer Separation, Characterization, and Photophysics. Inorganic Chemistry, 2011, 50, 6093-6106.	1.9	50
3777	Quantum-Chemical Calculations and IR Spectra of the (F₂)MF₂ Molecules (M =) Tj ETQq1 1 0.784314 rgBT /O Journal of the American Chemical Society, 2011, 133, 3768-3771.	6.6	13
3778	Environmental Effects on the Lignin Model Monomer, Vanillyl Alcohol, Studied by Raman Spectroscopy. Journal of Physical Chemistry B, 2011, 115, 11470-11480.	1.2	20
3779	Adsorption of Enterobactin to Metal Oxides and the Role of Siderophores in Bacterial Adhesion to Metals. Langmuir, 2011, 27, 10587-10596.	1.6	27
3780	Effects of Chemical Structure on the Thermodynamic Efficiency of Radical Chain Carriers for Organic Synthesis. Journal of Organic Chemistry, 2011, 76, 1715-1726.	1.7	19
3781	The Role of Multifunctional Kinetics during Early-Stage Silicon Hydride Pyrolysis: Reactivity of Si₂H₂ Isomers with SiH₄ and Si₂H₆. Journal of Physical Chemistry A, 2011, 115, 2409-2422.	1.1	16
3782	Theoretical Study of the Equilibrium Structure, Vibrational Spectrum, and Thermochemistry of the Peroxynitrate CF2BrCFBrOONO2. Journal of Physical Chemistry A, 2011, 115, 7744-7752.	1.1	4
3783	Modeling Solvation of Magnesium Centers by Ether Ligands: Gas-Phase Synthesis and Hydrolysis of the Organomagnesium Cations [CH₃Mg(3X-crown-X)]⁺(X=) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	17

#	Article	IF	Citations
3784	Validation of the Distal Effect of Electron-Withdrawing Groups on the Stability of Peptide Enolates and Its Exploitation in the Controlled Stereochemical Inversion of Amino Acid Derivatives. Journal of Organic Chemistry, 2011, 76, 5907-5914.	1.7	9
3786	Disulfide Passivation of the Ge(100)-2 Ã— 1 Surface. Langmuir, 2011, 27, 179-186.	1.6	24
3787	Rhenium in Homogeneous Catalysis: [ReBrH(NO)(labile ligand)(large-bite-angle diphosphine)] Complexes as Highly Active Catalysts in Olefin Hydrogenations. Journal of the American Chemical Society, 2011, 133, 8168-8178.	6.6	57
3788	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. Chemistry of Materials, 2011, 23, 2979-2986.	3.2	337
3789	Linear-Free Energy Relationships for Modeling Structureâ€“Reactivity Trends in Controlled Radical Polymerization. Macromolecules, 2011, 44, 7568-7583.	2.2	69
3790	Theoretical Study of Oâ€“O Single Bond Formation in the Oxidation of Water by the Ruthenium Blue Dimer. Journal of Physical Chemistry A, 2011, 115, 8003-8016.	1.1	46
3791	Thermochemical Property Estimation of Hydrogenated Silicon Clusters. Journal of Physical Chemistry A, 2011, 115, 8969-8982.	1.1	25
3792	Infrared Spectroscopy of Mn⁺(H₂O) and Mn²⁺(H₂O) via Argon Complex Predissociation. Journal of Physical Chemistry A, 2011, 115, 7602-7609.	1.1	45
3793	Charge Sensitive Vibrations and Electron-Molecular Vibration Coupling in Bis(ethylenedithio)-tetrathiafulvalene (BEDT-TTF). Journal of Physical Chemistry C, 2011, 115, 19371-19378.	1.5	54
3794	Quest for Even Higher Stabilized Foiled Carbenesâ€. Journal of Organic Chemistry, 2011, 76, 7491-7496.	1.7	1
3795	Kinetics and Mechanisms of the Allyl + Allyl and Allyl + Propargyl Recombination Reactions. Journal of Physical Chemistry A, 2011, 115, 7610-7624.	1.1	39
3797	Reaction of HOD+with NO2: Effects of OD and OH Stretching, Bending, and Collision Energy on Reactions on the Singlet and Triplet Potential Surfaces. Journal of Physical Chemistry A, 2011, 115, 1172-1185.	1.1	6
3798	Computational Study of the Chemistry of 3-Phenylpropyl Radicals. Journal of Physical Chemistry A, 2011, 115, 2431-2441.	1.1	3
3799	Early Events in the Photochemistry of 1,2,3-Thiadiazole Studied by Ultrafast Time-Resolved UVâ€“Vis and IR Spectroscopies. Journal of Physical Chemistry A, 2011, 115, 14300-14305.	1.1	19
3800	Polymorphism of Dehydrobenzo[14]annulene Possessing Two Methyl Ester Groups in Noncentrosymmetric Positions. Crystal Growth and Design, 2011, 11, 5488-5497.	1.4	28
3801	Infrared Spectrum of the CH3OCH2Radical in Solid Argon. Journal of Physical Chemistry A, 2011, 115, 3029-3033.	1.1	10
3802	Infrared Spectra of CX₃â^'MnX and CX₂â•MnX₂ (X = H, F, Cl) Prepared in Reactions of Laser-Ablated Manganese Atoms with Halomethanes. Organometallics, 2011, 30, 477-486.	1.1	19
3803	Polarization-Angle-Scanning Two-Dimensional Spectroscopy: Application to Dipeptide Structure Determination. Journal of Physical Chemistry A, 2011, 115, 3766-3777.	1.1	1

#	Article	IF	Citations
3804	Vibrational Spectra of the Ground and the Singlet Excited Ï€Ï€* State of 6,7-Dimethyl-8-ribityllumazine. Journal of Physical Chemistry B, 2011, 115, 3689-3697.	1.2	7
3805	Effects of Olefin Group and Its Position on the Kinetics for Intramolecular H-Shift and HO₂ Elimination of Alkenyl Peroxy Radicals. Journal of Physical Chemistry A, 2011, 115, 655-663.	1.1	46
3806	Anharmonicity of Weakly Bound M⁺â^'H₂ Complexes. Journal of Physical Chemistry A, 2011, 115, 3272-3278.	1.1	22
3807	Paracyclophanes as Model Compounds for Strongly Interacting Ï€-Systems, Part 3: Influence of the Substitution Pattern on Photoabsorption Properties. Journal of Physical Chemistry A, 2011, 115, 3583-3591.	1.1	16
3808	Theoretical Investigation of Raman Optical Activity Signatures of TrÃ¶gerâ€™s Base. Journal of Physical Chemistry A, 2011, 115, 13706-13713.	1.1	6
3809	Structures, Internal Rotor Potentials, and Thermochemical Properties for a Series of Nitrocarbonyls, Nitroolefins, Corresponding Nitrites, and Their Carbon Centered Radicals. Journal of Physical Chemistry A, 2011, 115, 13921-13930.	1.1	7
3810	Spectroscopy of Free-Base N-Confused Tetraphenylporphyrin Radical Anion and Radical Cation. Journal of Physical Chemistry A, 2011, 115, 6456-6471.	1.1	17
3811	Matrix Infrared Spectroscopic and Theoretical Investigations of Uranium Atom and Methanol Reaction Products. Inorganic Chemistry, 2011, 50, 7099-7105.	1.9	14
3812	Understanding Thermodynamic Properties at the Molecular Level: Multiple Temperature Charge Density Study of Ribitol and Xylitol. Journal of Physical Chemistry A, 2011, 115, 7794-7804.	1.1	31
3813	Ultrafast Infrared Spectroscopy of an Isotope-Labeled Photoactivatable Flavoprotein. Biochemistry, 2011, 50, 1321-1328.	1.2	36
3814	Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F₄-TCNQ): A Density Functional Theory Study. Chemistry of Materials, 2011, 23, 5149-5159.	3.2	102
3815	Electron Distribution in Partially Reduced Mixed Metal Oxide Systems: Infrared Spectroscopy of Ce_mV_nO_o⁺ Gas-Phase Clusters. Journal of Physical Chemistry A, 2011, 115, 11187-11192.	1.1	42
3816	DFT Study on the Cycloreversion of Thietane Radical Cations. Journal of Physical Chemistry A, 2011, 115, 5443-5448.	1.1	4
3817	Matrix Infrared Spectroscopic and Computational Investigations of the Lanthanideâ^'Methylene Complexes CH₂LnF₂ with Single Lnâ^'C Bonds. Journal of Physical Chemistry A, 2011, 115, 1913-1921.	1.1	31
3818	Time-Resolved Resonance Raman Spectroscopic Studies on the Triplet Excited State of Thioxanthone. Journal of Physical Chemistry A, 2011, 115, 7566-7573.	1.1	11
3819	Infrared Spectra of Rh Atom Reaction Products with C₂H₂: The HRhCCH, RhCCH, RhCCH₂, and Rh-Î·²-C₂H₂ Molecules. Journal of Physical Chemistry A, 2011, 115, 9447-9455.	1.1	21
3820	The Distal Effect of N-Electron-withdrawing Groups on the Stability of Peptide Carbon Radicals. Australian Journal of Chemistry, 2011, 64, 403.	0.5	8
3821	Understanding Optoelectronic Properties of Cyano-Terminated Oligothiophenes in the Context of Intramolecular Charge Transfer. Journal of Physical Chemistry B, 2011, 115, 10573-10585.	1.2	23

#	Article	IF	Citations
3822	Hydrogenated cation vacancies in semiconducting oxides. Journal of Physics Condensed Matter, 2011, 23, 334212.	0.7	237
3823	Photoinduced Rearrangement of Aromatic N-Chloroamides to Chloroaromatic Amides in the Solid State: Inverted Î_Nâ€“Î£_N Occupational Stability of Amidyl Radicals. Journal of Physical Chemistry A, 2011, 115, 7834-7848.	1.1	8
3824	Synthesis and stability of 2-tetrazenium salts. New Journal of Chemistry, 2011, 35, 1640.	1.4	9
3825	Diazotization of the Amino Acid [closo-1-CB9H8-1-COOH-6-NH3] and Reactivity of the [closo-1-CB9H8-1-COO-6-N2]â^'Anion. Inorganic Chemistry, 2011, 50, 2654-2660.	1.9	22
3826	Study of Energetics and Structure of 1,2,3-Benzotriazin-4(3H)-one and its 1H and Enol Tautomers. Journal of Physical Chemistry B, 2011, 115, 6616-6622.	1.2	14
3827	Mechanistic Insights on N-Heterocyclic Carbene-Catalyzed Annulations: The Role of Base-Assisted Proton Transfers. Journal of Organic Chemistry, 2011, 76, 5606-5613.	1.7	86
3828	A Simplified Process for the Manufacture of AZD0530, a Potent SRC Kinase Inhibitor. Organic Process Research and Development, 2011, 15, 688-692.	1.3	5
3829	Intramolecular Charge Transfer and Z-Scan Studies of a Semiorganic Nonlinear Optical Material Sodium Acid Phthalate Hemihydrate: A Vibrational Spectroscopic Study. Journal of Physical Chemistry A, 2011, 115, 8216-8226.	1.1	58
3830	Computational Studies of Lewis Acidities of Tris(fluorophenyl)-Substituted Boranes: An Additive Relationship between Lewis Acidity and Fluorine Position. Inorganic Chemistry, 2011, 50, 7871-7879.	1.9	35
3831	A theoretical study on the structures, thermodynamic properties and detonation performances of azidamines. Molecular Simulation, 2011, 37, 893-898.	0.9	0
3832	Combined Triple and Double Bonds to Uranium: The Nâ‰¡Uâ•Nâ^'H Uranimine Nitride Molecule Prepared in Solid Argon. Inorganic Chemistry, 2011, 50, 3826-3831.	1.9	43
3833	Analytical approach for the excited-state Hessian in time-dependent density functional theory: Formalism, implementation, and performance. Journal of Chemical Physics, 2011, 135, 184111.	1.2	107
3834	The HRuCCH, RuCCH₂, and Ru-Î·²-C₂H₂ Molecules: Infrared Spectra and Density Functional Calculations. Journal of Physical Chemistry A, 2011, 115, 12194-12200.	1.1	18
3835	Convert graphene sheets to boron nitride and boron nitrideâ€“carbon sheets via a carbon-substitution reaction. Applied Physics Letters, 2011, 98, .	1.5	60
3836	Synthesis and evaluation of sesquiterpene lactone inhibitors of phospholipase A2 from Bothrops jararacussu. Toxicon, 2011, 57, 100-108.	0.8	22
3837	Absorption, Photoluminescence, and Polarized Raman Spectra of a Fourfold Alkoxy-Substituted Phthalocyanine Liquid Crystal. Journal of Physical Chemistry C, 2011, 115, 12150-12157.	1.5	25
3839	Substituent Effects on the Properties Related to Detonation Performance and Sensitivity for 2,2â€²,4,4â€²,6,6â€²-Hexanitroazobenzene Derivatives. Journal of Physical Chemistry A, 2011, 115, 1754-1762.	1.1	72
3840	Theoretical Studies on the Heats of Formation, Detonation Properties, and Pyrolysis Mechanisms of Energetic Cyclic Nitramines. Journal of Physical Chemistry A, 2011, 115, 13858-13864.	1.1	67

#	Article	IF	Citations
3841	Surface-Enhanced Raman Scattering on Semiconducting Oxide Nanoparticles: Oxide Nature, Size, Solvent, and pH Effects. Journal of Physical Chemistry C, 2011, 115, 8994-9004.	1.5	79
3842	Vibrational Spectra of Î±-Glucose, Î²-Glucose, and Sucrose: Anharmonic Calculations and Experiment. Journal of Physical Chemistry A, 2011, 115, 5859-5872.	1.1	63
3843	Solvation and Crystal Effects in Bilirubin Studied by NMR Spectroscopy and Density Functional Theory. Journal of Physical Chemistry A, 2011, 115, 11696-11714.	1.1	10
3844	Sulfur Dioxide in Water: Structure and Dynamics Studied by an Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation. Inorganic Chemistry, 2011, 50, 3379-3386.	1.9	15
3845	The Structures and Stabilities of the Complexes of Biologically Available Ligands with Fe(III)â˜Porphine: An Ab Initio Study. Journal of Physical Chemistry B, 2011, 115, 569-579.	1.2	15
3846	Dinuclear Zn(II) Complex Catalyzed Phosphodiester Cleavage Proceeds via a Concerted Mechanism: A Density Functional Theory Study. Journal of the American Chemical Society, 2011, 133, 2904-2915.	6.6	55
3847	The Nature of In-Plane Skeleton Raman Modes of P3HT and Their Correlation to the Degree of Molecular Order in P3HT:PCBM Blend Thin Films. Journal of the American Chemical Society, 2011, 133, 9834-9843.	6.6	350
3848	Ï€-conjugation and charge polarization in fluorene-dibenzothiophene-S,S-dioxide co-oligomers by Raman spectroscopy and quantum chemistry. Journal of Chemical Physics, 2011, 134, 044520.	1.2	13
3849	Understanding the Electronic Reorganization along the Nonpolar [3 + 2] Cycloaddition Reactions of Carbonyl Ylides.. Journal of Organic Chemistry, 2011, 76, 373-379.	1.7	89
3850	The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. Journal of Chemical Theory and Computation, 2011, 7, 2804-2817.	2.3	87
3851	DFT Study of Trichloroethene Reaction with Permanganate in Aqueous Solution. Environmental Science & Technology, 2011, 45, 3006-3011.	4.6	29
3852	Quantitative Infrared Intensity Studies of Vapor-Phase Glyoxal, Methylglyoxal, and 2,3-Butanedione (Diacetyl) with Vibrational Assignments. Journal of Physical Chemistry A, 2011, 115, 9886-9900.	1.1	48
3853	The Joining of Measurement and Prediction: The Enthalpy of Formation of 1,4-Cubanedicarboxylic Acid. Journal of Chemical & Engineering Data, 2011, 56, 1220-1228.	1.0	14
3854	Quantum Mechanical Modeling of Catalytic Processes. Annual Review of Chemical and Biomolecular Engineering, 2011, 2, 453-477.	3.3	68
3856	Reaction of N-Acyloxy-N-alkoxyamides with Biological Thiol Groups. Australian Journal of Chemistry, 2011, 64, 443.	0.5	12
3857	Intermediates of CO oxidation on iron oxides: An experimental and theoretical study. Journal of Chemical Physics, 2011, 134, 034305.	1.2	11
3858	Proton transfer reactions and dynamics of sulfonic acid group in NafionÂ®. Physical Chemistry Chemical Physics, 2011, 13, 10923.	1.3	30
3859	Î²-Carotene Radical Cation Addition to Green Tea Polyphenols. Mechanism of Antioxidant Antagonism in Peroxidizing Liposomes. Journal of Agricultural and Food Chemistry, 2011, 59, 12643-12651.	2.4	32

#	Article	IF	Citations
3860	Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study. Journal of Chemical & Engineering Data, 2011, 56, 4516-4523.	1.0	12
3861	Direct Calculations of Mid- and Near-IR Absorption and Circular Dichroism Spectra of Chiral Molecules Using QM/MM Molecular Dynamics Simulation Method. Journal of Chemical Theory and Computation, 2011, 7, 4097-4103.	2.3	29
3862	Stereocontrolled Ring-Opening of a Hindered Sulfamidate with Nitrogen-Containing Aromatic Heterocycles: Synthesis of Chiral Quaternary Imidazole Derivatives. Journal of Organic Chemistry, 2011, 76, 4034-4042.	1.7	25
3863	Infrared Spectra of CH₃â€“MF and Several Fragments Prepared by Methyl Fluoride Reactions with Laser-Ablated Cu, Ag, and Au Atoms. Inorganic Chemistry, 2011, 50, 10319-10327.	1.9	20
3864	Anharmonic Vibrational Modes of Nucleic Acid Bases Revealed by 2D IR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 15650-15660.	6.6	108
3865	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. Organic and Biomolecular Chemistry, 2011, 9, 6616.	1.5	45
3866	Manganese substituted Compound I of cytochrome P450 biomimetics: A comparative reactivity study of MnV-oxo versus MnIV-oxo species. Archives of Biochemistry and Biophysics, 2011, 507, 4-13.	1.4	39
3867	Nitrogen dioxide solubility and permeation in lipid membranes. Archives of Biochemistry and Biophysics, 2011, 512, 190-196.	1.4	36
3868	Polymerization of aqueous silica in H2Oâ€“K2O solutions at 25â€“200Â°C and 1bar to 20kbar. Chemical Geology, 2011, 283, 161-170.	1.4	59
3869	Density functional theory studies of energetic nitrogen-rich derivatives of substituted carbon-bridged diiminotetrazoles. Computational and Theoretical Chemistry, 2011, 967, 257-264.	1.1	14
3870	Calculation of vibrational spectroscopic and NMR parameters of 2-Dicyanovinyl-5-(4-N,N-dimethylaminophenyl) thiophene by ab initio HF and density functional methods. Computational and Theoretical Chemistry, 2011, 969, 27-34.	1.1	61
3871	Density functional theory study of electronic structure and spectra of tetraoxa[8]circulenes. Computational and Theoretical Chemistry, 2011, 972, 68-74.	1.1	43
3872	Electronic structure, electric moments and vibrational analysis of 5-nitro-2-furaldehyde semicarbazone: A D.F.T. study. Computational and Theoretical Chemistry, 2011, 973, 20-27.	1.1	19
3873	Comprehensive computational study of gas-phase conformations of neutral, protonated and deprotonated glutamic acids. Computational and Theoretical Chemistry, 2011, 976, 42-50.	1.1	23
3874	Electronic structure, vibrational spectra and 1H NMR of halide ion (Fâˆ’, Clâˆ’ and Brâˆ’) encapsulated bambus[6]uril from density functional theory. Computational and Theoretical Chemistry, 2011, 976, 76-82.	1.1	16
3875	Computational outlook on the ribosome as an entropy trap. Computational and Theoretical Chemistry, 2011, 976, 148-152.	1.1	6
3876	Calculation of equilibrium stable isotope partition function ratios for aqueous zinc complexes and metallic zinc. Geochimica Et Cosmochimica Acta, 2011, 75, 769-783.	1.6	83
3877	Equilibrium mass-dependent fractionation relationships for triple oxygen isotopes. Geochimica Et Cosmochimica Acta, 2011, 75, 7435-7445.	1.6	109

#	Article	IF	Citations
3878	Kinetic and thermodynamic aspects of the chain-breaking antioxidant activity of ascorbic acid derivatives in non-aqueous media. Organic and Biomolecular Chemistry, 2011, 9, 3792.	1.5	55
3879	Time-Resolved Resonance Raman Spectroscopy: Exploring Reactive Intermediates. Applied Spectroscopy, 2011, 65, 1087-1115.	1.2	53
3880	To Bend or Not to Bend! The Dilemma of Allenes. Journal of Organic Chemistry, 2011, 76, 2558-2567.	1.7	49
3881	Theoretical Prediction of Properties of Aliphatic Polynitrates. Journal of Physical Chemistry A, 2011, 115, 795-804.	1.1	27
3882	Synthesis and structural characterization of group 6 transition metal complexes with terminal fluoromethylidyne (CF) ligands; a DFT/NBO/NRT comparison of bonding characteristics of terminal NO, CF and CH ligands. Dalton Transactions, 2011, 40, 47-55.	1.6	19
3883	Development of CHARMM Polarizable Force Field for Nucleic Acid Bases Based on the Classical Drude Oscillator Model. Journal of Physical Chemistry B, 2011, 115, 580-596.	1.2	121
3884	Computational Studies on the Crystal Structure, Thermodynamic Properties, Detonation Performance, and Pyrolysis Mechanism of 2,4,6,8-Tetranitro-1,3,5,7-tetraazacubane as a Novel High Energy Density Material. Journal of Physical Chemistry A, 2011, 115, 11788-11795.	1.1	63
3885	Proton transfer reactions and dynamics in protonated water clusters. Physical Chemistry Chemical Physics, 2011, 13, 4562.	1.3	31
3886	CHARMM Additive All-Atom Force Field for Carbohydrate Derivatives and Its Utility in Polysaccharide and Carbohydrateâ€“Protein Modeling. Journal of Chemical Theory and Computation, 2011, 7, 3162-3180.	2.3	559
3887	Entropy Calculations of Single Molecules by Combining the Rigidâ€“Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2638-2653.	2.3	56
3888	Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals. Organic and Biomolecular Chemistry, 2011, 9, 3636.	1.5	63
3889	Infrared Multiple Photon Dissociation Action Spectroscopy and Computational Studies of Mass-Selected Gas-Phase Fluorescein and 2â€²,7â€²-Dichlorofluorescein Ions. Journal of Physical Chemistry A, 2011, 115, 9739-9747.	1.1	23
3890	Organocatalytic, Enantioselective Intramolecular [6 + 2] Cycloaddition Reaction for the Formation of Tricyclopentanoids and Insight on Its Mechanism from a Computational Study. Journal of the American Chemical Society, 2011, 133, 20175-20185.	6.6	66
3891	Electrophilic organic selenium reagentsâ€”protonated seleninic acids as precursors for unsymmetrical aromatic selenides. Tetrahedron, 2011, 67, 2633-2643.	1.0	26
3892	On the Involvement of Copper Binding to the N-Terminus of the Amyloid Beta Peptide of Alzheimer's Disease: A Computational Study on Model Systems. International Journal of Alzheimer's Disease, 2011, 2011, 1-15.	1.1	18
3893	Tert-butyl esters of 2,3-diaryl-3-arylaminopropanoic acids - stereoselective synthesis, isolation, spectroscopic and structural elucidation. Polish Journal of Chemical Technology, 2011, 13, 12-17.	0.3	1
3894	Thermochemistry and Kinetics for 2-Butanone-3yl Radical (CH₃C(=O)CH^{â€¢}CH₃) Reactions with O₂. Zeitschrift Fur Physikalische Chemie, 2011, 225, 993-1018.	1.4	26
3895	Silver-Catalyzed Carbon Dioxide Incorporation and Rearrangement on Propargylic Derivatives. Bulletin of the Chemical Society of Japan, 2011, 84, 698-717.	2.0	116

#	Article	IF	Citations
3896	Intercluster Reactions Show That (CH₃)₂S⁺CH₂CO₂H is a Better Methyl Cation Donor Than (CH₃)₃N⁺CH₂CO₂H. European Journal of Mass Spectrometry, 2011, 17, 159-166.	0.5	7
3898	Hydrogen and oxygen adsorption on a nanosilicate - a quantum chemical study. Monthly Notices of the Royal Astronomical Society, 2011, 414, 1285-1291.	1.6	27
3899	Conformational search for zwitterionic leucine and hydrated conformers of both the canonical and zwitterionic leucine using the DFT-CPCM model. Vibrational Spectroscopy, 2011, 56, 74-81.	1.2	19
3900	Terahertz, infrared and Raman vibrational assignments of [FeFe]-hydrogenase model compounds. Vibrational Spectroscopy, 2011, 56, 219-227.	1.2	11
3901	The effect of electron charge transfer in biological activity and vibrational wavenumbers of 2â€²-Deoxyuridine and 5-Fluoro-2â€²-Deoxyuridine: DFT approach. Solid State Sciences, 2011, 13, 1906-1915.	1.5	4
3902	1,3-Dipolar cycloaddition of 1H-pyrazinium-3-olate and N1- and C-methyl substituted pyrazinium-3-olates with methyl acrylate: a density functional theory study. Tetrahedron, 2011, 67, 8383-8391.	1.0	9
3903	Characterization of the structure and dynamics of an aqueous Hg2+ solution by an ab initio molecular dynamics study. Journal of Molecular Liquids, 2011, 163, 147-152.	2.3	7
3904	Extensive study of the autooxidation products of apomorphine and its pharmacologically active derivatives. Journal of Molecular Structure, 2011, 1002, 37-44.	1.8	7
3905	On the photochemistry of 4-azidoquinoline 1-oxide: Structural elucidation of primary photoproduct. Journal of Molecular Structure, 2011, 1003, 41-46.	1.8	1
3906	Fluorine radical interception with radical traps: An experimental and DFT study. Journal of Molecular Structure, 2011, 1002, 121-127.	1.8	5
3907	The structure elucidation of mequindox and 1,4-bisdesoxymequindox: NMR analyses, FT-IR spectra, DFT calculations and thermochemical studies. Journal of Molecular Structure, 2011, 1004, 109-115.	1.8	8
3908	Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UVâ€“Visible) and DFT studies of 2-amino-5-chlorobenzoxazole. Journal of Molecular Structure, 2011, 1003, 92-102.	1.8	19
3909	Study of vibrational spectra and molecular structure of intermolecular hydrogen bonded 2-thiohydantoin using Density Functional Theory. Journal of Molecular Structure, 2011, 1004, 237-247.	1.8	22
3910	Molecular structures and preferred conformations of stabilized keto diester phosphonium ylides. Journal of Molecular Structure, 2011, 1004, 284-291.	1.8	3
3911	Analysis of molecular structure and vibrational spectra of 2-(2â€²-thienyl)pyridine. Journal of Molecular Structure, 2011, 1005, 100-106.	1.8	20
3912	Structure of 4-(trimethylammonium)benzoate hydrate studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra. Journal of Molecular Structure, 2011, 1005, 144-151.	1.8	8
3913	Vibrational, nuclear magnetic resonance and electronic spectra, quantum chemical investigations of 2-amino-6-fluorobenzothiazole. Journal of Molecular Structure, 2011, 1006, 247-258.	1.8	26
3914	Structure of methyl 4-(trimethylammonium)benzoate iodide studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra. Journal of Molecular Structure, 2011, 1006, 330-336.	1.8	6

#	Article	IF	Citations
3915	Intermolecular CHâ‹¯O hydrogen bonds in formyl-substituted diphenylhexatriene, a [2+2] photoreactive organic solid: Crystal structure and IR, NMR spectroscopic evidence. Journal of Molecular Structure, 2011, 1006, 366-374.	1.8	12
3916	Synthesis, crystal structure, vibrational spectral and density functional studies of 4-(2,5-dioxo-2H-pyrrol-1(5H)-yl)antipyrine. Journal of Molecular Structure, 2011, 1006, 383-394.	1.8	7
3917	Experimental and theoretical investigation on the vibrational spectroscopy of l-theanine. Journal of Molecular Structure, 2011, 1006, 559-565.	1.8	2
3918	Vibrational spectra of (4E)-4-((E)-3-phenyl-allylideneamino)-1,2-dihydro-2,3-dimethyl-1-phenylpirazol-5-one. Journal of Molecular Structure, 2011, 1006, 589-595.	1.8	2
3919	One-pot synthesis, FT-IR, NMR and density functional method (B3LYP) studies on 2-(cyclohexylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 64-71.	2.0	14
3920	Natural bond orbital analysis, electronic structure, non-linear properties and vibrational spectral analysis of l-histidinium bromide monohydrate: A density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 85-98.	2.0	139
3921	Structure and vibrational spectroscopy investigation of 2-(4-chlorophenyliminomethyl)-8-hydroxyquinoline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 251-6.	2.0	0
3922	Conformational stability, the spectroscopic (FT-IR and UV), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 6,8-diphenylimidazo[1,2-Î±]pyrazine molecule by ab initio HF and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 339-352.	2.0	4
3923	Vibrational spectroscopic, electronic and quantum chemical investigations on 2,3-hexadiene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 81, 620-630.	2.0	20
3924	Molecular structure, vibrational spectra and HOMO, LUMO analysis of yohimbine hydrochloride by density functional theory and ab initio Hartreeâ€“Fock calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 270-278.	2.0	19
3925	DFT, FT-Raman and FT-IR investigations of 5-methoxysalicylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 504-512.	2.0	33
3926	Enhanced Raman spectrum of lawsone on Ag surface: Vibrational analyses, frequency shifts, and molecular geometry. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 425-431.	2.0	24
3927	Quantum mechanical and spectroscopic (FT-IR, FT-Raman, 13C, 1H and UV) investigations of antiepileptic drug Ethosuximide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 478-489.	2.0	12
3928	FT-IR, UVâ€“vis, 1H and 13C NMR spectra and the equilibrium structure of organic dye molecule disperse red 1 acrylate: A combined experimental and theoretical analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 561-569.	2.0	62
3929	FT-IR, FT-Raman and quantum chemical calculations of (E)-N-carbamimidoyl-4-((3,4-dimethoxybenzylidene) amino) benzenesulfonamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 156-163.	2.0	6
3930	Spectroscopic, electronic structure and natural bond orbital analysis of o-fluoronitrobenzene and p-fluoronitrobenzene: A comparative study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 196-209.	2.0	16
3931	Vibrational spectroscopic investigation (FT-IR and FT-Raman) on 1,2-dibromobenzene by HF and hybrid (LSDA and B3LYP) calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 86, 449-55.	2.0	2
3932	Infrared optical properties and Raman spectra of n-pentane and n-pentane-d12. Vibrational Spectroscopy, 2011, , .	1.2	4

#	Article	IF	Citations
3933	Vibrational spectra and structure of methyl-derivatives of imidazo[4,5-c]pyridine based on DFT quantum chemical calculations and XRD studies. Vibrational Spectroscopy, 2011, 57, 229-241.	1.2	9
3934	Raman, infrared and computational analysis of genistein and its methoxy derivatives. Vibrational Spectroscopy, 2011, 57, 306-314.	1.2	20
3935	The influence of fragment size and intermediate barriers on competing near-identical simple cleavage reactions: A variational RRKM study. International Journal of Mass Spectrometry, 2011, 306, 175-181.	0.7	6
3936	Deprotonated N-(2,4-dinitrophenyl)amino acids undergo cyclization in solution and the gas phase. International Journal of Mass Spectrometry, 2011, 306, 232-240.	0.7	8
3937	Unimolecular reactivity upon collision of uracilâ€“Ca2+ complexes in the gas phase: Comparison with uracilâ€“M+ (M=H, alkali metals) and uracilâ€“M2+ (M=Cu, Pb) systems. International Journal of Mass Spectrometry, 2011, 306, 27-36.	0.7	37
3938	Thermal rate constants of the pyrolysis of n-Heptane. Combustion and Flame, 2011, 158, 2314-2324.	2.8	36
3939	Ligand redox non-innocent behaviour in ruthenium complexes of ethynyl tolans. Inorganica Chimica Acta, 2011, 374, 461-471.	1.2	16
3940	Examining the impact of steric and electronic variation in N2S scorpionate ligands on the properties of zinc(II) and cadmium(II) complexes. Inorganica Chimica Acta, 2011, 376, 562-573.	1.2	12
3941	OH stretching frequencies in systems with intramolecular hydrogen bonds: Harmonic and anharmonic analyses. Chemical Physics, 2011, 389, 107-115.	0.9	30
3942	S-Oxidation of Thiazolidinedione with Hydrogen Peroxide, Peroxynitrous Acid, and C4a-Hydroperoxyflavin: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 891-898.	1.1	22
3943	Hammett Correlations in the Chemistry of 3-Phenylpropyl Radicals. Journal of Physical Chemistry A, 2011, 115, 14687-14696.	1.1	8
3944	Toxic Metabolite Formation from Troglitazone (TGZ): New Insights from a DFT Study. Chemical Research in Toxicology, 2011, 24, 1113-1122.	1.7	28
3945	High temperature shock-tube study of the reaction of gallium with ammonia. Physical Chemistry Chemical Physics, 2011, 13, 4149.	1.3	6
3946	Divalent N(I) Compounds with Two Lone Pairs on Nitrogen. Journal of Physical Chemistry A, 2011, 115, 7645-7655.	1.1	62
3947	Structures and Stabilities of Fe2+/3+Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	1.1	27
3948	Molecular structure and vibrational spectra of phenobaraitone by density functional theory and ab initio hartree-Fock calculations. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2011, 6, 358-366.	0.4	13
3949	Computational study on decomposition kinetics of CH 3 CFClO radical. Journal of Chemical Sciences, 2011, 123, 733-741.	0.7	7
3950	Study of structure and spectral characteristics of the binuclear zinc complex with (E)-2-({2-[3-(pyridin-2-yl)-1H-1,2,4-triazol-5-yl]phenylimino}methyl)phenol. Russian Journal of General Chemistry, 2011, 81, 2332-2344.	0.3	13

#	Article	IF	Citations
3951	Reactions of heterocumulenes with organometallic reagents: XVIII. Quantum-chemical study on the mechanisms of formation of thiophene ring from lithium and potassium buta-2,3-dienimidothioates. Russian Journal of Organic Chemistry, 2011, 47, 1841-1850.	0.3	2
3952	A study of the radical polymerization of styrene in the presence of ferrocene. Russian Journal of Physical Chemistry B, 2011, 5, 131-138.	0.2	3
3953	SERS approach for Zn(II) detection in contaminated soil. Open Chemistry, 2011, 9, 410-414.	1.0	6
3954	FTIR spectroscopic and quantum-chemical studies on some tribromoindenes and their isomers. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2011, 111, 894-903.	0.2	3
3955	Reaction Mechanism and Chemoselectivity of Intermolecular Cycloaddition Reactions between Phenyl-Substituted Cyclopropenone Ketal and Methyl Vinyl Ketone. Journal of Organic Chemistry, 2011, 76, 3086-3095.	1.7	11
3957	Ab initio Calculations. , 2011, , 175-390.		1
3958	Semiempirical Calculations. , 2011, , 391-444.		1
3959	Density Functional Calculations. , 2011, , 445-519.		3
3960	Density Functional Theory Study of Hydrogen Atom Abstraction from a Series ofpara-Substituted Phenols: Why is the Hammett Ïƒp+Constant Able to Represent Radical Reaction Rates?. Journal of Organic Chemistry, 2011, 76, 4564-4570.	1.7	14
3961	Firstâ€principles prediction of acidities in the gas and solution phase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 649-660.	6.2	94
3962	Theoretical studies of furoxan-based energetic nitrogen-rich compounds. Structural Chemistry, 2011, 22, 149-159.	1.0	30
3963	Insights into amine-based CO2 capture: an ab initio self-consistent reaction field investigation. Structural Chemistry, 2011, 22, 537-549.	1.0	21
3964	Theoretical studies on a series of 1,2,3-triazoles derivatives as potential high energy density compounds. Structural Chemistry, 2011, 22, 577-587.	1.0	12
3965	DFT studies on the structures and stabilities of N5 +-containing salts. Structural Chemistry, 2011, 22, 1067-1073.	1.0	11
3966	Theoretical Study of Peroxo- and Diperoxomolybdate Formation as Catalysts in the Oxidative Desulfurization of Diesel. Topics in Catalysis, 2011, 54, 527-534.	1.3	4
3967	Density functional theory study on (LiNH2)n (nâ€‰=â€‰1â€“5) clusters. Journal of Molecular Modeling, 2011, 17, 235-242.	0.8	2
3968	Ab initio studies on the decomposition kinetics of CF3OCF2O radical. Journal of Molecular Modeling, 2011, 17, 415-422.	0.8	26
3969	Computer-aided molecular design of 1H-imidazole-2,4-diamine derivatives as potential inhibitors of Plasmodium falciparum DHFR enzyme. Journal of Molecular Modeling, 2011, 17, 657-667.	0.8	33

#	Article	IF	Citations
3970	Extrapolation of water and formaldehyde harmonic and anharmonic frequencies to the B3LYP/CBS limit using polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2029-2040.	0.8	30
3971	Estimation of formamide harmonic and anharmonic modes in the Kohn-Sham limit using the polarization consistent basis sets. Journal of Molecular Modeling, 2011, 17, 2265-2274.	0.8	28
3972	Hydrogenated amorphous silicon nanostructures: novel structureâ€“reactivity relationships for cyclization and ring opening in the gas phase. Theoretical Chemistry Accounts, 2011, 128, 91-113.	0.5	23
3973	Functionalized pentacenes: a combined theoretical, Raman and UVâ€“Vis spectroscopic study. Theoretical Chemistry Accounts, 2011, 128, 521-530.	0.5	22
3974	Avoiding gas-phase calculations in theoretical pK a predictions. Theoretical Chemistry Accounts, 2011, 130, 1-13.	0.5	65
3975	DFT and ONIOM study on the alkylation of the lithium enolate in solution: microsolvation cluster models for CH2=CHOLiÂ+ÂCH3ClÂ+Â(THF)0â€“6. Theoretical Chemistry Accounts, 2011, 130, 323-331.	0.5	13
3976	A quantum mechanical study of bioactive 3-chloro-2,5-dihydroxybenzyl alcohol through substitutions. Theoretical Chemistry Accounts, 2011, 130, 965-979.	0.5	5
3977	Crystal structure and spectroscopic properties of the complex of trigonelline hydrate with p-hydroxybenzoic acid. Journal of Molecular Structure, 2011, 985, 219-226.	1.8	11
3978	Infrared, Raman and NMR spectra, conformational stability, normal coordinate analysis and B3LYP calculations of 5-amino-4-cyano-3-(methylthio)-1H-pyrazole-1-carbothioamide. Journal of Molecular Structure, 2011, 985, 277-291.	1.8	15
3979	Synthesis and comparison of bis(4-amino-5-mercapto-1,2,4-triazol-3-yl)butane using DFT study. Journal of Molecular Structure, 2011, 996, 1-11.	1.8	2
3980	IR, Raman, SERS and DFT study of pindolol and verapamil. Journal of Molecular Structure, 2011, 993, 308-315.	1.8	3
3981	Hostâ€“guest complex of cypermethrin with Î²-cyclodextrin: A spectroscopy and theoretical investigation. Journal of Molecular Structure, 2011, 990, 244-252.	1.8	28
3982	Molecular structure of hydrated complex of trigonelline with l(+)-tartaric acid. Journal of Molecular Structure, 2011, 991, 178-185.	1.8	6
3983	Experimental and theoretical investigations on the ketoâ€“enol tautomerism of 4-substituted Structure, 2011, 994, 313-320.	1.8	14
3984	Spectroscopic and computational insight into weak noncovalent interactions in crystalline pyrimidine. Chemical Physics Letters, 2011, 501, 319-323.	1.2	22
3985	Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H,4H)-one. Journal of Chemical Thermodynamics, 2011, 43, 635-644.	1.0	13
3986	Molecular geometry and vibrational studies of 3,5-diamino-1,2,4-triazole using quantum chemical calculations and FT-IR and FT-Raman spectroscopies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 347-353.	2.0	26
3987	Vibrational spectroscopy (FTIR and FTRaman) investigation using ab initio (HF) and DFT (B3LYP) calculations on the structure of 3-Bromo phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 575-581.	2.0	18

#	Article	IF	Citations
3988	Density functional theory studies on vibrational and electronic spectra of 2-chloro-6-methoxypyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1625-1632.	2.0	26
3989	Investigation of structure, vibrational and NMR spectra of oxycodone and naltrexone: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 574-582.	2.0	14
3990	Experimental (FT-IR and FT-Raman) and theoretical (HF and DFT) investigation, IR intensity, Raman activity and frequency estimation analyses on 1-bromo-4-chlorobenzene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 920-927.	2.0	29
3991	Vibrational spectroscopic analysis of 2-bromobenzoic and anthranilic acids: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 2003-2011.	2.0	3
3992	DFT Calculations on the Molecular Structure, Vibrational and Chemical Shift Assignments of 4-Allyl-2-(morpholin-4-ylmethyl)-5-(pyridin-4-yl)-2,4-Dihydro-3H-1,2,4-Triazole-3-Thione. Arabian Journal for Science and Engineering, 2011, 36, 607-620.	1.1	5
3993	Experimental and Theoretical Investigation of the Proton-Bound Dimer of Lysine. Journal of the American Society for Mass Spectrometry, 2011, 22, 1651-9.	1.2	36
3994	Synthesis and Comprehensive Characterization of Hydrated Alkaline Earth Metal Salts of 5â€Aminoâ€1Hâ€tetrazole. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 1490-1501.	0.6	8
3995	Remote substituent effects on homolytic Fe–C bond energies of pâ€Gâ€C₆H₄CH₂Fe(CO)₂(Î·⁵â€C₅H<su> and pâ€Gâ€C₆H₄(H)(CN)CFe(CO)₂(Î·⁵â€C₅H₅</su> studied by Hartreeâ€“Fock and density functional theory methods. Journal of Physical Organic Chemistry, 2011, 24, 1058-1066.	0.9	2
3996	Mild route to generate gaseous metal anions. Rapid Communications in Mass Spectrometry, 2011, 25, 681-688.	0.7	20
3997	Theoretical investigation of solvent effects on tautomeric equilibrium of 2â€diazoâ€4,6â€dinitrophenol. International Journal of Quantum Chemistry, 2011, 111, 1115-1126.	1.0	13
3998	On experimental versus theoretically calculated properties of thiadiazole derivatives. International Journal of Quantum Chemistry, 2011, 111, 1879-1884.	1.0	2
3999	A density functional theory study on diazotization and nitration of 3,5-diamino-1,2,4-triazole. International Journal of Quantum Chemistry, 2011, 111, 2332-2339.	1.0	3
4000	Reactivity of polynuclear zincâ€thiolate sites. International Journal of Quantum Chemistry, 2011, 111, 1239-1247.	1.0	9
4001	Theoretical study on the solvent effect of the nitrosyl cation (NO⁺) generating reaction. International Journal of Quantum Chemistry, 2011, 111, 3571-3577.	1.0	0
4002	Quantum confinement effects on the surface enhanced Raman spectra of hybrid systems moleculeâ€TiO₂ nanoparticles. International Journal of Quantum Chemistry, 2011, 111, 1659-1670.	1.0	29
4003	Calculations of the infrared and Raman spectra of simple thiols and thiolâ€“water complexes. International Journal of Quantum Chemistry, 2011, 111, 1843-1857.	1.0	11
4004	The reaction mechanism of the gasâ€phase thermal decomposition kinetics of neopentyl halides: A DFT study. International Journal of Quantum Chemistry, 2011, 111, 4011-4019.	1.0	3
4005	Quantum Monte Carlo calculations of bond dissociation energies for some nitro and amino molecules. International Journal of Quantum Chemistry, 2011, 111, 4452-4456.	1.0	3

#	Article	IF	Citations
4006	Ab initio studies of the conformers and conformational distribution of gasâ€phase N,Nâ€dimethylaminopropanol. International Journal of Quantum Chemistry, 2011, 111, 4296-4302.	1.0	4
4007	A quantum chemical study on the antioxidant properties of aureusidin and bracteatin. International Journal of Quantum Chemistry, 2011, 111, 4483-4496.	1.0	16
4008	Structural analysis of sterically hindered 1,4â€diols from the naturally occurring lignan hydroxymatairesinol a quantum chemical study. International Journal of Quantum Chemistry, 2011, 111, 4309-4317.	1.0	6
4009	Theoretical study of the kojic acid structure in gas phase and aqueous solution. International Journal of Quantum Chemistry, 2011, 111, 4318-4329.	1.0	13
4010	Computational study toward understanding the photodissociation mechanism of sarin. International Journal of Quantum Chemistry, 2011, 111, 4410-4417.	1.0	2
4011	Betulin and its natural resource as potential anticancer drug candidate seen by FTâ€Raman and FTâ€IR spectroscopy. Journal of Raman Spectroscopy, 2011, 42, 97-107.	1.2	43
4012	New insights on surfaceâ€enhanced Raman scattering based on controlled aggregation and spectroscopic studies, DFT calculations and symmetry analysis for 3,6â€bisâ€2â€pyridylâ€1,2,4,5â€tetrazine adsorbed onto citrateâ€stabilized gold nanoparticles. Journal of Raman Spectroscopy, 2011, 42, 644-652.	1.2	17
4013	Vibrational spectroscopy and density functional theory calculations of polyâ€<scp>D</scp>â€mannuronate and heteropolymeric fractions from sodium alginate. Journal of Raman Spectroscopy, 2011, 42, 870-878.	1.2	45
4014	DFT and MP2 based quantum mechanical calculations and a theoretical vibrational spectroscopic investigation on roscovitine, a potential drug to treat cancers. Journal of Raman Spectroscopy, 2011, 42, 719-732.	1.2	8
4015	Retinal in bacteriorhodopsin and related molecular models investigated with Raman spectroscopy and density functional theory calculations. Journal of Raman Spectroscopy, 2011, 42, 1207-1214.	1.2	7
4016	Raman, infrared, SERS and theoretical study of 3â€(1â€phenylpropanâ€2â€ylamino) propanenitrile, fenproporex. Journal of Raman Spectroscopy, 2011, 42, 1497-1504.	1.2	2
4017	Synthesis and Raman spectroscopic investigation of a new selfâ€assembly monolayer material 4â€[Nâ€phenylâ€Nâ€(3â€methylphenyl)â€amino]â€benzoic acid for organic lightâ€emitting devices. Journal of Raman Spectroscopy, 2011, 42, 1682-1689.	1.2	3
4018	Vibrational properties of levulinic acid and furan derivatives: Raman spectroscopy and theoretical calculations. Journal of Raman Spectroscopy, 2011, 42, 2069-2076.	1.2	71
4019	Characterization of antioxidant olive oil biophenols by spectroscopic methods. Journal of the Science of Food and Agriculture, 2011, 91, 309-314.	1.7	29
4020	Experimental and theoretical NMR and IR studies of the sideâ€chain orientation effects on the backbone conformation of dehydrophenylalanine residue. Magnetic Resonance in Chemistry, 2011, 49, 343-349.	1.1	16
4021	Electronic Structure Calculations for Holeâ€Transporting Triphenylamine Derivatives in Polymer Lightâ€Emitting Diodes. Macromolecular Theory and Simulations, 2011, 20, 790-805.	0.6	0
4022	New Umpolung Catalysts: Reactivity and Selectivity of Terpenolâ€Based Lithium Phosphonates in Enantioselective Benzoinâ€Type Couplings. European Journal of Organic Chemistry, 2011, 2011, 256-263.	1.2	18
4023	Density Functional Theory Study on (Cl₂GaN₃)_n(n=1â€“4) Clusters. Chinese Journal of Chemistry, 2011, 29, 1817-1823.	2.6	1

#	Article	IF	Citations
4024	Assessing Spinâ€Componentâ€Scaled Secondâ€Order MÃ¸llerâ€“Plesset Theory Using Anharmonic Frequencies. ChemPhysChem, 2011, 12, 3383-3391.	1.0	7
4025	Harmonic vibrational frequencies: Scale factors for pure, hybrid, hybrid meta, and doubleâ€hybrid functionals in conjunction with correlation consistent basis sets. Journal of Computational Chemistry, 2011, 32, 2339-2347.	1.5	61
4026	Computational study of energetic nitrogenâ€rich derivatives of 1,1â€²â€•and 5,5â€²â€bridged ditetrazoles. Journal of Computational Chemistry, 2011, 32, 2298-2312.	1.5	43
4027	Energetic Salts of the Binary 5â€Cyanotetrazolate Anion ([C₂N₅]^{â^'}) with Nitrogenâ€Rich Cations. Chemistry - A European Journal, 2011, 17, 1683-1695.	1.7	26
4028	Highly Efficient Visibleâ€Light Driven Photochromism: Developments towards a Solidâ€State Molecular Switch Operating through a Tripletâ€Sensitised Pathway. Chemistry - A European Journal, 2011, 17, 4385-4395.	1.7	48
4029	Competitive Reactions of Organophosphorus Radicals on Coke Surfaces. Chemistry - A European Journal, 2011, 17, 12027-12036.	1.7	23
4030	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 2,4,6-trinitrophenol. Computational and Theoretical Chemistry, 2011, 963, 34-39.	1.1	12
4031	Design and density functional theoretical study of three novel pyrazine-based high-energy density compounds. Computational and Theoretical Chemistry, 2011, 963, 221-226.	1.1	15
4032	Rate coefficients of the reactions of isopentane with H and CH3 radicals: Quantum mechanical approach. Computational and Theoretical Chemistry, 2011, 963, 357-364.	1.1	7
4033	A DFT study of the structural units in SBA-15 mesoporous molecular sieve. Computational and Theoretical Chemistry, 2011, 963, 403-411.	1.1	37
4034	Modified enthalpies of formation for hydrocarbons from DFT and ab initio thermal energies. Computational and Theoretical Chemistry, 2011, 964, 100-107.	1.1	2
4035	Quantum-chemical studies of amideâ€“iminol tautomerism for inhibitor of lactate dehydrogenase: Oxamic acid. Computational and Theoretical Chemistry, 2011, 964, 310-317.	1.1	8
4036	Additivity of substituent effects on the proton affinity and gas-phase basicity of pyridines. Computational and Theoretical Chemistry, 2011, 966, 31-37.	1.1	22
4037	DFT studies on Meisenheimer rearrangement. Computational and Theoretical Chemistry, 2011, 966, 383-390.	1.1	6
4038	Experimental and theoretical study of the reactions of iron and manganese oxides with dinitrogen in a cryogenic matrix. Chemical Physics Letters, 2011, 503, 33-38.	1.2	6
4039	A theoretical study of experimentally unknown metallosubphthalocyanines. Chemical Physics Letters, 2011, 511, 51-56.	1.2	7
4040	The effect molecular structural variations has on the CO2 absorption characteristics of heterocyclic amines. Energy Procedia, 2011, 4, 224-231.	1.8	4
4041	In situ FTIR spectra at the Pt electrode/Î³-butyrolactone solution interface. Electrochimica Acta, 2011, 56, 7078-7083.	2.6	11

#	Article	IF	Citations
4042	Photoinduced activation of CO2 on TiO2 surfaces: Quantum chemical modeling of CO2 adsorption on oxygen vacancies. Fuel Processing Technology, 2011, 92, 805-811.	3.7	47
4043	Influence of diosgenin structure on the polymerization kinetics of acrylamide: An experimental and theoretical approach. Journal of Molecular Structure, 2011, 985, 34-47.	1.8	2
4044	FT-IR and FT-Raman spectra, vibrational assignments, NBO analysis and DFT calculations of 2-amino-4-chlorobenzonitrile. Journal of Molecular Structure, 2011, 985, 148-156.	1.8	69
4045	Synthesis, characterization, and computational study of N,Nâ€²-bis (2â€²,4â€²-dihydroxyphenyl)-1.4-quinonediimine, a hydroxyl-capped three-ring quinonediimine with sterically hindered substituent on outer rings. Journal of Molecular Structure, 2011, 985, 299-306.	1.8	7
4046	Spectroscopic investigations of newly formed betulin-cyclodextrin guestâ€“host type complexes as potential anti skin cancer candidates. Journal of Molecular Structure, 2011, 993, 297-301.	1.8	10
4047	Theoretical and experimental investigation on the spectroscopic properties of indigo dye. Journal of Molecular Structure, 2011, 993, 43-51.	1.8	61
4048	IR, Raman, SERS and DFT study of amoxicillin. Journal of Molecular Structure, 2011, 993, 52-56.	1.8	66
4049	X-ray, DFT, FTIR and NMR structural study of 2,3-dihydro-2-(R-phenylacylidene)-1,3,3-trimethyl-1H-indole. Journal of Molecular Structure, 2011, 987, 106-118.	1.8	21
4050	Spectroscopic and DFT study of atenolol and metoprolol and their copper complexes. Journal of Molecular Structure, 2011, 993, 357-366.	1.8	14
4051	The synthesis, molecular structure, FT-IR and XRD spectroscopic investigation of 4-[(2-{[(2-furylmethyl)imino]methyl}-4-methoxyphenoxy)methyl]benzonitrile: A comparative DFT study. Journal of Molecular Structure, 2011, 991, 12-17.	1.8	4
4052	DFT, FT-Raman, FT-IR and FT-NMR studies of 4-phenylimidazole. Journal of Molecular Structure, 2011, 990, 14-20.	1.8	67
4053	Ab initio and semi-empirical computational studies on 5-hydroxy-4-methyl-5,6-di-pyridin-2-yl-4,5-dihydro-2H-[1,2,4]triazine-3-thione. Journal of Molecular Structure, 2011, 991, 186-201.	1.8	12
4054	Density functional theory studies on 2,5-bis(4-hydroxy-3-methoxybenzylidene)cyclopentanone. Journal of Molecular Structure, 2011, 999, 2-9.	1.8	10
4055	Unusual molecular structure of the 1:2.5:2 complex of DABCO di-betaine (1,4-diacetate-1,4-diazoniumbicyclo[2.2.2]octane) with p-hydroxybenzoic acid and water. Journal of Molecular Structure, 2011, 994, 131-136.	1.8	5
4056	Molecular structure of the 1:2 complex of 2-quinuclidinium-butyrate with p-hydroxybenzoic acid. Journal of Molecular Structure, 2011, 994, 144-149.	1.8	5
4057	The structure of 4-(trimethylammonium)benzoic acid chloride studied by X-ray diffraction, DFT calculations, NMR and FTIR spectroscopy. Journal of Molecular Structure, 2011, 996, 75-81.	1.8	19
4058	Raman experimental and DFT theoretical studies on the adsorption behavior of MHBA on silver nanoparticles. Journal of Molecular Structure, 2011, 998, 49-52.	1.8	4
4059	FT-IR, FT-Raman spectra and scaled quantum mechanical study of 4-amino-1-benzylpiperidine. Journal of Molecular Structure, 2011, 998, 69-78.	1.8	13

#	Article	IF	Citations
4060	Diastereomeric complex of (R/S)-piperidine-3-carboxylic acid with (2R,3R)-tartaric acid: Structural, spectroscopic and computational studies. Journal of Molecular Structure, 2011, 999, 98-105.	1.8	6
4061	OHâ‹¯O and OHâ‹¯N hydrogen bonds in the complex of DABCO mono-betaine with p-hydroxybenzoic acid studied by X-ray diffraction, DFT calculations and spectroscopic methods. Journal of Molecular Structure, 2011, 1000, 127-134.	1.8	10
4062	Synthesis and structure of 9,10-bis(2,4,6-triisopropylphenyl)-9,10-dihydro-9,10-disilaanthracene. Journal of Organometallic Chemistry, 2011, 696, 982-985.	0.8	2
4063	Molecular structure, vibrational spectra and nonlinear optical properties of l-Valine Hydrobromide: DFT study. Journal of Molecular Structure, 2011, 985, 48-56.	1.8	34
4064	When theory and experiment hold hands: The thermochemistry of Î³-pyrone derivatives. Journal of Chemical Thermodynamics, 2011, 43, 1159-1163.	1.0	5
4065	Calorimetric and computational study of 7-hydroxycoumarin. Journal of Chemical Thermodynamics, 2011, 43, 1435-1440.	1.0	7
4066	The reaction of iso-propyl radicals with oxygen atoms: Rate coefficient, product branching, and relevance for combustion modeling. Proceedings of the Combustion Institute, 2011, 33, 283-291.	2.4	4
4067	Synthesis, X-ray crystallography characterization, vibrational spectroscopic, molecular electrostatic potential maps, thermodynamic properties studies of N,Nâ€²-di(p-thiazole)formamidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 88-95.	2.0	15
4068	Intramolecular charge delocalization and nonlinear optical properties of pushâ€“pull chromophore 1-(4-N,N-dimethylaminopyridinium) acetic acid bromide monohydrate from vibrational spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 264-272.	2.0	13
4069	Molecular structure and vibrational spectra of three substituted 4-thioflavones by density functional theory and ab initio Hartreeâ€“Fock calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 528-536.	2.0	38
4070	Molecular structure, vibrational spectroscopic, first order hyperpolarizability and HOMOâ€“LUMO studies of 7-amino-8-oxo-3-vinyl-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 660-669.	2.0	16
4071	Experimental and theoretical investigation of the molecular and electronic structure of anticancer drug camptothecin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1058-1067.	2.0	36
4072	Structure and vibrational spectra of some 8-oxa[5]helicenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1090-1096.	2.0	1
4073	Vibrational spectroscopy [FTIR and FTRaman] investigation, computed vibrational frequency analysis and IR intensity and Raman activity peak resemblance analysis on 4-chloro 2-methylaniline using HF and DFT [LSDA, B3LYP and B3PW91] calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1149-1161.	2.0	12
4074	Quantum chemical computational studies on 5-(4-bromophenylamino)-2-methylsulfanylmethyl-2H-1,2,3-triazol-4-carboxylic acid ethyl ester. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1201-1211.	2.0	18
4075	Quantum chemical study of p-toluenesulfonic acid, p-toluenesulfonate anion and the waterâ€“p-toluenesulfonic acid complex. Comparison with experimental spectroscopic data. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 27-34.	2.0	33
4076	Density functional theory calculations and vibrational spectral analysis of 3,5-(dinitrobenzoic acid). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1437-1444.	2.0	59
4077	FT-IR, Raman and DFT study of 2-amino-5-fluorobenzoic acid and its biological activity with other halogen (Cl, Br) substitution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 332-337.	2.0	24

#	Article	IF	Citations
4078	Surface-enhanced Raman scattering and DFT investigation of Eriochrome Black T metal chelating compound. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 226-231.	2.0	15
4079	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of butylated hydroxy toluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 562-569.	2.0	42
4080	Experimental (FT-IR and FT-Raman), electronic structure and DFT studies on 1-methoxynaphthalene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 646-653.	2.0	54
4081	FT-IR and FT-Raman, vibrational assignments, molecular geometry, ab initio (HF) and DFT (B3LYP) calculations for 1,3-dichlorobenzene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 962-969.	2.0	20
4082	Vibrational spectra, tautomerism and thermodynamics of anticarcinogenic drug: 5-Fluorouracil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 970-977.	2.0	44
4083	Nonplanar property study of antifungal agent tolnaftate-spectroscopic approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 993-1003.	2.0	20
4084	DFT, FT-Raman and FT-IR investigations of 5-o-tolyl-2-pentene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1077-1083.	2.0	1
4085	Synthesis, experimental and theoretical characterization of palladium(II) and platinum(II) saccharinate complexes with 2-(2-pyridyl)benzimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1171-1178.	2.0	13
4086	Spectroscopic and quantum chemical studies on 4-acryloyl morpholine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1386-1394.	2.0	7
4087	A combined experimental and theoretical quantum chemical studies on 4-morpholinecarboxaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1395-1401.	2.0	3
4088	Synthesis, vibrational spectral and nonlinear optical studies of N-(4-hydroxy-phenyl)-2-hydroxybenzaldehyde-imine: A combined experimental and theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1475-1482.	2.0	30
4089	Structural and spectroscopic characterization of 2,3-difluorobenzoic acid and 2,4-difluorobenzoic acid with experimental techniques and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1511-1519.	2.0	33
4090	Vibrational assignments, normal coordinate analysis, B3LYP calculations and conformational analysis of methyl-5-amino-4-cyano-3-(methylthio)-1H-pyrazole-1-carbodithioate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 1722-1730.	2.0	10
4091	Chemical, spectroscopic characterization, DFT studies and initial pharmacological assays of a silver(I) complex with N-acetyl-l-cysteine. Polyhedron, 2011, 30, 579-583.	1.0	24
4092	Preparation and evaluation of 2-azinyl-2H-benzotriazoles as bidentate ligands: Synthesis and characterization of [2-(2-pyridynyl)-2H-benzotriazole](bpy)2Ru2+. Polyhedron, 2011, 30, 1339-1348.	1.0	4
4093	Improved DFT calculation of Raman spectra of silicates. Vibrational Spectroscopy, 2011, 56, 265-272.	1.2	29
4094	Coverage dependence of glycine adsorption on the Ge(100)â˜2Ã—1 surface. Surface Science, 2011, 605, 760-769.	0.8	16
4095	DFT study of isocyanate chemisorption on Cu(100). Surface Science, 2011, 605, 1202-1208.	0.8	10

#	Article	IF	Citations
4096	Synthesis and structural, spectroscopic, and electrochemical characterization of benzo[c]quinolizinium and its 5-aza-, 6-aza, and 5,6-diaza analogues. Tetrahedron, 2011, 67, 3317-3327.	1.0	10
4097	Three-component conformational equilibria of some flexible pyrrolidin-2-(thi)ones in solution by NMR data (ÎˊC, ÎˆH, and nJHH) and their DFT predictions: a confrontation of different approaches. Tetrahedron, 2011, 67, 6901-6916.	1.0	16
4098	K2Ca3Si3O10, a novel trisilicate: high-pressure synthesis, structural, spectroscopic and computational studies. European Journal of Mineralogy, 2011, 23, 425-435.	0.4	13
4099	Vibrational Spectroscopy of Fluorescent Proteins: A Tool to Investigate the Structure of the Chromophore and Its Environment. Springer Series on Fluorescence, 2011, , 133-169.	0.8	1
4100	Tuning the electronic coupling in a low-bandgap donorâ€“acceptor copolymer via the placement of side-chains. Journal of Chemical Physics, 2011, 134, 114901.	1.2	34
4101	Molecular Structure and Vibrational Analysis of 1-Bromo-2-Chlorobenzene Using ab initio HF and Density Functional Theory (B3LYP) Calculations. Journal of Atomic, Molecular, and Optical Physics, 2011, 2011, 1-10.	0.5	8
4102	Spectroscopy of a Gamma Irradiated Poly(Acrylic Acid)-Clotrimazole System. Chinese Physics Letters, 2011, 28, 128201.	1.3	10
4103	Computational IR Spectroscopy for PAHs: from the early years to the present status. EAS Publications Series, 2011, 46, 75-93.	0.3	9
4104	Theoretical Study on the Mechanism and Kinetic of the Reactions between Elemental Mercury and Oxidizing Radicals. , 2011, , .		0
4105	Raman, FT-IR spectroscopic analysis and first-order hyperpolarisability of 3-benzoyl-5-chlorouracil by first principles. Molecular Simulation, 2011, 37, 153-163.	0.9	123
4106	Synthesis, FT-IR, FT-Raman and quantum chemical investigations of N-(3-methylphenyl)-2,2-dichloroacetamide. European Journal of Chemistry, 2011, 2, 70-76.	0.3	12
4107	Infrared spectroscopy of Sc+(H2O) and Sc2+(H2O) via argon complex predissociation: The charge dependence of cation hydration. Journal of Chemical Physics, 2011, 134, 014302.	1.2	36
4108	In vivomolecular labeling of halogenated volatile anesthetics via intrinsic molecular vibrations using nonlinear Raman spectroscopy. Journal of Chemical Physics, 2011, 134, 024525.	1.2	9
4109	H+ versus D+ transfer from HOD+ to CO2: Bond-selective chemistry and the anomalous effect of bending excitation. Journal of Chemical Physics, 2011, 134, 064312.	1.2	5
4110	Density functional theory and Raman spectroscopy applied to structure and vibrational mode analysis of 1,1â€²,3,3â€²-tetraethyl-5,5â€²,6,6â€²-tetrachloro- benzimidazolocarbocyanine iodide and its aggregate. Journal of Chemical Physics, 2011, 134, 064325.	1.2	13
4111	Vibrational solvatochromism and electrochromism of infrared probe molecules containing Câ‰¡O, Câ‰¡N, C=O, or Câ^'F vibrational chromophore. Journal of Chemical Physics, 2011, 134, 154513.	1.2	82
4112	Comment on â€œUncertainties in scaling factors for ab initio vibrational zero-point energiesâ€•[J. Chem. Phys. 130, 114102 (2009)] and â€œCalibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functionalâ€•[J. Chem. Phys. 133, 114109 (2010)]. Journal of Chemical Physics, 2011, 134, 167101; author reply 167102-3.	1.2	14
4113	Response to â€œComment on â€˜Uncertainties in scaling factors for ab initio vibrational zero-point energiesâ€™ and â€˜Calibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functionalâ€™â€•[J. Chem. Phys. 134, 167101 (2011)]. Journal of Chemical Physics, 2011, 134, 167103.	1.2	2

#	Article	IF	Citations
4114	Theoretical and experimental studies on 2-(2-methyl-5-nitro-1-imidazolyl)ethanol. European Journal of Chemistry, 2011, 2, 136-145.	0.3	32
4116	Theoretical density functional study of gas-phase tautomerization and acidity of 5-methylhydantoin and its thio derivatives. European Journal of Chemistry, 2012, 3, 348-355.	0.3	6
4117	Interaction Mechanism of Nano-silicon Dioxide Modified by Poly(amidoamine) Dendrimers. Chinese Journal of Chemical Physics, 2012, 25, 592-604.	0.6	5
4118	Theoretical Study on Vibrational Spectra, Detonation Properties and Pyrolysis Mechanism for Cyclic 2-Diazo-4,6-dinitrophenol. Chinese Journal of Chemical Physics, 2012, 25, 545-551.	0.6	1
4119	Structural variability in transition metal oxide clusters: gas phase vibrational spectroscopy of V3O6â€“8+. Physical Chemistry Chemical Physics, 2012, 14, 9377.	1.3	55
4120	Near-threshold shape resonance in the photoionization of 2-butyne. Journal of Chemical Physics, 2012, 136, 154303.	1.2	23
4121	Gas Phase Conformations of Tetrapeptide Glycine-Phenylalanine-Glycine-Glycine. Chinese Journal of Chemical Physics, 2012, 25, 77-85.	0.6	5
4122	Orientational order parameters of a de Vriesâ€“type ferroelectric liquid crystal obtained by polarized Raman spectroscopy and x-ray diffraction. Physical Review E, 2012, 85, 061703.	0.8	23
4123	THEORETICAL STUDY OF THE STRUCTURES AND PROPERTIES OF (Cl₂AlN₃)_n(n = 2â€“4) CLUSTERS. Journal of Theoretical and Computational Chemistry, 2012, 11, 941-952.	1.8	1
4124	HYPERCONJUGATION EFFECT ON THE STRUCTURAL STABILITY OF A TERT-BUTYL AND ITS DERIVED C4Hn(n =) Tj ETQq1 1 0.784314 rgBT	1.8	2
4125	Correlation of TrpGly and GlyTrp Rotamer Structure with W7 and W10 UV Resonance Raman Modes and Fluorescence Emission Shifts. Journal of Amino Acids, 2012, 2012, 1-10.	5.8	4
4126	Prediction of Thermodynamic and Kinetic Parameters for Interfacial Reactions of the SIO2System by Quantum Chemistry Methods. Soft Materials, 2012, 10, 285-312.	0.8	3
4127	Factors That Differentiate the H-bond Strengths of Water Near the Schiff Bases in Bacteriorhodopsin and Anabaena Sensory Rhodopsin*. Journal of Biological Chemistry, 2012, 287, 34009-34018.	1.6	21
4128	Theoretical Studies of the Structure and Properties of Anticancer Drug Taxol. Current Organic Chemistry, 2012, 16, 2321-2331.	0.9	3
4129	Comparison of Visible and Near-Infrared Raman Cross-Sections of Explosives in Solution and in the Solid State. Applied Spectroscopy, 2012, 66, 636-643.	1.2	14
4130	Regio- and Stereoselectivity of the 1,3-Dipolar Cycloaddition of Pyridinium-3-olates and Pyrazinium-3-olates with Methyl Methacrylate: A Density Functional Theory Exploration. Current Organic Chemistry, 2012, 16, 1711-1722.	0.9	7
4131	THE INFRARED AND UV-VISIBLE SPECTRA OF POLYCYCLIC AROMATIC HYDROCARBONS CONTAINING (5,) Tj ETQq0 0 0 rgBT /Overlock 1	1.6	14
4132	Rapid anharmonic vibrational corrections derived from partial Hessian analysis. Journal of Chemical Physics, 2012, 136, 224102.	1.2	20

#	Article	IF	Citations
4133	Theoretical investigation of the oxidation pathways of the Cl-initiated reaction of 2-methyl-3-buten-2-ol. Molecular Physics, 2012, 110, 2901-2917.	0.8	4
4134	Benzo[b]trithiophene Polymer Network Prepared by Electrochemical Polymerization with a Combination of Thermal Conversion. Chemistry Letters, 2012, 41, 140-141.	0.7	4
4135	On the Effects of Changing Gaussian Program Version and SCRF Defining Parameters: Isopropylamine as a Case Study. Bulletin of the Chemical Society of Japan, 2012, 85, 962-975.	2.0	10
4136	Insights into the structure and dynamics of liquid water: A comparative study of conventional QM/MM and ONIOM-XS MD simulations. Journal of Molecular Liquids, 2012, 174, 26-33.	2.3	13
4137	Relationships between DFT/RRKM Branching Ratios of the Complementary Fragment Ions [C5H5O]+ and [M â€“ C5H5O]+ and Relative Abundances in the EI Mass Spectrum of N-(2-Furylmethyl)aniline. Journal of Physical Chemistry A, 2012, 116, 12136-12147.	1.1	5
4138	ATRâ€“FTIR and Density Functional Theory Study of the Structures, Energetics, and Vibrational Spectra of Phosphate Adsorbed onto Goethite. Langmuir, 2012, 28, 14573-14587.	1.6	142
4139	On the path to glycan conformer identification: Gas-phase study of the anomers of methyl glycosides of N-acetyl-d-glucosamine and N-acetyl-d-galactosamine. International Journal of Mass Spectrometry, 2012, 330-332, 285-294.	0.7	26
4140	The Structures and Stabilities of the Complexes of Biologically Available Ligands with Fe(II) Porphine: An Ab Initio Study. Journal of Physical Chemistry B, 2012, 116, 10301-10310.	1.2	14
4141	Valence structures of aromatic bioactive compounds: a combined theoretical and experimental study. Journal of Synchrotron Radiation, 2012, 19, 773-781.	1.0	3
4142	First-Principles Mode Grüneisen Parameters and Negative Thermal Expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>ZrW</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 195503.	7.6	51
4143	Exploring Câ€“HÂ·Â·Â·O hydrogen bonds in dihydrocoumarin from combined vibrational spectroscopy and DFT calculations. Chemical Physics Letters, 2012, 551, 86-91.	1.2	4
4144	Theoretical and experimental characterization of pyrazolato-based Ni(ii) metalâ€“organic frameworks. Journal of Materials Chemistry, 2012, 22, 22592.	6.7	17
4145	The Ï€-conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors. Physical Chemistry Chemical Physics, 2012, 14, 14832.	1.3	23
4146	Mechanism of Photo-Oxidation of Heptafluorobutyric Anhydride in the Presence of NO2. Synthesis and Characterization of Heptafluoropropyl Peroxynitrate, CF3CF2CF2OONO2. Journal of Physical Chemistry A, 2012, 116, 9904-9910.	1.1	5
4147	A computational proposal for the experimentally observed discriminatory behavior of hypoxanthine, a weak universal nucleobase. Physical Chemistry Chemical Physics, 2012, 14, 2743.	1.3	12
4148	fac-Re(CO)3 complexes of 2,6-bis(4-substituted-1,2,3-triazol-1-ylmethyl)pyridine â€œclickâ€•ligands: synthesis, characterisation and photophysical properties. Dalton Transactions, 2012, 41, 14625.	1.6	43
4149	Synthesis, crystal structure, vibrational spectral and density functional studies of 4-(1,3-dioxoisoindolin-2-yl)antipyrine. Journal of Molecular Structure, 2012, 1030, 113-124.	1.8	3
4150	The Binding of Fe(II)â€“Heme to the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations. Journal of Chemical Theory and Computation, 2012, 8, 5150-5158.	2.3	10

#	Article	IF	Citations
4151	Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations. Journal of Chemical Information and Modeling, 2012, 52, 1199-1212.	2.5	99
4152	A detailed test study of barrier heights for the HO2 + H2O + O3 reaction with various forms of multireference perturbation theory. Journal of Chemical Physics, 2012, 136, 114312.	1.2	10
4153	Ruthenium Carbonyl Complexes Bearing Bis(pyrazol-1-yl)carboxylato Ligands. Organometallics, 2012, 31, 2166-2174.	1.1	24
4154	Some cyclization reactions of 1,3-diphenylbenzo[e][1,2,4]triazin-7(1H)-one: preparation and computational analysis of non symmetrical zwitterionic biscyanines. Organic and Biomolecular Chemistry, 2012, 10, 1339.	1.5	22
4155	Investigating the Calculation of Anharmonic Vibrational Frequencies Using Force Fields Derived from Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 4417-4425.	1.1	42
4156	Characterization of nitrogen-bridged 1,2,4,5-tetrazine-, furazan-, and 1H-tetrazole-based polyheterocyclic compounds: heats of formation, thermal stability, and detonation properties. Journal of Molecular Modeling, 2012, 18, 3467-3479.	0.8	34
4157	Carbonylâ€Functionalized Quaterthiophenes: A Study of the Vibrational Raman and Electronic Absorption/Emission Properties Guided by Theoretical Calculations. ChemPhysChem, 2012, 13, 168-176.	1.0	8
4158	Formation of nano-plate silver particles in the presence of polyampholyte copolymer. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 414, 17-25.	2.3	19
4159	Structural characterization of a thirdâ€generation commercial cement superplasticizer by Raman spectroscopy and DFT calculations. Journal of Raman Spectroscopy, 2012, 43, 1623-1629.	1.2	5
4160	Rapid detection method for nitrofuran antibiotic residues by surface-enhanced Raman Spectroscopy. European Food Research and Technology, 2012, 235, 555-561.	1.6	55
4161	Cooperativity effects in linear formaldehyde oligomers using density functional theory calculations. Journal of Molecular Modeling, 2012, 18, 3723-3729.	0.8	6
4162	XZP + 1d and XZP + 1d-DKH basis sets for second-row elements: application to CCSD(T) zero-point vibrational energy and atomization energy calculations. Journal of Molecular Modeling, 2012, 18, 4081-4088.	0.8	5
4163	Induced chirality in fisetin upon binding to serum albumin: experimental circular dichroism and TDDFT calculations. Journal of Molecular Modeling, 2012, 18, 4381-4387.	0.8	9
4164	Raman spectra of tetraoxa[8]circulenes. p-dinaphthalenodiphenylenotetrafuran and its tetraalkyl derivatives (DFT study and experiment). Journal of Applied Spectroscopy, 2012, 79, 695-707.	0.3	11
4165	Solvent Effects on IR Modes of (R)-3-Methylcyclopentanone Conformers: A Computational Investigation. Journal of Solution Chemistry, 2012, 41, 1495-1506.	0.6	12
4166	Cluster models of aqueous Na+ and Clâ^' in sea water/ice. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	4
4167	Spectral character of intermediate state in solid-state photoarrangement of Î±-santonin. Chemical Physics, 2012, 405, 40-45.	0.9	8
4168	Studies of the tautomeric equilibrium of 1,3-thiazolidine-2-thione: Theoretical and experimental approaches. Chemical Physics, 2012, 408, 62-68.	0.9	20

#	Article	IF	Citations
4169	First detection of the silylgermylene (H3SiGeH) and D4-silylgermylene (D3SiGeD) molecules in low temperature silaneâ€“germane ices. Chemical Physics, 2012, 409, 49-60.	0.9	6
4170	Silver(I) and gold(I) complexes of diethylmalonate. International Journal of Mass Spectrometry, 2012, 330-332, 226-232.	0.7	10
4171	FTIR, FT-Raman, SERS and DFT study on melamine. Vibrational Spectroscopy, 2012, 62, 165-171.	1.2	204
4172	Adsorption of the anthraquinone drug parietin on silver nanoparticles: A SERS and fluorescence study. Vibrational Spectroscopy, 2012, 63, 477-484.	1.2	9
4173	Probing the electronic structure of -fused quinoxalino porphyrins and tetraazaanthracene-bridged bis-porphyrins with resonance Raman spectroscopy and density functional theory. Journal of Molecular Structure, 2012, 1029, 187-198.	1.8	13
4174	A Crystallographic, Spectroscopic, Thermal, and DFT Investigation of Mixed Ligand Cu(II) Complexes of 2-benzoylbenzoate. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2012, 42, 1449-1458.	0.6	4
4175	Vibrational spectra of polyatomic molecules assisted by quantum thermal baths. Physical Chemistry Chemical Physics, 2012, 14, 10503.	1.3	29
4176	Reactions of o-benzyne with propargyl and benzyl radicals: potential sources of polycyclic aromatic hydrocarbons in combustion. Physical Chemistry Chemical Physics, 2012, 14, 9722.	1.3	32
4177	Infrared photodissociation spectra of mass selected homoleptic dinuclear iron carbonyl cluster anions in the gas phase. Chemical Science, 2012, 3, 1698.	3.7	47
4178	Time-resolved vibrational spectroscopy of a molecular shuttle. Physical Chemistry Chemical Physics, 2012, 14, 1865-1875.	1.3	31
4179	The stability of the acetic acid dimer in microhydrated environments and in aqueous solution. Physical Chemistry Chemical Physics, 2012, 14, 4162.	1.3	18
4180	Excited State Structure and Dynamics of the Neutral and Anionic Flavin Radical Revealed by Ultrafast Transient Mid-IR to Visible Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 5810-5818.	1.2	33
4181	A QMCF-MD Investigation of the Structure and Dynamics of Ce⁴⁺ in Aqueous Solution. Inorganic Chemistry, 2012, 51, 6746-6752.	1.9	22
4182	Ultrafast primary processes of an iron-(iii) azido complex in solution induced with 266 nm light. Physical Chemistry Chemical Physics, 2012, 14, 6165.	1.3	24
4183	A binuclear silver complex with l-buthionine sulfoximine: synthesis, spectroscopic characterization, DFT studies and antibacterial assays. RSC Advances, 2012, 2, 10372.	1.7	13
4184	Nanosecond time-resolved IR study of thiobenzoylnitrene. Physical Chemistry Chemical Physics, 2012, 14, 10438.	1.3	11
4185	Computational study on the thermal decomposition and isomerization of the CH3OCF2Oâ€¢ radical. Canadian Journal of Chemistry, 2012, 90, 403-409.	0.6	14
4186	Characterization of structure and dynamics of an aqueous scandium(iii) ion by an extended ab initio QM/MM molecular dynamics simulation. Dalton Transactions, 2012, 41, 11889.	1.6	14

#	Article	IF	Citations
4187	Theoretical and Experimental Studies of the Spin Trapping of Inorganic Radicals by 5,5-Dimethyl-1-pyrroline N-Oxide (DMPO). 3. Sulfur Dioxide, Sulfite, and Sulfate Radical Anions. Journal of Physical Chemistry A, 2012, 116, 7210-7218.	1.1	145
4188	Photoproduct Channels from BrCD₂CD₂OH at 193 nm and the HDO + Vinyl Products from the CD₂CD₂OH Radical Intermediate. Journal of Physical Chemistry A, 2012, 116, 6394-6407.	1.1	9
4189	Guest Inclusion in Cucurbiturils Studied by ESR and DFT: The Case of Nitroxide Radicals and Spin Adducts of DMPO and MNP. Journal of Physical Chemistry A, 2012, 116, 8475-8483.	1.1	13
4190	Infrared Spectra of CH₃â€“MH through Methane Activation by Laser-Ablated Sn, Pb, Sb, and Bi Atoms. Journal of Physical Chemistry A, 2012, 116, 8500-8506.	1.1	19
4191	Transmission of Electronic Effects through the {closo-1-CB₉} and {closo-1-CB₁₁} Cages: Apparent Dissociation Constants for Series of [closo-1-CB₉H₈-1-COOH-10-X] and [closo-1-CB₁₁H₁₀-1-COOH-12-X] Acids. Inorganic Chemistry, 2012, 51, 5353-5359.	1.9	32
4192	Infrared Spectra of the Î·²-M(NC)-CH₃, CH₃-MNC, and CH₂â•M(H)NC Complexes Prepared by Reactions of Thorium and Uranium Atoms with Acetonitrile. Organometallics, 2012, 31, 535-544.	1.1	27
4193	Ab Initio Quantum Mechanical Charge Field Molecular Dynamics Simulation (QMCF-MD) of Bi³⁺ in Water. Journal of Physical Chemistry A, 2012, 116, 8008-8014.	1.1	12
4194	An Evaluation of Scaling Factors for Multiparameter Scaling Procedures Based on DFT Force Fields. Journal of Physical Chemistry A, 2012, 116, 3866-3880.	1.1	40
4195	Oscillator Strength of Symmetry-Forbidden d-d Absorption of Octahedral Transition Metal Complex: Theoretical Evaluation. Inorganic Chemistry, 2012, 51, 2785-2792.	1.9	11
4196	Theoretical Study on the Ring-Opening of 1,3-Disilacyclobutane and H₂ Elimination. Journal of Physical Chemistry A, 2012, 116, 11806-11816.	1.1	20
4197	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. Journal of Chemical Theory and Computation, 2012, 8, 1212-1222.	2.3	46
4198	Tautomeric transitions of isocytosine isolated in argon and neon matrices induced by UV irradiation. Journal of Molecular Structure, 2012, 1025, 92-104.	1.8	21
4199	Dissociative Adsorption of Dimethyl Sulfoxide at the Ge(100)-2 Ã— 1 Surface. Journal of Physical Chemistry C, 2012, 116, 26422-26430.	1.5	10
4200	Bond Energies and Structures of Ammoniaâ€“Sulfuric Acid Positive Cluster Ions. Journal of Physical Chemistry A, 2012, 116, 5886-5899.	1.1	36
4201	Reliability of Approximate Methods to Study Tip-Functionalized Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 25401-25406.	1.5	12
4202	Vibrational and Electronic Spectroscopy of Neutral Antimony Coordination Compounds of the 1,3-Dithiole-2-thione-4,5-dithiolate (dmit). Journal of Physical Chemistry A, 2012, 116, 2244-2260.	1.1	10
4203	FT-IR Investigation of Methoxy Substituted Benzenes Adsorbed on Solid Acid Catalysts. Journal of Physical Chemistry C, 2012, 116, 21308-21317.	1.5	10
4204	N-Acylated Dipeptide Tags Enable Precise Measurement of Ion Temperature in Peptide Fragmentation. Journal of Physical Chemistry B, 2012, 116, 13982-13990.	1.2	3

#	Article	IF	Citations
4205	Infrared Spectra of the Complexes Osâ†NCCH₃, Reâ†NCCH₃, CH₃â€“ReNC, CH₂â•Re(H)NC, and CHâ‰¡Re(H)₂NC and their Mn Counterparts Prepared by Reactions of Laser-Ablated Os, Re, and Mn Atoms with Acetonitrile in Excess Argon. Organometallics, 2012, 31, 6095-6105.	1.1	17
4206	Unusual Low-Vibrational Câ•O Mode of COOH Can Distinguish between Carboxylated Zigzag and Armchair Single-Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 26072-26083.	1.5	13
4207	Transition State Analysis of Acid-Catalyzed Hydrolysis of an Enol Ether, Enolpyruvylshikimate 3-Phosphate (EPSP). Journal of the American Chemical Society, 2012, 134, 12947-12957.	6.6	8
4208	Twisted Imide Bond in Noncyclic Imides. Synthesis and Structural and Vibrational Properties of N,N-Bis(furan-2-carbonyl)-4-chloroaniline. Journal of Organic Chemistry, 2012, 77, 4688-4695.	1.7	19
4209	Vibrational Assignment of the Ultrafast Infrared Spectrum of the Photoactivatable Flavoprotein AppA. Journal of Physical Chemistry B, 2012, 116, 10722-10729.	1.2	21
4210	Delocalization-to-Localization Charge Transition in Diferrocenyl-Oligothienylene-Vinylene Molecular Wires as a Function of the Size by Raman Spectroscopy. Journal of the American Chemical Society, 2012, 134, 5675-5681.	6.6	33
4211	Cisâ€“Trans Isomerization of Chemically Activated 1-Methylallyl Radical and Fate of the Resulting 2-Buten-1-peroxy Radical. Journal of Physical Chemistry A, 2012, 116, 7603-7614.	1.1	17
4212	Synthesis of Tris-hydroxymethyl-Based Nitrone Derivatives with Highly Reactive Nitronyl Carbon. Journal of Organic Chemistry, 2012, 77, 938-948.	1.7	6
4213	Theoretical Study of Nascent Hydration in the Fe⁺(H₂O)_n System. Journal of Physical Chemistry A, 2012, 116, 1906-1913.	1.1	23
4214	Influence of Connector Groups on the Interactions of Substituents with Carbon-Centered Radicals. Journal of Physical Chemistry A, 2012, 116, 10203-10208.	1.1	9
4215	Picosecond Rotational Interconversion Adjacent to a Câ•O Bond Studied by Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 11292-11301.	1.2	13
4216	Dynamics and Thermodynamics of Crystalline Polymorphs: Î±-Glycine, Analysis of Variable-Temperature Atomic Displacement Parameters. Journal of Physical Chemistry A, 2012, 116, 8092-8099.	1.1	24
4217	Molybdenum(VI) Complexes of a 2,2â€²-Biphenyl-bridged Bis(amidophenoxide): Competition between Metalâ€“Ligand and Metalâ€“Amidophenoxide Ï€ Bonding. Inorganic Chemistry, 2012, 51, 1239-1250.	1.9	26
4218	Infrared Spectra of IrCCH₂, HIrCCH, and Ir-Î·²-C₂H₂ Prepared in Reaction of Laser-Ablated Iridium Atom with Acetylene. Journal of Physical Chemistry A, 2012, 116, 9261-9270.	1.1	10
4219	Implementation of the Solvent Macromolecule Boundary Potential and Application to Model and Realistic Enzyme Systems. Journal of Physical Chemistry B, 2012, 116, 12522-12534.	1.2	14
4220	Single versus Dual Attachment in the Adsorption of Diisocyanates at the Ge(100)-2 Ã— 1 Surface. Journal of Physical Chemistry C, 2012, 116, 12670-12679.	1.5	16
4221	1H-Pyrrolo[3,2-h]quinoline: A Benchmark Molecule for Reliable Calculations of Vibrational Frequencies, IR Intensities, and Raman Activities. Journal of Physical Chemistry A, 2012, 116, 11973-11986.	1.1	13
4222	Transition State Analysis ofVibrio choleraeSialidase-Catalyzed Hydrolyses of Natural Substrate Analogues. Journal of the American Chemical Society, 2012, 134, 3748-3757.	6.6	16

#	Article	IF	Citations
4223	Experimental (FT-IR and FT-Raman) and theoretical (HF and DFT) investigation, NMR, NBO, electronic properties and frequency estimation analyses on 2,4,5-trichlorobenzene sulfonyl chloride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 311-325.	2.0	8
4224	A comparative study on vibrational, conformational and electronic structure of 1,2-dimethyl-5-nitroimidazole and 2-methyl-5-nitroimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 176-188.	2.0	11
4225	FT-IR and FT-Raman spectra, thermo dynamical behavior, HOMO and LUMO, UV, NLO properties, computed frequency estimation analysis and electronic structure calculations on Î±-bromotoluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 411-422.	2.0	139
4226	Solid state simulation of tetramer form of 5-aminoorotic acid: The vibrational spectra and molecular structure study by using MP2 and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 948-962.	2.0	11
4227	FT-IR, FT-Raman, SERS and computational study of 5-ethylsulphonyl-2-(o-chlorobenzyl)benzoxazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 617-625.	2.0	77
4228	6-Phenyl-3-(4-pyridyl)-1,2,4-triazolo-[3,4-b][1,3,4]thiadiazole: Synthesis, experimental, theoretical characterization and biological activities. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 606-615.	2.0	15
4229	Molecular structure and vibrational study of diprotonated guanazolium using DFT calculations and FT-IR and FT-Raman spectroscopies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 975-985.	2.0	3
4230	Synthesis, vibrational and quantum chemical investigations of hydrogen bonded complex betaine dihydrogen selenite. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 744-758.	2.0	17
4231	N-cyclohexyl-2-[5-(4-pyridyl)-4-(p-tolyl)-4H-1,2,4-triazol-3-ylsulfanyl]-acetamide dihydrate: Synthesis, experimental, theoretical characterization and biological activities. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 923-934.	2.0	17
4232	Synthesis, structure, photo-responsive properties of 4-(2-fluorobenzylideneamino)antipyrine: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 1013-1022.	2.0	16
4233	A novel bonding of 6,7-dichloroquinoxlaine-2,3-dione, DCQX, to two molybdenum (0) metal centers: Synthesis, characterization, biological activity studies and semiempirical calculations of [(bpy)2Mo(Î¼2-Î²2:Î·6-DCQX)Mo(CO)3] complex. Polyhedron, 2012, 44, 238-244.	1.0	7
4234	Kinetic energy of structural protons in silica xerogels. Surface Science, 2012, 606, 1088-1092.	0.8	5
4235	Role of Explicit Solvents in Palladium(II)-Catalyzed Alkoxylation of Arenes: An Interesting Paradigm for Preferred Outer-Sphere Reductive Elimination over Inner-Sphere Pathway. Organometallics, 2012, 31, 6466-6481.	1.1	42
4236	A quantum chemical investigation of the electronic structure of thionine. Photochemical and Photobiological Sciences, 2012, 11, 397-408.	1.6	32
4237	Phenylpropargyl Radicals and Their Dimerization Products: An IR/UV Double Resonance Study. Journal of Physical Chemistry A, 2012, 116, 8515-8522.	1.1	31
4238	Reactive Nitrogen Species Reactivities with Nitrones: Theoretical and Experimental Studies. Chemical Research in Toxicology, 2012, 25, 1581-1597.	1.7	43
4239	Experimental (IR/Raman and ¹H/¹³C NMR) and Theoretical (DFT) Studies of the Preferential Conformations Adopted by <scp>l</scp>-Lactic Acid Oligomers and Poly(<scp>l</scp>-lactic acid) Homopolymer. Journal of Physical Chemistry B, 2012, 116, 9-21.	1.2	32
4240	A comparative study on vibrational, conformational and electronic structure of 2-(hydroxymethyl)pyridine and 3-(hydroxymethyl)pyridine. Journal of Molecular Structure, 2012, 1018, 156-170.	1.8	20

#	Article	IF	Citations
4241	Synthesis, characterization and electrochemistry of novel unsymmetrical zinc phthalocyanines sensitizer with extended conjugation. Journal of Molecular Structure, 2012, 1022, 153-158.	1.8	22
4242	Conformation of a MnCp(CO)2-thienothiophene carbene complex: A spectroscopic and computational study. Journal of Molecular Structure, 2012, 1021, 76-83.	1.8	6
4243	Structural and spectroscopic characterization of a novel potential chemotherapeutic agent 3-(1-adamantyl)-1-{[4-(2-methoxyphenyl)piperazin-1-yl]methyl}-4-methyl-1H-1,2,4-triazole-5(4H)-thione by first principle calculations. Journal of Molecular Structure, 2012, 1022, 49-60.	1.8	37
4244	Monomeric and dimeric structures, electronic properties and vibrational spectra of azelaic acid by HF and B3LYP methods. Journal of Molecular Structure, 2012, 1022, 81-88.	1.8	8
4245	Ab initio and semi-empirical computational studies on 5-hydroxy-5,6-di-pyridin-2-yl-4,5-dihidro-2H-[1,2,4]triazine-3-thione. Journal of Molecular Structure, 2012, 1024, 176-188.	1.8	3
4246	FTIR, FT-Raman and quantum chemical investigations of 4,5-dimethyl-1,3-dioxol-2-one. Journal of Molecular Structure, 2012, 1024, 54-64.	1.8	4
4247	Unusual hydrogen-bonding aggregation in 4-amino-1-(2-carboxyethyl)pyridinium bromide hemihydrate. Journal of Molecular Structure, 2012, 1026, 150-158.	1.8	5
4248	Valence XPS, IR, and C13 NMR spectral analysis of 6 polymers by quantum chemical calculations. Journal of Molecular Structure, 2012, 1027, 20-30.	1.8	8
4249	Raman spectroscopy and DFT calculations of intermediates in the hydrolysis of methylmethoxysilanes. Journal of Molecular Structure, 2012, 1023, 204-211.	1.8	14
4250	An experimental and theoretical approach of spectroscopic and structural properties of the bis(diethyldithiocarbamate)â€“cobalt(II). Journal of Molecular Structure, 2012, 1029, 119-134.	1.8	6
4251	Infrared spectra and density functional calculations of the Mâ†NCCCH3, Î·2â€“M(NC)â€“CH3, CH3â€“MNC, CH2M(H)NC, and CHM(H)2NC complexes produced by reactions of Group 6 metal atoms with acetonitrile. Journal of Organometallic Chemistry, 2012, 703, 25-33.	0.8	14
4252	A quantum chemical study on the antioxidant activity of bioactive polyphenols from peanut (Arachis) Tj ETQq1 1 0.784314 rgBT /Ove 2012, 981, 38-46.	1.1	5
4253	Binding of viologen derivatives to cucurbit[8]uril. Computational and Theoretical Chemistry, 2012, 983, 16-24.	1.1	13
4254	Kinetic study of the formation of triphenylene from the condensation of C12H10+C6H5. Computational and Theoretical Chemistry, 2012, 985, 1-7.	1.1	13
4255	Theoretical studies on intramolecular methyl transfer in the 2-methoxy-pyridine derivative radical cations. Computational and Theoretical Chemistry, 2012, 989, 51-58.	1.1	3
4256	Mechanism of SO2 elimination from the aromatic sulfonamide anions: A theoretical study. Computational and Theoretical Chemistry, 2012, 991, 74-81.	1.1	12
4257	Computational studies on the heats of formation, energetic properties, and thermal stability of energetic nitrogen-rich furazano[3,4-b]pyrazine-based derivatives. Computational and Theoretical Chemistry, 2012, 992, 110-119.	1.1	50
4258	DFT study on the intramolecular nitroneâ€“alkene cycloaddition reaction of the N-3-alkenylnitrone. Computational and Theoretical Chemistry, 2012, 992, 128-133.	1.1	2

#	Article	IF	Citations
4259	Computational study of the cerium(III) ion in aqueous environment. Chemical Physics Letters, 2012, 539-540, 50-53.	1.2	13
4260	Theoretical estimation of the equilibrium distribution of clumped isotopes in nature. Geochimica Et Cosmochimica Acta, 2012, 77, 292-303.	1.6	44
4261	The Element Effect Revisited: Factors Determining Leaving Group Ability in Activated Nucleophilic Aromatic Substitution Reactions. Journal of Organic Chemistry, 2012, 77, 9535-9540.	1.7	47
4262	Formation of Metal Oxyfluorides from Specific Metal Reactions with Oxygen Difluoride: Infrared Spectroscopic and Theoretical Investigations of the OScF₂ Radical and OScF with Terminal Single and Triple Sc–O Bonds. Chemistry - A European Journal, 2012, 18, 12446-12451.	1.7	11
4263	Hartreeâ€“Fock and density functional theory study of remote substituent effects on heterolytic Feâ€“N bond energies of pâ€Câ€₆H₄NHFe(CO)₂(Î·⁵â€C₅H₅) and pâ€Câ€₆H₄N(COMe)Fe(CO)₂(Î·⁵â€C₅H₅). Journal of Physical Organic Chemistry, 2012, 25, 1275-1285.	0.9	7
4264	DFT, AIM, and NBO analyses of 1-methyl-2-thioxoimidazolidin-4-one tautomers and their complexes with iodine. Journal of Structural Chemistry, 2012, 53, 649-658.	0.3	8
4265	Improving anharmonic infrared spectra using semiclassically prepared molecular dynamics simulations. Physical Chemistry Chemical Physics, 2012, 14, 2381.	1.3	27
4266	Divalent N(I) Character in 2-(Thiazol-2-yl)guanidine: An Electronic Structure Analysis. Journal of Physical Chemistry A, 2012, 116, 9071-9079.	1.1	31
4267	Detection of Mercuryâ€“TpT Dinucleotide Binding by Raman Spectra: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 8313-8320.	1.1	19
4268	Intrinsic point-defect equilibria in tetragonal ZrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: Density functional theory analysis with finite-temperature effects. Physical Review B, 2012, 86, .	1.1	74
4269	Density Functional Study on the Cytochrome-Mediated S-Oxidation: Identification of Crucial Reactive Intermediate on the Metabolic Path of Thiazolidinediones. Journal of Physical Chemistry A, 2012, 116, 10441-10450.	1.1	20
4270	Structural, Spectroscopic (NMR, IR, and Raman), and DFT Investigation of the Self-Assembled Nanostructure of Pravastatin-LDH (Layered Double Hydroxides) Systems. Chemistry of Materials, 2012, 24, 1415-1425.	3.2	66
4271	Why Are S_nN₄ (n = 1â€“4) Species â€œMissingâ€? Answers in a Broader Theoretical Context of Binary Sâ€“N Compounds. Inorganic Chemistry, 2012, 51, 13321-13327.	1.9	18
4272	Reactivities of Superoxide and Hydroperoxyl Radicals with Disubstituted Cyclic Nitrones: A DFT Study. Journal of Physical Chemistry A, 2012, 116, 886-898.	1.1	11
4273	Solid-state vibrational spectroscopic investigation of cocrystals and salt of indomethacin. CrystEngComm, 2012, 14, 6665.	1.3	24
4274	Axial Ligand Effect On The Rate Constant of Aromatic Hydroxylation By Iron(IV)â€“Oxo Complexes Mimicking Cytochrome P450 Enzymes. Journal of Physical Chemistry B, 2012, 116, 718-730.	1.2	64
4275	Photoactivated linkage isomerism in single crystals of nickel, palladium and platinum di-nitro complexes â€“ a photocrystallographic investigation. Dalton Transactions, 2012, 41, 13173.	1.6	35
4276	Conformational polymorphism in bicalutamide: a quantum chemical study. Structural Chemistry, 2012, 23, 1857-1866.	1.0	10

#	Article	IF	Citations
4277	Theoretical studies of molecular structure and vibrational spectra of free, H-bonded and coordinated nicotinamide. Computational and Theoretical Chemistry, 2012, 988, 27-33.	1.1	10
4278	Theoretical studies on intramolecular methyl transfer in the S-2-alkenyl-dimethylsulfonium ion. Computational and Theoretical Chemistry, 2012, 997, 25-33.	1.1	2
4279	Atmospheric reaction of OH radicals with 2-methyl-3-buten-2-ol (MBO): Quantum chemical investigation on the reaction mechanism. Computational and Theoretical Chemistry, 2012, 999, 109-120.	1.1	6
4280	Energetic and vibrational assignment of tautomerizm of (Hydroxyphosphino)silanethione: A theoretical study. Computational and Theoretical Chemistry, 2012, 999, 251-258.	1.1	2
4281	Dihydropyridine-fused and pyridine-fused coumarins: Reduction on a glassy carbon electrode in dimethylformamide. Electrochimica Acta, 2012, 85, 336-344.	2.6	10
4282	Molecular structure and vibrational spectra of Irinotecan: A density functional theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 1-6.	2.0	22
4283	Quantum chemical studies and vibrational analysis of 4-acetyl benzonitrile, 4-formyl benzonitrile and 4-hydroxy benzonitrile â€“ A comparative study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 156-169.	2.0	16
4284	Vibrational analyses of 1,3-dibenzoyl-4,5-dihydro-1H-imidazole-2-thione and 1,3-dibenzoyl tetrahydropyrimidine-2(1H)-thione by normal coordinate treatment. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 384-395.	2.0	12
4285	Vibrational spectral investigation and Natural Bond Orbital analysis of anti-rheumatoid drug Ethyl 4-nitrophenylacetate â€“ DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 413-422.	2.0	5
4286	Crystal structure and theoretical studies of the keto-enol isomerism of N,Nâ€²-bis(salicylidene)-o-phenylenediamine (salophen). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 110-115.	2.0	44
4287	Efficient synthesis of trifluoromethylated dihydrochalcones, aryl vinyl ketones and indanones by superelectrophilic activation of 4,4,4-trifluoro/3-(trifluoromethyl)crotonic acids. Journal of Fluorine Chemistry, 2012, 143, 292-302.	0.9	20
4288	Syntheses, structures and redox properties of tris(pyrazolyl)borate-capped ruthenium vinyl complexes. Journal of Organometallic Chemistry, 2012, 721-722, 173-185.	0.8	4
4289	Mass spectrometric and theoretical studies on dissociation of the CS bond in the benzenesulfonic acid and benzenesulfinic acid anion series: Homolytic cleavage vs heterolytic cleavage. Journal of Molecular Structure, 2012, 1028, 1-6.	1.8	7
4290	Salts of 1-(chloromethyl)-1,1-dimethylhydrazine and ionic liquids. RSC Advances, 2012, 2, 3691.	1.7	18
4291	Optimized Structure and Vibrational Properties by Error Affected Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2012, 8, 4204-4215.	2.3	22
4292	Mechanistic Investigation of Enediyne-Connected Amino Ester Rearrangement. Theoretical Rationale for the Exclusive Preference for 1,6- or 1,5-Hydrogen Atom Transfer Depending on the Substrate. A Potential Route to Chiral Naphthoazepines. Journal of Organic Chemistry, 2012, 77, 2773-2783.	1.7	23
4293	A Density Functional Theory Study on Carbon Monoxide Adsorption on Platinumâ€“Osmium and Platinumâ€“Rutheniumâ€“Osmium Alloys. Journal of Physical Chemistry C, 2012, 116, 21447-21458.	1.5	13
4294	Evaluation of Accuracy of Ideal-Gas Heat Capacity and Entropy Calculations by Density Functional Theory (DFT) for Rigid Molecules. Journal of Chemical & Engineering Data, 2012, 57, 227-232.	1.0	52

#	Article	IF	Citations
4295	Metal salts of the 4,5-dicyano-2H-1,2,3-triazole anion ([C4N5]â˜). Dalton Transactions, 2012, 41, 3817.	1.6	24
4296	Optimization of CHARMM force field parameters for the chalcone fragment. Science China Chemistry, 2012, 55, 2580-2586.	4.2	0
4297	Theoretical studies on a series of 1,2,4-triazoles derivatives as potential high energy density compounds. Journal of Chemical Sciences, 2012, 124, 995-1006.	0.7	8
4298	Phase transition in organicâ€“inorganic perovskite (C9H19NH3)2 PbI2Br2 of long-chain alkylammonium. Results in Physics, 2012, 2, 71-76.	2.0	35
4299	A joint application of vibrational spectroscopic and quantum mechanical methods in quantitative analysis of baicalein structure. Monatshefte FÃ¼r Chemie, 2012, 143, 1369-1378.	0.9	1
4300	Colour tuning from green to red by substituent effects in phosphorescent tris-cyclometalated iridium(iii) complexes of carbazole-based ligands: synthetic, photophysical, computational and high efficiency OLED studies. Journal of Materials Chemistry, 2012, 22, 6419.	6.7	96
4301	The Mechanism of Permanganate Oxidation of Sulfides and Sulfoxides. Journal of Organic Chemistry, 2012, 77, 351-356.	1.7	20
4302	Thermochemistry and Bond Dissociation Energies of Ketones. Journal of Physical Chemistry A, 2012, 116, 5707-5722.	1.1	45
4303	Molecular Vibration Spectroscopy Studies on Novel Trinuclear Rhodium-7-Hydride Complexes of the General Type {[Rh(PP*)X]₃(Î¼₂-X)₃(Î¼₃-X)}(BF₄)₂ (X = H, D). Inorganic Chemistry, 2012, 51, 7377-7383.	1.9	10
4304	Thermochemical Properties for Hydrogenated and Oxy-Hydrogenated Aluminum Species. Soft Materials, 2012, 10, 313-343.	0.8	4
4305	Anti-Stokes-enhanced tunneling ionization of molecules. Physical Review A, 2012, 86, .	1.0	15
4306	Depth Profile Assignments of nm and Î¼m Orders by Quantum Chemical Calculations for Chitosan Films Modified by Kr+ Beam Bombardment. Progress in Theoretical Chemistry and Physics, 2012, , 475-485.	0.2	0
4307	A Stepwise Solvent-Promoted SNi Reaction of Î±-d-Glucopyranosyl Fluoride: Mechanistic Implications for Retaining Glycosyltransferases. Journal of the American Chemical Society, 2012, 134, 1212-1220.	6.6	53
4309	Thermally reversible Dielsâ€“Alder-based polymerization: an experimental and theoretical assessment. Polymer Chemistry, 2012, 3, 628-639.	1.9	50
4310	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	22
4311	Electronic Structure, Nonlinear Optical Properties, and Vibrational Analysis of Gemifloxacin by Density Functional Theory. Spectroscopy, 2012, 27, 185-206.	0.8	24
4312	Synthesis, Characterization, and Energetic Properties of Nitroso Compounds. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 336-344.	0.6	1
4313	On QM/MM and MO/MO cluster calculations of all-atom anisotropic displacement parameters for molecules in crystal structures. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 110-116.	0.3	27

#	Article	IF	Citations
4314	The role of hydrogen bonds in proteinâ€“ligand interactions. DFT calculations in 1,3â€dihydrobenzimidazoleâ€2 thione derivatives with glycinamide as model HIV RT inhibitors. International Journal of Quantum Chemistry, 2012, 112, 1786-1795.	1.0	10
4315	Combined experimental and computational modeling studies on 3,5â€dimethylâ€pyrazoleâ€1â€carbodithioic acid benzyl ester. International Journal of Quantum Chemistry, 2012, 112, 373-381.	1.0	4
4316	Ab initio and semiempirical computational studies on 1â€{(2E)â€2â€[(aminocarbonothioyl)hydrazono]â€2â€(3â€mesitylâ€3â€methylcyclobutyl)ethyl}â€pyrrolidineâ€2,5â€dione. International Journal of Quantum Chemistry, 2012, 112, 394-413.	1.0	1
4317	Ab initio and RRKM calculations for the reaction channels of O(¹D) + CH₃CHF₂. International Journal of Quantum Chemistry, 2012, 112, 1353-1362.	1.0	0
4318	Theoretical study on the adduct of chlorine trifluoride oxide and boron trifluorideâ€”molecular and crystal structures, vibrational spectrum, and thermodynamic properties. International Journal of Quantum Chemistry, 2012, 112, 1291-1298.	1.0	3
4319	Remote substituent effects on homolytic Feâ€C bond energies of pâ€C₆H₄CH₂Fe(CO)₂(Î·⁵â€C₅H₅) and pâ€C₆H₄(H)(CN)CFe(CO)₂(Î·⁵â€C₅H₅). Journal of Physical Organic Chemistry, 2012, 25, 1221-1231.	0.9	8
4320	Computational study on structures, thermochemical properties, and bond energies of disulfide oxygen (Sâ€“Sâ€“O)â€bridged CH₃SSOH and CH₃SS(=O)H and radicals. Journal of Physical Organic Chemistry, 2012, 25, 475-485.	0.9	9
4321	Computational study on the conformational preferences in nateglinide. Journal of Physical Organic Chemistry, 2012, 25, 649-657.	0.9	8
4322	Remote substituent effects on homolytic Feâ€N bond energies of pâ€C₆H₄NHFe(CO)₂(Î·⁵â€C₅H₅) and pâ€C₆H₄(COMe)NFe(CO)₂(Î·⁵â€C₅H₅) studied using Hartreeâ€“Fock and density functional theory methods. Journal of Physical Organic Chemistry, 2012, 25, 1119-1126.	0.9	6
4323	Experimental and quantum chemical calculational studies on Nâ€[4â€(3â€Methylâ€3â€phenylâ€cyclobutyl)â€thiazolâ€2â€yl]â€Nâ€²â€pyridinâ€3ylmethyleneâ€hydrazine. International Journal of Quantum Chemistry, 2012, 112, 2775-2781.	1.0	0
4324	Density functional theory and ab initio study on the reaction mechanisms of the homogeneous, unimolecular elimination kinetics of selected 1â€chloroalkenes in the gas phase. International Journal of Quantum Chemistry, 2012, 112, 3729-3738.	1.0	6
4325	Decomposition of Malonic Anhydrides. Journal of the American Chemical Society, 2012, 134, 9698-9707.	6.6	13
4326	Numerical Study of the Zirconium Oxide System. Soft Materials, 2012, 10, 344-368.	0.8	0
4327	The mechanism of hexamethylenetetramine (HMT) formation in the solid state at low temperature. Physical Chemistry Chemical Physics, 2012, 14, 12309.	1.3	52
4328	Theoretical Determination of the Infrared Spectra of Amorphous Polymers. Journal of Physical Chemistry A, 2012, 116, 7424-7435.	1.1	14
4329	Metabolicâ€intermediate complex formation with cytochrome P450: Theoretical studies in elucidating the reaction pathway for the generation of reactive nitroso intermediate. Journal of Computational Chemistry, 2012, 33, 1740-1747.	1.5	30
4330	Gasâ€phase reactions of SiH_n⁺ (n = 1,2) with NF₃: A computational investigation on the detailed mechanistic aspects. Journal of Computational Chemistry, 2012, 33, 1918-1926.	1.5	3
4331	M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198.	1.5	59

#	Article	IF	Citations
4332	Extension of the CHARMM general force field to sulfonylâ€containing compounds and its utility in biomolecular simulations. Journal of Computational Chemistry, 2012, 33, 2451-2468.	1.5	659
4333	Vibrational frequency scale factors for density functional theory and the polarization consistent basis sets. Journal of Computational Chemistry, 2012, 33, 2380-2387.	1.5	186
4334	Kinetic Study of 1,5â€Hydrogen Transfer Reactions of Methyl Acrylate and Butyl Acrylate Using Quantum Chemistry. Macromolecular Theory and Simulations, 2012, 21, 461-469.	0.6	31
4335	Role of wobble base pair geometry for codon degeneracy: purine-type bases at the anticodon wobble position. Journal of Molecular Modeling, 2012, 18, 3805-3820.	0.8	12
4336	Hydrogen bond donating ability of meta and parahydroxy phenoxyl radicals. Organic and Biomolecular Chemistry, 2012, 10, 814-818.	1.5	12
4337	Ring splitting of azetidin-2-ones via radical anions. Organic and Biomolecular Chemistry, 2012, 10, 7928.	1.5	13
4339	Goldâ€“Gold Cooperation in the Addition of Methanol to Alkynes. Angewandte Chemie - International Edition, 2012, 51, 8378-8382.	7.2	78
4340	Density Functional Theoretical Study of Polynitrogen Compounds N₅⁺Y^{â^'} (Y=B(CF₃)₄, BF₄,) Tj ETQq1 1 0.784314 rgBT	2.1	13
4341	Influence of an Unnatural Amino Acid Side Chain on the Conformational Dynamics of Peptides. ChemPhysChem, 2012, 13, 1522-1534.	1.0	10
4342	Microheterogeneities in Ionicâ€Liquidâ€“Methanol Solutions Studied by FTIR Spectroscopy, DFT Calculations and Molecular Dynamics Simulations. ChemPhysChem, 2012, 13, 1708-1717.	1.0	51
4343	Vibrational Davydov Splittings and Collective Mode Polarizations in Oriented Organic Semiconductor Crystals. Journal of Physical Chemistry C, 2012, 116, 14491-14503.	1.5	25
4344	Spectroscopic and DFT Study of Ferraaziridine Complexes Formed in the Transfer Hydrogenation of Acetophenone Catalyzed Using trans-[Fe(CO)(NCMe)(PPh₂C₆H₄CHâ•NCH₂â^')₂]⁴ Organometallics, 2012, 31, 3056-3064.	1.1	46
4345	Density functional study of substituted (â€“SH, â€“S, â€“OH, â€“Cl) hydrated ions of Hg2+. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	12
4346	Performance assessment of density functional theory-based models using orbital momentum distributions. Molecular Simulation, 2012, 38, 468-480.	0.9	4
4347	Modeling and Analysis of Hydrogen Atoms. Structure and Bonding, 2012, , 21-52.	1.0	18
4348	Thermochemical Properties and Bond Dissociation Energies of C3â€“C5 Cycloalkyl Hydroperoxides and Peroxy Radicals: Cycloalkyl Radical + 3O2 Reaction Thermochemistry. Journal of Physical Chemistry A, 2012, 116, 7550-7563.	1.1	13
4349	New Protein Footprinting: Fast Photochemical Iodination Combined with Top-Down and Bottom-Up Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2012, 23, 1306-1318.	1.2	43
4350	Establishment of rapid detection method of methamidophos in vegetables by surface enhanced Raman spectroscopy. European Food Research and Technology, 2012, 234, 1091-1098.	1.6	29

#	Article	IF	Citations
4351	Molecular design of new nitramine explosives: 1,3,5,7-tetranitro-8-(nitromethyl)-4-imidazolino[4,5-b]4-imidazolino-[4,5-e] pyridine and its N-oxide. Journal of Molecular Modeling, 2012, 18, 1325-1331.	0.8	17
4352	Quantum chemical modeling of the kinetic isotope effect of the carboxylation step in RuBisCO. Journal of Molecular Modeling, 2012, 18, 1877-1883.	0.8	4
4353	Estimating the carbonyl anharmonic vibrational frequency from affordable harmonic frequency calculations. Journal of Molecular Modeling, 2012, 18, 2471-2478.	0.8	10
4354	Theoretical studies on vibrational spectra, thermodynamic properties, detonation properties and pyrolysis mechanism for 1,2-bis(2,4,6-trinitrophenyl) hydrazine. Journal of Molecular Modeling, 2012, 18, 2897-2905.	0.8	4
4355	Design and selection of nitrogen-rich bridged di-1,3,5-triazine derivatives with high energy and reduced sensitivity. Journal of Molecular Modeling, 2012, 18, 3125-3138.	0.8	44
4356	Probing the linear and nonlinear optical properties of nitrogen-substituted carbon nanotube. Journal of Molecular Modeling, 2012, 18, 3219-3225.	0.8	15
4357	Antibacterial Activities of 4â€Substitutedâ€2â€[(E)â€{(1S,2R)/(1R,2S)â€1â€Hydroxyâ€1â€Phenylpropanâ€2â€Ylimino]-3-methyl-4,5-dihydroisoxazol-5-ones. Chemical Biology and Drug Design, 2012, 79, 177-185.	1.3	3
4358	The synthesis, molecular and electronic structure of cyanovinylidene complexes. Inorganica Chimica Acta, 2012, 380, 358-371.	1.2	14
4359	Fabrication of succinic acid-Î³-Fe2O3 nano coreâ€“shells. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 403, 96-102.	2.3	17
4360	Thermally-driven isotope separation across nanoporous graphene. Chemical Physics Letters, 2012, 521, 118-124.	1.2	69
4361	A theoretical study on 2â€²-deoxyguanosine and its mono-hydration: Intermolecular hydrogen bonding weakening induces the fluorescence strengthening. Chemical Physics Letters, 2012, 528, 53-58.	1.2	15
4362	Infrared spectroscopy of V2+(H2O) complexes. Chemical Physics Letters, 2012, 530, 10-15.	1.2	23
4363	Hydration of trivalent lanthanum revisited â€“ An ab initio QMCF-MD approach. Chemical Physics Letters, 2012, 536, 50-54.	1.2	25
4364	Merocyanine dyes containing an isoxazolone nucleus: Synthesis, X-ray crystal structures, spectroscopic properties and DFT studies. Dyes and Pigments, 2012, 93, 1408-1415.	2.0	58
4365	Gas-phase acidities of lysine homologues and proline analogs from the extended kinetic method. International Journal of Mass Spectrometry, 2012, 316-318, 126-132.	0.7	9
4366	A theoretical elucidation of coordination properties of histidine and lysine to Mn2+. International Journal of Mass Spectrometry, 2012, 313, 47-57.	0.7	10
4367	Electronic absorption and vibrational spectra and nonlinear optical properties of l-valinium succinate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 66-73.	2.0	10
4368	FT-IR spectroscopy and DFT calculation study on the solvent effects of benzaldehyde in organic solvents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 86, 51-55.	2.0	17

#	Article	IF	Citations
4369	Comparison of DFT methods for molecular structure and vibration spectra of ofloxacin calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 85, 303-309.	2.0	13
4370	Photoactive azoimine dyes: 4-(2-Pyridylazo)-N,N-diethylaniline and 4-(2-pyridylazo)-N,N-dimethylaniline: Computational and experimental investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 86, 538-546.	2.0	20
4371	FT-Raman, FT-IR spectral and DFT studies on (E)-1-4-nitrobenzylidenethiocarbonohydrazide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 87, 86-95.	2.0	25
4372	Application of the multi-parameter SQM harmonic force field, and ESFF harmonic frequencies scaling procedures to the determination of the vibrational spectra of silicon- and sulfur(II)-containing compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 86, 571-585.	2.0	6
4373	FT-IR and Raman spectroscopic and quantum chemical investigations of some metal halide complexes of 1-phenylpiperazine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 144-155.	2.0	13
4374	Experimental, quantum chemical and natural bond orbital investigations of N-(2,4-dimethylphenyl)-2,2-dichloroacetamide and N-(3,5-dimethylphenyl)-2,2-dichloroacetamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 192-209.	2.0	6
4375	FTIR, FT-Raman, FT-NMR, UVâ€“visible and quantum chemical investigations of 2-amino-4-methylbenzothiazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 88, 220-231.	2.0	35
4376	DFT, FT-Raman and FT-IR investigations of 1-cyclobutylpiperazine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 90, 109-117.	2.0	5
4377	FT-IR, FT-Raman, ab initio, HF and DFT studies, NBO, HOMOâ€“LUMO and electronic structure calculations on 4-chloro-3-nitrotoluene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 89, 137-148.	2.0	73
4378	2-Methoxyphenyl isocyanate and 2-Methoxyphenyl isothiocyanate: Conformers, vibration structure and multiplet Fermi resonance. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 261-268.	2.0	5
4379	4-Allyl-5-pyridin-4-yl-2,4-dihydro-3H-1,2,4-triazole-3-thione: Synthesis, experimental and theoretical characterization. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 136-145.	2.0	14
4380	Experimental (FT-IR, FT-Raman, NMR) and theoretical spectroscopic properties of intermolecular hydrogen bonded 1-acetyl-2-thiohydantoin polymorphs. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 90, 141-151.	2.0	6
4381	â€œAdditiveâ€•cooperativity of hydrogen bonds in complexes of catechol with proton acceptors in the gas phase: FTIR spectroscopy and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 75-82.	2.0	7
4382	Molecular structure and vibrational spectra of 3-and 4-amino-2-bromopyridine by density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 206-216.	2.0	10
4383	Density functional theory study on characterization of 3-chloro-1,2-benzisothiazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 248-255.	2.0	29
4384	Calculated infrared spectra of nerve agents and simulants. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 256-260.	2.0	24
4385	A comparative study on vibrational, conformational and electronic structure of Î±,Î±â€²-diol-o-xylene, Î±,Î±â€²-diol-m-xylene and Î±,Î±â€²-diol-p-xylene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 92, 1-15.	2.0	2
4386	Experimental and quantum chemical computational study of (E)-1-[5-(3,4-dimethylphenyldiazenyl)-2-hydroxyphenyl]ethanone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 208-213.	2.0	19

#	Article	IF	Citations
4387	A comparative study on vibrational, conformational and electronic structure of 2-chloro-4-methyl-3-nitropyridine and 2-chloro-6-methylpyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 92, 305-317.	2.0	9
4388	The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMOâ€“LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 33-46.	2.0	106
4389	SERS and DFT investigation of 1-(2-pyridylazo)-2-naphthol and its metal complexes with Al(III), Mn(II), Fe(III), Cu(II), Zn(II) and Pb(II). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 266-273.	2.0	30
4390	Vibrational spectroscopic studies, NLO, HOMOâ€“LUMO and electronic structure calculations of Î±,Î±,Î±-trichlorotoluene using HF and DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 94, 53-64.	2.0	26
4391	Structural, vibrational (FT-IR and FT-Raman) and UVâ€“Vis spectral analysis of 1-phenyl-3-(1,2,3-thiadiazol-5-yl)urea by DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 331-340.	2.0	12
4392	Ab initio Hartreeâ€“Fock and density functional theory investigations on the conformational stability, molecular structure and vibrational spectra of 5-chloro-3-(2-(4-methylpiperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one drug molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 282-299.	2.0	18
4393	Structural, proton-transfer, thermodynamic and nonlinear optical studies of (E)-2-((2-hydroxyphenyl)iminiomethyl)phenolate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 42-50.	2.0	30
4394	DFT simulations and vibrational analysis of FTIR and FT-Raman spectra of 2-amino-4-methyl benzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 480-484.	2.0	7
4395	Experimental (FT-IR, FT-Raman and UVâ€“Vis) spectra and theoretical DFT investigations of 2,3-diaminophenazine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 401-412.	2.0	16
4396	Tautomeric purine forms of 2-amino-6-chloropurine (N9H10 and N7H10): Structures, vibrational assignments, NBO analysis, hyperpolarizability, HOMOâ€“LUMO study using B3 based density functional calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 340-351.	2.0	48
4397	Experimental and theoretical quantum chemical investigations of 8-hydroxy-5-nitroquinoline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 96, 506-516.	2.0	32
4398	IR spectra and structure of 2-{5,5-dimethyl-3-[(2-phenyl)vinyl]cyclohex-2-enylidene}-malononitrile and its potassium cyanide and sodium methoxide carbanionic adducts: Experimental and B3LYP theoretical studies. Journal of Molecular Structure, 2012, 1009, 42-48.	1.8	1
4399	Measurement and applications of absolute infrared intensities. Journal of Molecular Structure, 2012, 1009, 111-122.	1.8	17
4400	Three hydrogen-bonded complexes of trigonelline with squaric acid: Crystallographic, spectroscopic and theoretical studies. Journal of Molecular Structure, 2012, 1007, 113-121.	1.8	20
4401	A comparative spectroscopic, electronic structure and chemical shift investigations of o-Chloronitrobenzene, p-Chloronitrobenzene and m-Chloronitrobenzene. Journal of Molecular Structure, 2012, 1007, 122-135.	1.8	14
4402	The experimental and DFT studies of 1,3-dimethyl-2-[4-chloro-styryl]-benzimidazolium iodide. Journal of Molecular Structure, 2012, 1007, 275-281.	1.8	0
4403	Low temperature Raman and DFT study of creatinine. Journal of Molecular Structure, 2012, 1012, 141-150.	1.8	20
4404	FT-IR, FT-Raman, surface enhanced Raman scattering and computational study of 2-(p-fluorobenzyl)-6-nitrobenzoxazole. Journal of Molecular Structure, 2012, 1012, 22-30.	1.8	37

#	Article	IF	Citations
4405	Structure of 2,3-dicarboxy-1-methylpyridinium monohydrate studied by X-ray diffraction, DFT calculations, FTIR, Raman and NMR spectra. Journal of Molecular Structure, 2012, 1013, 1-10.	1.8	6
4406	Comparison of the performance of different DFT methods in the calculations of the molecular structure and vibration spectra of serotonin (5-hydroxytryptamine, 5-HT). Journal of Molecular Structure, 2012, 1013, 111-118.	1.8	9
4407	Vibrational spectra and DFT calculations of the vibrational modes of Schiff base C18H17N3O2. Journal of Molecular Structure, 2012, 1013, 126-133.	1.8	4
4408	Structural, spectroscopic and theoretical studies of the 1:1 complex of N-methylpiperidine betaine with squaric acid. Journal of Molecular Structure, 2012, 1015, 86-93.	1.8	11
4409	Combined spectroscopic and DFT studies on 2-chloro-4-nitrotoluene and 4-chloro-2-nitrotoluene. Journal of Molecular Structure, 2012, 1016, 82-96.	1.8	5
4410	Structure of methyl 3-(trimethylammonium)benzoate iodide studied by X-ray diffraction, DFT calculations, NMR and FTIR spectra. Journal of Molecular Structure, 2012, 1017, 115-122.	1.8	6
4411	Molecular structure and vibrational spectra of free and coordinated 3-bromoquinoline: Unexpected intramolecular CHâ‹¯O interactions. Journal of Molecular Structure, 2012, 1017, 135-142.	1.8	7
4412	Polyamines â€“ V: The structure of tetramethylene-1,4-bis(N-deoxyglucitolammonium chloride) studied by X-ray diffraction, DFT calculations, NMR and FTIR spectroscopy. Journal of Molecular Structure, 2012, 1020, 41-47.	1.8	3
4413	Synthesis, spectroscopic characterization and molecular modeling of a tetranuclear platinum(II) complex with thiazolidine-4-carboxylic acid. Journal of Molecular Structure, 2012, 1019, 21-26.	1.8	1
4414	Molecular structure, vibrational spectra, first order hyper polarizability, NBO and HOMOâ€“LUMO analysis of 4-amino-3(4-chlorophenyl) butanoic acid. Solid State Sciences, 2012, 14, 476-487.	1.5	61
4415	On the relation between the solvent parameters and the physical properties of methyl-4,6-O-benzylidene-Î±-d-glucopyranoside organogels. Tetrahedron, 2012, 68, 3803-3810.	1.0	25
4416	Dynamics of Dielsâ€“Alder reactions involving 2-trialkylsilyloxyfurans. Tetrahedron Letters, 2012, 53, 179-181.	0.7	2
4417	Charge transfer in thin films of donorâ€“acceptor complexes studied by infrared spectroscopy. Organic Electronics, 2012, 13, 1237-1244.	1.4	24
4418	Experimental and quantum-chemical studies of histamine complexes with copper(II) ion. Polyhedron, 2012, 31, 285-293.	1.0	7
4419	Synthesis and X-ray crystal structure of the first dinuclear 1,1,2-tris(pyrazol-1-yl)etheneâ€“zinc chloride complex. Polyhedron, 2012, 33, 252-256.	1.0	3
4420	Silver(I) and gold(I) complexes with penicillamine: Synthesis, spectroscopic characterization and biological studies. Polyhedron, 2012, 34, 210-214.	1.0	29
4421	Synthesis, spectroscopic characterization, DFT studies and antibacterial assays of a novel silver(I) complex with the anti-inflammatory nimesulide. Polyhedron, 2012, 36, 112-119.	1.0	40
4422	2,1,3-Benzothiadiazole: Study of its structure, energetics and aromaticity. Journal of Chemical Thermodynamics, 2012, 50, 30-36.	1.0	19

#	Article	IF	Citations
4423	The quinones of bicyclo[3.1.0]hexatriene: A computational study of their chemistry and thermochemistry. Journal of Chemical Thermodynamics, 2012, 52, 43-56.	1.0	3
4424	A conformational analysis and vibrational spectroscopic investigation on 1,2-bis(o-carboxyphenoxy) ethane molecule. Vibrational Spectroscopy, 2012, 58, 27-43.	1.2	7
4425	Raman spectral studies on 2â€²-hydroxyacetophenone in binary liquid mixtures. Vibrational Spectroscopy, 2012, 61, 30-37.	1.2	1
4426	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	1.2	51
4427	Copper(II) and cobalt(II) complexes of 2,6-diacetylpyridine bis(O-methyloxime): A theoretical investigation. Journal of Structural Chemistry, 2012, 53, 251-259.	0.3	2
4428	Computer modeling of the structure of supramolecular systems: An example of ion exchangers. Journal of Analytical Chemistry, 2012, 67, 312-320.	0.4	0
4429	The Photochemistry of [Fe^{III}N₃(cyclamâ€ac)]PF₆ at 266â€…nm. Chemistry - A European Journal, 2012, 18, 3043-3055.	1.7	31
4430	Dynamics and mechanism of structural diffusion in linear hydrogen bond. Journal of Computational Chemistry, 2012, 33, 175-188.	1.5	13
4431	Energetic Salts of Symmetrical Dimethylhydrazine (SDMH). European Journal of Inorganic Chemistry, 2012, 2012, 866-877.	1.0	9
4432	Rate coefficients for intramolecular homolytic substitution of oxyacyl radicals at selenium. International Journal of Chemical Kinetics, 2012, 44, 51-58.	1.0	13
4433	Computational study on the recombination reaction between benzyl and propargyl radicals. International Journal of Chemical Kinetics, 2012, 44, 206-218.	1.0	63
4434	Theoretical Studies of Molecular Structure and Vibrational Spectra of Melaminium Salt: 2,4,6-Triamino-1,3,5-triazin-1,3-ium Tartrate Monohydrate. Arabian Journal for Science and Engineering, 2012, 37, 171-181.	1.1	8
4435	Examining the impact of ancillary ligand basicity on copper(I)â€“ethylene binding interactions: a DFT study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
4436	Computational DFT studies on a series of toluene derivatives as potential high energy density compounds. Structural Chemistry, 2012, 23, 515-524.	1.0	12
4437	Density functional theory study on (F2AlN3) n (nÂ=Â1â€“4) clusters. Structural Chemistry, 2012, 23, 545-550.	1.0	5
4438	methyl-2, 4, 6, 8, 12-hexanitrohexaazaisowurtzitane. Journal of Molecular Modeling, 2012, 18, 165-170.	0.8	21
4439	Theoretical study of substituent effects on the gasâ€phase stabilities of phenoxide anions. Journal of Physical Organic Chemistry, 2013, 26, 115-123.	0.9	6
4440	Protonation of 5â€methylhydantoin and its thio derivatives in the gas phase: A theoretical study. International Journal of Quantum Chemistry, 2013, 113, 908-915.	1.0	14

#	Article	IF	Citations
4441	Theoretical analysis of correlation between ionization threshold fluence in IRâ€MALDI and IR absorption spectrum of matrix molecules. International Journal of Quantum Chemistry, 2013, 113, 125-129.	1.0	2
4442	Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?. Journal of Physical Chemistry A, 2013, 117, 6664-6670.	1.1	33
4443	Study of the Gas-Phase Intramolecular Aryltrifluoromethylation of Phenyl(Trifluoromethyl)Iodonium by ESI-MS/MS. Journal of the American Society for Mass Spectrometry, 2013, 24, 761-767.	1.2	8
4444	Charge Reversal Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2013, 24, 213-221.	1.2	2
4445	Theoretical study on the structures and properties of (Br2AlN3) n (n = 1â€“4) clusters. Journal of Structural Chemistry, 2013, 54, 32-39.	0.3	0
4446	Comparative vibrational spectroscopic studies, HOMOâ€“LUMO and NBO analysis of N-(phenyl)-2,2-dichloroacetamide, N-(2-chloro phenyl)-2,2-dichloroacetamide and N-(4-chloro) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Chemistry, 2013, 1016, 8-21.	1.1	116
4447	The Molecule Calculator: A Web Application for Fast Quantum Mechanics-Based Estimation of Molecular Properties. Journal of Chemical Education, 2013, 90, 1093-1095.	1.1	36
4448	Molecular structure, spectroscopic properties, NLO and NBO analysis of 3,4-Lutidine and [Ag(3,4-Lutidine)2NO3] complex. Journal of Molecular Structure, 2013, 1048, 308-320.	1.8	7
4449	Tracking of Tuning Effects in Bis-Cyclometalated Iridium Complexes: A Combined Time Resolved Infrared Spectroscopy, Electrochemical, and Computational Study. Inorganic Chemistry, 2013, 52, 8795-8804.	1.9	30
4450	3-Formylchromone based topoisomerase IIÎ± inhibitors: discovery of potent leads. MedChemComm, 2013, 4, 1257.	3.5	11
4451	FT-IR, Micro-Raman and UVâ€“vis spectroscopic and quantum chemical investigations of free 2,2â€²-dithiodipyridine and its metal (Co, Cu and Zn) halide complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 61-73.	2.0	50
4452	A THEORETICAL STUDY ON THE INFRARED SPECTRA, THERMODYNAMIC FUNCTIONS, AND DETONATION PARAMETERS FOR THE â€“CN, â€“NC, â€“NNO₂and â€“ONO₂DERIVATIVES OF HNS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1250095.	1.8	0
4453	Polymerization of Methyl Methacrylate with Lithium Triflate. A Kinetic and Structural Study. Macromolecules, 2013, 46, 5445-5454.	2.2	14
4454	Significant Oâ€“H Bond Weakening in CpMn(CO)2(CH3OH): Evidence for the Generation of the CpMn(CO)2(CH3O) Radical upon H Atom Abstraction by O2. Organometallics, 2013, 32, 4359-4365.	1.1	5
4455	QVibeplot: A Program To Visualize Molecular Vibrations in Two Dimensions. Journal of Chemical Education, 2013, 90, 944-946.	1.1	31
4456	Structure and conformation of 2,3-diethoxycarbonyl-1-methylpyridinium iodide studied by NMR, FTIR, Raman, X-ray diffraction and DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 208-218.	2.0	4
4457	Vibrational spectral investigation and natural bond orbital analysis of pharmaceutical compound 7-Amino-2,4-dimethylquinolinium formate â€“ DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 595-602.	2.0	62
4458	Vibrational spectral studies and non-linear optical properties of l-leucine l-leucinium picrate: A Density Functional Theory approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 437-444.	2.0	35

#	Article	IF	Citations
4459	Gold(III) Complexes of Pyridyl- and Isoquinolylamido Ligands: Structural, Spectroscopic, and Biological Studies of a New Class of Dual Topoisomerase I and II Inhibitors. Inorganic Chemistry, 2013, 52, 7889-7906.	1.9	33
4460	Multi-photon absorption effect and intra-molecular charge transfer of donor-Ï€-acceptor chromophore ethyl p-amino benzoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 108, 197-210.	2.0	12
4461	Raman spectra of alkyl-substituted azaoxa[8]circulenes: DFT calculation and experiment. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2013, 114, 509-521.	0.2	10
4462	FT-IR, FT-Raman, NMR spectra and DFT simulations of 4-(4-fluoro-phenyl)-1H-imidazole. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2013, 114, 525-536.	0.2	24
4463	Site Preferences of Carboyxl Groups on the Periphery of Graphene and Their Characteristic IR Spectra. Journal of Physical Chemistry C, 2013, 117, 18206-18215.	1.5	12
4464	Molecular Design of Tetrazole- and Tetrazine-Based High-Density Energy Compounds with Oxygen Balance Equal to Zero. Journal of Chemical & Engineering Data, 2013, 58, 2748-2762.	1.0	47
4465	Quantum chemical investigation on the influence of amino substitution on proton affinity of oxazolidin-2-one. Structural Chemistry, 2013, 24, 2173-2191.	1.0	2
4466	Computational study on the crystal structure, thermodynamic properties, detonation performance and pyrolysis mechanism of a novel high density cage compound 10-(5-nitrimino-1,2,3,4-tetrazol-1-yl)methyl-2,4,6,8,12-pentanitrohexaazaisowurtzitane. Structural Chemistry, 2013, 24, 1655-1663.	1.0	5
4467	Theoretical investigation of a high density cage compound 1,3,5,7,9,11-hexanitrotetradecahydro-1H-1,3,4,5,7,7b,9,11,12a,12b1,12b2,13-dodecaaza-4,8,12-(epimethanetriyl)cyclohepta[2,1]cyclopentaphenanthrene. Structural Chemistry, 2013, 24, 1411-1417.		
4468	A First-Principles Study of the Role of Quaternary-N Doping on the Oxygen Reduction Reaction Activity and Selectivity of Graphene Edge Sites. Topics in Catalysis, 2013, 56, 1623-1633.	1.3	67
4469	Multivariate curve resolution combined with on-line infrared spectroscopy for researching the synthesis mechanism of 3,4-bis(4â€²-aminofurazano-3â€²)furoxan. Chemical Research in Chinese Universities, 2013, 29, 759-764.	1.3	4
4470	5-S-Lipoylhydroxytyrosol, a Multidefense Antioxidant Featuring a Solvent-Tunable Peroxyl Radical-Scavenging 3-Thio-1,2-dihydroxybenzene Motif. Journal of Organic Chemistry, 2013, 78, 9857-9864.	1.7	34
4471	Rapid parameterization of small molecules using the force field toolkit. Journal of Computational Chemistry, 2013, 34, 2757-2770.	1.5	403
4472	Theoretical investigations on vibrational spectra of pillar[5]arene-bis(pyridinium) complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 368-376.	2.0	13
4473	A comparative study on the antioxidant properties of bractein and cernuoside by the DFT method. Monatshefte FÃ¼r Chemie, 2013, 144, 1513-1524.	0.9	5
4474	Competing geometric and electronic effects in adsorption of phenylenediamine structural isomers on the Ge(100)-2Ã—1 surface. Surface Science, 2013, 615, 72-79.	0.8	13
4475	Looking for high energy density compounds among polynitraminepurines. Journal of Molecular Modeling, 2013, 19, 3491-3499.	0.8	10
4476	Theoretical design of energetic nitrogen-rich derivatives of 1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane. Journal of Molecular Modeling, 2013, 19, 2945-2954.	0.8	13

#	Article	IF	Citations
4477	Computational study of energetic nitrogen-rich derivatives of 1,4-bis(1-azo-2,4-dinitrobenzene)-iminotetrazole. Journal of Molecular Modeling, 2013, 19, 1853-1864.	0.8	18
4478	Aryl Nitrene Rearrangements: Spectroscopic Observation of a Benzazirine and Its Ring Expansion to a Ketenimine by Heavy-Atom Tunneling. Journal of the American Chemical Society, 2013, 135, 10246-10249.	6.6	67
4479	Rapid estimation of vibrational zero-point energies of silicon compounds. Computational and Theoretical Chemistry, 2013, 1017, 182-187.	1.1	5
4480	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	1.2	50
4481	Fe(III)â€“Heme Complexes with the Amyloid Beta Peptide of Alzheimerâ€™s Disease: QM/MM Investigations of Binding and Redox Properties of Heme Bound to the His Residues of AÎ²(1â€“42). Journal of Chemical Theory and Computation, 2013, 9, 4233-4242.	2.3	7
4482	HCl Adsorption on Copper-Modified ZSM-5: FTIR and DFT Study. Journal of Physical Chemistry C, 2013, , 130912084723007.	1.5	7
4483	Density Functional Theoretical Study on 5,5â€²-azotetrazolate Nonmetallic Salts. Defence Technology, 2013, 9, 105-109.	2.1	1
4484	Vibrational, DFT, and thermal analysis of 2,4,6-triamino-1,3,5-triazin-1-ium 3-(prop-2-enoyloxy) propanoate acrylic acid monosolvate monohydrate. Journal of Molecular Structure, 2013, 1054-1055, 307-320.	1.8	21
4485	Importance of Câ€“HÂ·Â·Â·O Intramolecular Hydrogen Bonding Across a Nonproteinogenic Î³-Aminobenzoic Acid Residue: Stabilization of a Flat Î²-Strand-like Template. Crystal Growth and Design, 2013, 13, 2004-2012.	1.4	9
4486	DFT computation and spectroscopic analysis of N-(p-methoxybenzylidene)aniline, a potentially useful NLO material. Journal of Molecular Structure, 2013, 1047, 249-261.	1.8	11
4487	NBO, NMR, UV, FT-IR, FT-Raman spectra and molecular structure (monomeric and dimeric structures) investigation of 4-Chloro-3,5-Xylenol: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 170-182.	2.0	7
4488	Predictive correlations for ideal gas heat capacities of pure hydrocarbons and petroleum fractions. Fluid Phase Equilibria, 2013, 356, 338-370.	1.4	11
4489	Molecular structure of tetraaqua adenosine 5â€²-triphosphate aluminium(III) complex: A study involving Raman spectroscopy, theoretical DFT and potentiometry. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 88-101.	2.0	11
4490	Structural and vibrational spectral investigations of melaminium maleate monohydrate by FTIR, FT-Raman and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 107, 90-101.	2.0	15
4491	A density functional theory study of the regio- and stereoselectivity of the 1,3-dipolar cycloaddition of C-methyl substituted pyrazinium-3-olates with methyl acrylate and methyl methacrylate. Computational and Theoretical Chemistry, 2013, 1025, 58-66.	1.1	5
4492	Raman spectroscopic and ab initio studies on the molecular interactions in the binary liquid mixtures of 4â€²-fluoroacetophenone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 381-388.	2.0	1
4493	Electronic structure analysis of isomeric preferences of canonical and zwitterionic forms of lornoxicam. Computational and Theoretical Chemistry, 2013, 1023, 51-58.	1.1	4
4494	Nitro â‡Œ aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study. RSC Advances, 2013, 3, 25268.	1.7	12

#	Article	IF	Citations
4495	Vibrational (FT-IR and FT-Raman) spectra, NBO, HOMOâ€“LUMO, Molecular electrostatic potential surface and computational analysis of 4-(trifluoromethyl)benzylbromide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 84-95.	2.0	24
4496	Dynamics and Thermodynamics of Crystalline Polymorphs. 2. Î²-Glycine, Analysis of Variable-Temperature Atomic Displacement Parameters. Journal of Physical Chemistry A, 2013, 117, 8001-8009.	1.1	18
4497	Theoretical modelling of the epoxidation of vinylallenes to give cyclopentenones. Tetrahedron Letters, 2013, 54, 6607-6610.	0.7	3
4498	Two-dimensional stimulated resonance Raman spectroscopy study of the Trp-cage peptide folding. Physical Chemistry Chemical Physics, 2013, 15, 19457.	1.3	17
4499	A novel solid-state photochromic compound containing double heterocycles. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 267, 55-59.	2.0	9
4500	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. Molecular Physics, 2013, 111, 1526-1538.	0.8	6
4501	Structure and dynamics of the Th4+-ion in aqueous solution â€“ An ab initio QMCF-MD study. Computational and Theoretical Chemistry, 2013, 1022, 94-102.	1.1	16
4502	Structural analysis of a sulfo cation exchanger in the form of glycine. Journal of Structural Chemistry, 2013, 54, 668-675.	0.3	2
4503	Computational Study of the Fe(CN)₂CO Cofactor and Its Binding to HypC Protein. Journal of Physical Chemistry B, 2013, 117, 13523-13533.	1.2	5
4504	Structure and spectral characteristics of diquat-cucurbituril complexes from density functional theory. Journal of Molecular Modeling, 2013, 19, 5113-5127.	0.8	7
4505	Single electron transfer between selectfluor and chloride: A mass spectrometric and theoretical study. Journal of Molecular Structure, 2013, 1050, 21-25.	1.8	6
4506	Interpretation of the infrared and Raman spectra of zwitterionic pushâ€“pull dyes based on quinoidal thiazole. Journal of Molecular Structure, 2013, 1044, 55-60.	1.8	2
4507	Analysis of heat-treated graphite oxide by X-ray photoelectron spectroscopy. Journal of Materials Science, 2013, 48, 8171-8198.	1.7	147
4508	Molecular structure and vibrational spectral investigation of charge transfer NLO crystal Naphthalene Picrate for THz application. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 108, 256-267.	2.0	19
4509	Selected hydroxycoumarins as antioxidants in cells: physicochemical and reactive oxygen species scavenging studies. Journal of Physical Organic Chemistry, 2013, 26, 773-783.	0.9	14
4510	A theoretical study on 1,5-diazido-3-nitrazapentane (DANP) and 1,7-diazido-2,4,6-trinitrazaheptane (DATNH): molecular and crystal structures, thermodynamic and detonation properties, and pyrolysis mechanism. Journal of Molecular Modeling, 2013, 19, 5367-5376.	0.8	16
4511	Trastuzumab-Peptide Interactions: Mechanism and Application in Structure-Based Ligand Design. International Journal of Molecular Sciences, 2013, 14, 16836-16850.	1.8	21
4512	Molecular insight into the amineâ€“water interaction: A combined vibrational, energetic and NBO/NEDA study. Computational and Theoretical Chemistry, 2013, 1023, 74-82.	1.1	10

#	Article	IF	Citations
4513	Manipulating the singletâ€“triplet energy gaps of arene-fused bis(1,2,3-dithiazoles): A computational study. Polyhedron, 2013, 64, 172-180.	1.0	17
4514	Raman study of a photochromic diarylethene molecule: a combined theoretical and experimental study. Journal of Raman Spectroscopy, 2013, 44, 1777-1785.	1.2	5
4515	Tautomerism, Raman, infrared and ultravioletâ€“visible spectra, vibrational assignments, MP2 and B3LYP calculations of dienol 3,4-dihydroxypyridine, keto-enol 3-hydroxypyridin-4-one and keto-enol dimer. Journal of Molecular Structure, 2013, 1043, 52-67.	1.8	7
4516	Antimicrobial Investigation and Structural Study of 4â€²â€Methylazobenzeneâ€2â€sulfenyl Thiocyanate by Xâ€Ray Diffraction, DFT, and Ab Initio HF Calculations. Heteroatom Chemistry, 2013, 24, 502-509.	0.4	2
4517	Structure and detonation performance of a novel HMX/LLMâ€105 cocrystal explosive. Journal of Physical Organic Chemistry, 2013, 26, 898-907.	0.9	53
4518	Optimized CGenFF force-field parameters for acylphosphate and N-phosphonosulfonimidoyl functional groups. Journal of Molecular Modeling, 2013, 19, 5075-5087.	0.8	2
4519	Calculation of Vibrational Spectra of p-Ethylbenzenesulfonic Acid Hydrates. Journal of Applied Spectroscopy, 2013, 80, 499-504.	0.3	0
4520	Analysis of Vibrational Spectra of Pyridoxazinone Based on Density Functional Theory Calculations. Journal of Applied Spectroscopy, 2013, 80, 492-498.	0.3	11
4521	DFT, FT-Raman, and FT-IR investigations of 1-cyclopropylpiperazine. Journal of Structural Chemistry, 2013, 54, 1044-1054.	0.3	4
4522	A study of aliphatic amino acids using simulated vibrational circular dichroism and Raman optical activity spectra. European Physical Journal D, 2013, 67, 1.	0.6	21
4523	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	1.2	159
4524	A Facile Method to Determine the Absolute Structure of Achiral Molecules: Supramolecularâ€Tilt Structures. Chemistry - A European Journal, 2013, 19, 6044-6051.	1.7	5
4525	Structural and Vibrational Properties of Imidazo[4,5-c]pyridine, a Structural Unit in Natural Products. Journal of Natural Products, 2013, 76, 1637-1646.	1.5	4
4526	Conformations of monoylidic diester triphenylphosphonium ylides. Journal of Molecular Structure, 2013, 1034, 51-56.	1.8	1
4527	Synthesis, structural characterization, and computational study of novel (E)-Nâ€²-(1-p-tolylethylidene)furan-2-carbohydrazide. Journal of Molecular Structure, 2013, 1051, 345-353.	1.8	1
4528	Computational design and structure-property relationship studies on (I2GaN3) n (n = 1â€“4) clusters. Russian Journal of Physical Chemistry A, 2013, 87, 2047-2053.	0.1	3
4529	Photochemical formation of thiirene and thioketene in 1,2,3-thiadiazoles with phenyl substituents studied by time-resolved spectroscopy. Photochemical and Photobiological Sciences, 2013, 12, 895-901.	1.6	13
4530	Analytic second derivatives of the energy in the fragment molecular orbital method. Journal of Chemical Physics, 2013, 138, 164103.	1.2	40

#	Article	IF	Citations
4531	Infrared spectroscopic characterization of hydrogen-bonded propylene oxide â˜ ethanol and propylene oxide â˜ 2-fluoroethanol complexes isolated in solid neon matrices. Canadian Journal of Chemistry, 2013, 91, 1292-1302.	0.6	2
4532	(4,4â€²)-Bipyridinein vacuo and in solvents: a quantum chemical study of a prototypical floppy molecule from a molecular transport perspective. Physical Chemistry Chemical Physics, 2013, 15, 1918-1928.	1.3	35
4533	Cyclopalladation of dimesityl selenide: synthesis, reactivity, structural characterization, isolation of an intermediate complex with Câ€“Hâ‹¯Pd intra-molecular interaction and computational studies. Dalton Transactions, 2013, 42, 10828.	1.6	11
4534	Spectroscopy of the Câ€“H Stretching Vibrational Band in Selected Organic Molecules. Journal of Physical Chemistry A, 2013, 117, 7442-7452.	1.1	22
4535	Torsionâ€“Inversion Tunneling Patterns in the CH-Stretch Vibrationally Excited States of the G₁₂ Family of Molecules Including Methylamine. Journal of Physical Chemistry A, 2013, 117, 13356-13367.	1.1	6
4536	X-ray, vibrational spectra and density functional studies on cynacure. Vibrational Spectroscopy, 2013, 64, 68-77.	1.2	7
4537	Effects of hydrogen-bond and cooperativity in the vibrational spectra of Luminol. Vibrational Spectroscopy, 2013, 64, 119-125.	1.2	4
4538	Thermochemical Properties for Isooctane and Carbon Radicals: Computational Study. Journal of Physical Chemistry A, 2013, 117, 421-429.	1.1	20
4539	Vibrational spectroscopic and DFT study of trimethoprim. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 52-58.	2.0	9
4540	A silver complex with tryptophan: Synthesis, structural characterization, DFT studies and antibacterial and antitumor assays in vitro. Journal of Molecular Structure, 2013, 1031, 125-131.	1.8	33
4541	Density functional theory characterization of phosphate and sulfate adsorption on Fe-(hydr)oxide: Reactivity, pH effect, estimation of Gibbs free energies, and topological analysis of hydrogen bonds. Computational and Theoretical Chemistry, 2013, 1005, 16-24.	1.1	54
4542	Structural changes of Î²-carotene and some retinoid pharmaceuticals induced by environmental factors. Journal of Molecular Structure, 2013, 1037, 99-108.	1.8	9
4543	Zwitterions are the most stable form for neutral arginylglycine in gas phase: Clear theoretical evidence. Computational and Theoretical Chemistry, 2013, 1008, 96-102.	1.1	9
4544	Fourier Transform Infrared and Raman spectra, DFT: B3LYP/6-311G(d, p) calculations and structural properties of bis(diethyldithiocarbamate)copper(II). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 259-266.	2.0	20
4545	Mechanistic Aspects of Ketene Formation Deduced from Femtosecond Photolysis of Diazocyclohexadienone, o-Phenylene Thioxocarbonate, and 2-Chlorophenol. Journal of Organic Chemistry, 2013, 78, 2026-2032.	1.7	21
4546	QM and QM/MM Simulations of Proteins. Methods in Molecular Biology, 2013, 924, 91-124.	0.4	18
4547	Proton affinity of para-substituted acetophenones in gas phase and in solution: a theoretical study. Journal of Molecular Modeling, 2013, 19, 631-646.	0.8	5
4548	Theoretical investigation of a novel high density cage compound 4,8,11,14,15â€“pentanitro-2,6,9,13â€“tetraoxa-4,8,11,14,15-pentaazaheptacyclo[5.5.1.13,11. 15,9] pentadecane Journal of Molecular Modeling, 2013, 19, 1019-1026.	0.8	12

#	Article	IF	Citations
4549	Structural, electronic, thermodynamical and charge transfer properties of Chloramphenicol Palmitate using vibrational spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 335-342.	2.0	22
4550	Analysis of UV and vibrational spectra (FT-IR and FT-Raman) of hexachlorocyclotriphosphazene based on normal coordinate analysis, MP2 and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 446-455.	2.0	9
4551	Conformational analysis, spectroscopic and quantum chemical investigations of 2-bromo-3-nitroacetophenone. Journal of Molecular Structure, 2013, 1037, 73-84.	1.8	6
4552	Structural conformations and density functional study on the intramolecular charge transfer based on vibrational spectra of 2,4-dihydroxy-Nâ€²-(4-methoxybenzylidene)benzohydrazide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 157-168.	2.0	8
4553	Structural, vibrational, electronic investigations and quantum chemical studies of 2-amino-4-methoxybenzothiazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 327-340.	2.0	13
4554	Impact of the Synergistic Collaboration of Oligothiophene Bridges and Ruthenium Complexes on the Optical Properties of Dumbbellâ€Shaped Compounds. Chemistry - A European Journal, 2013, 19, 1476-1488.	1.7	9
4555	Oxalic Amidines â€“ Protonation Studies and Activity in Lactide Polymerisation. European Journal of Inorganic Chemistry, 2013, 2013, 99-108.	1.0	2
4556	Calculating excited state properties using Kohn-Sham density functional theory. Journal of Chemical Physics, 2013, 138, 064101.	1.2	47
4557	Crystal structures, infrared spectra, thermal stabilities and burning properties of RDX derivatives: A computational study. Computational and Theoretical Chemistry, 2013, 1018, 13-18.	1.1	7
4558	Vibrational spectroscopic investigation and conformational analysis of 1-heptylamine: A comparative density functional study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 668-680.	2.0	22
4559	Identification of isotopomers in natural abundance using two dimensional laser induced fluorescence: S1â€“S0 spectral shifts for the four 13C isotopomers of fluorobenzene. Chemical Physics Letters, 2013, 555, 38-43.	1.2	10
4560	On the surface structure of 1,3-dithiol-protected gold nanoparticles interpreted by the size effect of IR absorption properties. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2013, 426, 39-46.	2.3	4
4561	Synthesis, structure, vibrational spectral, nonlinear optical and electron-behavioral studies of N-(5-chloro-2-hydroxyphenyl)-(3-hydroxyphenyl)-methalimine. Optical Materials, 2013, 35, 2519-2526.	1.7	7
4562	Quantitative vapor-phase IR intensities and DFT computations to predict absolute IR spectra based on molecular structure: I. Alkanes. Journal of Quantitative Spectroscopy and Radiative Transfer, 2013, 129, 298-307.	1.1	27
4563	Probing the â€˜Venus fly-trapâ€™ parameters of cyclo-octadiene in selected Î²-diketonato complexes of platinum(II) and the nickel-triad from a spectroscopic, X-ray crystallographic and DFT study. Polyhedron, 2013, 50, 82-89.	1.0	5
4564	Unimolecular reactions of gaseous picoline radical cations. A new experimental and computational study. International Journal of Mass Spectrometry, 2013, 336, 1-16.	0.7	7
4565	One trinucleus dimethine cyanine dye: Experimental and theoretical studies on molecular structure as well as absorption and fluorescence properties. Journal of Molecular Structure, 2013, 1039, 84-93.	1.8	0
4566	4-Hydroxy-2,5-dimethylphenyl-benzophenone: Conformational stability, FT-IR and Raman investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 386-392.	2.0	10

#	Article	IF	Citations
4567	FT-IR and FT-Raman spectroscopies and DFT calculations of 2,2-dimethyl-5-(4H-1,2,4-triazol-4-ylaminomethylene)-1,3-dioxane-4,6-dione monohydrate. Journal of Molecular Structure, 2013, 1038, 170-176.	1.8	4
4568	DFT study on the reaction of the Î±-amino acid anion catalyzed by the aldehyde: Decarboxylation vs. intramolecular CO2 transfer. Computational and Theoretical Chemistry, 2013, 1006, 1-8.	1.1	2
4569	FT-Raman, FT-IR, UV spectroscopic, NBO and DFT quantum chemical study on the molecular structure, vibrational and electronic transitions of clopidogrel hydrogen sulfate form 1: A comparison to form 2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 409-418.	2.0	11
4570	Vibrational spectral investigations and density functional theory study of 4-Formylbenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 502-508.	2.0	7
4571	Ultrafast optical nonlinearity, electronic absorption, vibrational spectra and solvent effect studies of ninhydrin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 109, 331-343.	2.0	20
4572	Optimized structures and ring strain energies of isoelectronic homo- and heterogermiranes c-AX2GeH2GeH2q (A/qÂ=ÂGa/â^'1, Ge/0, As/+1): Variable trends across triads. Journal of Organometallic Chemistry, 2013, 740, 110-115.	0.8	2
4573	Adsorption of Enantiomers on Metal Surfaces: Application to D- and L-Alanine on Cu, Ni and Zn Electrodes. Journal of the Electrochemical Society, 2013, 160, G102-G110.	1.3	2
4575	Mechanism-Based Inactivation of Cytochromes by Furan Epoxide: Unraveling the Molecular Mechanism. Inorganic Chemistry, 2013, 52, 13496-13508.	1.9	23
4576	Statistical Validation of Absolute Configuration Assignment in Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 5504-5512.	2.3	19
4577	Cyclization of acyl radical onto NC bond: Application in the synthesis of Î²-lactam. Computational and Theoretical Chemistry, 2013, 1008, 83-89.	1.1	2
4578	Molecular level investigations of phosphate sorption on corundum (Î±-Al2O3) by 31P solid state NMR, ATR-FTIR and quantum chemical calculation. Geochimica Et Cosmochimica Acta, 2013, 107, 252-266.	1.6	94
4579	Synthesis, crystal growth, thermal studies and scaled quantum chemical studies of structural and vibrational spectra of the highly efficient organic NLO crystal: 1-(4-Aminophenyl)-3-(3,4-dimethoxyphenyl)-prop-2-en-1-one. Materials Chemistry and Physics, 2013, 141, 248-262.	2.0	38
4580	Raman study of 2,7-bis(biphenyl-4-yl-)2â€²,7â€²-ditertbutyl-9,9â€²-spirobifluorene adsorbed on oxide surfaces. Chemical Physics Letters, 2013, 584, 74-78.	1.2	4
4581	Experimental and theoretical approaches for identification of p-benzophenoneoxycarbonylphenyl acrylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 80-91.	2.0	15
4582	Synthesis and characterization of p-benzophenoneoxycarbonylphenyl acrylate by means of experimental measurements and theoretical approaches, and bulk melt polymerization. Journal of Molecular Structure, 2013, 1049, 479-487.	1.8	14
4583	Methyl-to-double bond transfer in the gas phase: A theoretical study. Computational and Theoretical Chemistry, 2013, 1020, 7-13.	1.1	0
4584	Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. Vibrational Spectroscopy, 2013, 66, 123-131.	1.2	42
4585	Quantum chemistry study on the destruction mechanism of 2,3,7,8-TCDD by OH and O3 radicals. Chemosphere, 2013, 92, 293-298.	4.2	6

#	Article	IF	Citations
4586	A combined experimental and quantum chemical (DFT and AIM) study on molecular structure, spectroscopic properties, NBO and multiple interaction analysis in a novel ethyl 4-[2-(carbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. Journal of Molecular Structure, 2013, 1035, 427-440.	1.8	84
4587	Structure of SnF2-SnO-P2O5 Glasses. Physics Procedia, 2013, 44, 159-165.	1.2	31
4588	Synthesis and mesomorphic investigation of calamitic liquid crystalline system ethyl-[4-(4â€²-decyloxy)benzoyloxy]-benzoate (4-EDBB): A temperature dependent micro-Raman study and DFT calculations. Vibrational Spectroscopy, 2013, 69, 40-48.	1.2	18
4589	DFT: B3LYP/6-311G (d, p) vibrational analysis of bis-(diethyldithiocarbamate)zinc (II) and natural bond orbitals. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 251-258.	2.0	29
4590	Investigation of spectroscopic, structural and non-linear optical properties of ethyl 3,5-dimethyl-4-[(benzenesulfonyl)-hydrazonoethyl]-1H-pyrrol-2-carboxylate. Journal of Molecular Structure, 2013, 1054-1055, 123-133.	1.8	18
4591	A study on the BF3 directed lithiation of 3-chloro- and 3-bromopyridine. Tetrahedron, 2013, 69, 10284-10291.	1.0	14
4592	Vibrational and conformational analysis on-N1-N2-bis((pyridine-4-yl)methylene) benzene-1,2-diamine. Journal of Molecular Structure, 2013, 1042, 37-44.	1.8	11
4593	First-Principles Prediction of the Effects of Temperature and Solvent Selection on the Dimerization of Benzoic Acid. Journal of Physical Chemistry B, 2013, 117, 868-876.	1.2	25
4594	Molecular structural, non-linear optical, second order perturbation and Fukui studies of Indole-3-Aldehyde using density functional calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 106, 299-309.	2.0	27
4595	â€œStructure-Makingâ€•Ability of Na⁺ in Dilute Aqueous Solution: An ONIOM-XS MD Simulation Study. Journal of Physical Chemistry A, 2013, 117, 1826-1833.	1.1	28
4596	New diethoxo-bridged dinuclear Cr(III) complexes with derivatives of the quinoxaline-2,3-dione ligand and 2,2â€²-bipyridine as a co-ligand: Syntheses, spectral characterizations, magnetic properties, antimicrobial inhibitory activities and interpretation of the electronic absorption spectra using the ZINDO/S-CI semi-empirical method. Polyhedron, 2013, 51, 243-254.	1.0	9
4597	Structure and Reactivity of Thiazolium Azo Dyes: UVâ€“Visible, Resonance Raman, NMR, and Computational Studies of the Reaction Mechanism in Alkaline Solution. Journal of Physical Chemistry A, 2013, 117, 1853-1871.	1.1	10
4598	Density functional investigation of the molecular structures, vibrational spectra and molecular properties of sulfonated pyridyl imine ligands and their palladium complexes. Computational and Theoretical Chemistry, 2013, 1013, 109-115.	1.1	12
4599	Theoretical studies on the thermodynamic properties, densities, detonation properties, and pyrolysis mechanisms of trinitromethyl-substituted aminotetrazole compounds. Journal of Molecular Modeling, 2013, 19, 2413-2422.	0.8	10
4600	PICVib: An accurate, fast, and simple procedure to investigate selected vibrational modes at high theoretical levels. Journal of Computational Chemistry, 2013, 34, 611-621.	1.5	3
4601	Molecular structure, spectroscopic (FT-IR, FT-Raman, UVâ€“vis), NBO, thermochemistry analysis of bis(thiourea)zinc(II) chloride crystals. Molecular Simulation, 2013, 39, 584-595.	0.9	5
4602	Computational studies on a high density cage compound hexanitrohexaazaisowurtzitane derivative. Canadian Journal of Chemistry, 2013, 91, 369-374.	0.6	6
4603	Theoretical and Experimental Spectroscopic Analysis of Cyano-Substituted Styrylpyridine Compounds. International Journal of Molecular Sciences, 2013, 14, 4005-4029.	1.8	27

#	Article	IF	Citations
4604	Mechanistic insights into the bioactivation of phenacetin to reactive metabolites: A DFT study. Computational and Theoretical Chemistry, 2013, 1007, 48-56.	1.1	20
4605	Molecular design of trinitromethyl-substituted nitrogen-rich heterocycle derivatives with good oxygen balance as high-energy density compounds. Structural Chemistry, 2013, 24, 1725-1736.	1.0	26
4606	The FTIR spectra of substituted tetraoxa[8]circulenes and their assignments based on DFT calculations. Vibrational Spectroscopy, 2013, 65, 147-158.	1.2	26
4607	A theoretical study on the red- and blue-shift hydrogen bonds of cis-trans formic acid dimer in excited states. Open Chemistry, 2013, 11, 171-179.	1.0	8
4608	Toward a Physically Based Quantitative Modeling of Impact Sensitivities. Journal of Physical Chemistry A, 2013, 117, 2253-2259.	1.1	42
4609	Rate Coefficients for Intramolecular Homolytic Substitution of Oxyacyl Radicals at Sulfur. Australian Journal of Chemistry, 2013, 66, 323.	0.5	5
4610	Anharmonic Vibrational Frequency Calculations Are Not Worthwhile for Small Basis Sets. Journal of Chemical Theory and Computation, 2013, 9, 951-954.	2.3	47
4611	Carbene Generation by Cytochromes and Electronic Structure of Heme-Iron-Porphyrin-Carbene Complex: A Quantum Chemical Study. Inorganic Chemistry, 2013, 52, 5097-5109.	1.9	40
4612	Vibrational self-consistent field calculations for spectroscopy of biological molecules: new algorithmic developments and applications. Physical Chemistry Chemical Physics, 2013, 15, 9468.	1.3	163
4613	Computer simulation of interactions in the NH3-CO2-H2O system. Russian Journal of General Chemistry, 2013, 83, 10-14.	0.3	6
4614	Electronic Elements Governing the Binding of Small Molecules to a [Fe]-Hydrogenase Mimic. European Journal of Inorganic Chemistry, 2013, 2013, 3993-3999.	1.0	7
4615	Structural, vibrational and nuclear magnetic resonance investigations of 4-bromoisoquinoline by experimental and theoretical DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 107, 62-71.	2.0	12
4616	A combined experimental and quantum chemical studies on molecular structure, spectral properties, intra and intermolecular interactions and first hyperpolarizability of 4-(benzyloxy)benzaldehyde thiosemicarbazone and its dimer. Journal of Molecular Structure, 2013, 1034, 374-385.	1.8	4
4617	Theoretical studies on vibrational spectra, thermodynamic properties, and detonation properties for 1,2,4,5-tetrazine derivatives. Canadian Journal of Chemistry, 2013, 91, 662-670.	0.6	4
4618	Existence of dynamic tautomerism and divalent N(I) character in Nâ€(pyridinâ€2â€yl)thiazolâ€2â€amine. Journal of Computational Chemistry, 2013, 34, 1577-1588.	1.5	29
4619	Effects of Hydrogen Bonding on Internal Conversion of GFP-like Chromophores. II. The meta-Amino Systems. Journal of Physical Chemistry B, 2013, 117, 2705-2716.	1.2	38
4620	Effects of Hydrogen Bonding on Internal Conversion of GFP-like Chromophores. I. The para-Amino Systems. Journal of Physical Chemistry B, 2013, 117, 2695-2704.	1.2	36
4621	Structure and spectroscopic studies of 2,3-diethoxycarbonyl-1-methylpyridinium nitrate. Journal of Molecular Structure, 2013, 1035, 348-357.	1.8	3

#	Article	IF	Citations
4622	Quasi-elastic Light Scattering (QELS). , 2013, , 2166-2166.		0
4623	Computational analysis of substituent effects and Hammett constants for the ionization of gas phase acids. Computational and Theoretical Chemistry, 2013, 1008, 46-51.	1.1	6
4624	Molecular Mechanisms in the Pyrolysis of Unsaturated Chlorinated Hydrocarbons: Formation of Benzene Rings. 1. Quantum Chemical Studies. Journal of Physical Chemistry A, 2013, 117, 4183-4197.	1.1	12
4625	Infrared Spectra of CH₃â€“MX and CH₂Xâ€“MH Prepared in Reactions of Laser-Ablated Gold, Platinum, Palladium, and Nickel Atoms with CH₃Cl and CH₃Br. Organometallics, 2013, 32, 2753-2759.	1.1	19
4626	Molecular Design of New Nitramine Explosive: 1,3,5,7-Tetraaza-1,2,3,5, 6,7-hexahydros-indacene Derivatives. Polycyclic Aromatic Compounds, 2013, 33, 297-309.	1.4	6
4627	Vibrational spectroscopy and DFT calculations of 1,3-dibromo-2,4,6-trimethylbenzene: Anharmonicity, coupling and methyl group tunneling. Vibrational Spectroscopy, 2013, 67, 27-43.	1.2	6
4628	Determination of the relationship between theoretical vibrational frequencies and experimental IR absorbance bands in organic molecules: computational study of oxane, chromane and flavan. Journal of Physical Organic Chemistry, 2013, 26, 327-334.	0.9	3
4629	A combined experimental and theoretical (DFT and AIM) studies on synthesis, molecular structure, spectroscopic properties and multiple interactions analysis in a novel Ethyl-4-[2-(thiocarbamoyl)hydrazinylidene]-3,5-dimethyl-1H-pyrrole-2-carboxylate and its dimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 112, 182-190.	2.0	62
4630	Recycling Nicotinamide. The Transition-State Structure of Human Nicotinamide Phosphoribosyltransferase. Journal of the American Chemical Society, 2013, 135, 3485-3493.	6.6	36
4631	Study of molecular structure, vibrational, electronic and NMR spectra of oncocalyxone A using DFT and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 367-377.	2.0	19
4632	FT-Raman, FT-IR and UVâ€“visible spectral investigations and ab initio computations of anti-epileptic drug: Vigabatrin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 633-641.	2.0	3
4633	Quinone Cofactors. , 2013, , 2166-2168.		1
4634	Azidoacetylene â€“ interpretation of gas phase infrared spectra based on high-level vibrational configuration interaction calculations. Physical Chemistry Chemical Physics, 2013, 15, 6719.	1.3	17
4635	Combined Ab Initio Computational and Infrared Spectroscopic Study of the cis- and trans-Bis(glycinato)copper(II) Complexes in Aqueous Environment. Journal of Physical Chemistry Letters, 2013, 4, 1502-1506.	2.1	17
4636	Raman Second Hyperpolarizability Determination Using Computational Raman Activities and a Comparison with Experiments. Journal of Physical Chemistry A, 2013, 117, 6217-6223.	1.1	5
4637	Some Ruthenium Derivatives of Penta-1,4-diyn-3-one. Organometallics, 2013, 32, 3286-3299.	1.1	37
4638	Isotope Effects and Mechanism of the Asymmetric BOROX BrÃ¸nsted Acid Catalyzed Aziridination Reaction. Journal of Organic Chemistry, 2013, 78, 5142-5152.	1.7	29
4639	The Photochemistry of 4,5-Carbomethoxy-1,2,3-thiadiazole: Direct Observation of Thiirene Formation and Its Decay in Solution. Journal of Physical Chemistry A, 2013, 117, 4551-4555.	1.1	11

#	Article	IF	Citations
4640	Fullerene C70 characterization by 13C NMR and the importance of the solvent and dynamics in spectral simulations. Physical Chemistry Chemical Physics, 2013, 15, 9223.	1.3	30
4641	On the detection of higher order carbon sulfides (CSx; x=4â€“6) in low temperature carbon disulfide ices. Chemical Physics Letters, 2013, 577, 42-47.	1.2	7
4642	Infrared Spectra of Manganese Insertion, Vinyl, and Cyclic Complexes Prepared in Reactions of Laser-Ablated Mn Atoms with Methane, Ethane, Ethyl Chloride, and 1,2-Dichloroethane. Organometallics, 2013, 32, 3458-3468.	1.1	10
4643	Synthesis, Insecticidal Activities, and SAR Studies of Novel Pyridylpyrazole Acid Derivatives Based on Amide Bridge Modification of Anthranilic Diamide Insecticides. Journal of Agricultural and Food Chemistry, 2013, 61, 5483-5493.	2.4	103
4644	Does the metalâ€“metal sextuple bond exist in the bimetallic sandwich compounds Cr₂(C₆H₆)₂, Mo₂(C₆H₆)₂, and W₂(C₆H₆)₂?^{â€}. Molecular Physics, 2013, 111, 2523-2535.	0.8	11
4645	Vibrational spectroscopic investigation of 1-pyrrolidino-1-cyclohexene: A comparative density functional study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 1-9.	2.0	5
4646	Infrared and NMR spectra, tautomerism, vibrational assignment, normal coordinate analysis, and quantum mechanical calculations of 4-amino-5-pyrimidinecarbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 111, 277-289.	2.0	10
4647	Vibrational, NMR spectrum and orbital analysis of 3,3â€²,5,5â€²-tetrabromobisphenol A: A combined experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 38-44.	2.0	11
4648	Quinazolin-4-yl-sulfanylacetyl-hydrazone derivatives; Synthesis, molecular structure and electronic properties. Journal of Molecular Structure, 2013, 1049, 177-188.	1.8	26
4649	Theoretical study of the molecular conformations, vibrational frequencies and thermochemistry of the FC(O)OOO(O)CF, FS(O2)OOO(O2)SF and FC(O)OOO(O2)SF trioxides. Computational and Theoretical Chemistry, 2013, 1009, 86-93.	1.1	5
4650	A new look into conformational, vibrational and electronic structure analysis of 3,4-dimethoxybenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 302-313.	2.0	4
4651	Study of polymorphism in imatinib mesylate: A quantum chemical approach using electronic and vibrational spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 325-332.	2.0	16
4652	Conformational, vibrational, NMR and DFT studies of N-methylacetanilide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 182-196.	2.0	17
4653	Mechanistic and kinetics study of the gas phase reactions of methyltrifluoroacetate with OH radical and Cl atom. Molecular Physics, 2013, 111, 860-867.	0.8	24
4654	A theoretical and spectroscopic study of co-amorphous naproxen and indomethacin. International Journal of Pharmaceutics, 2013, 453, 80-87.	2.6	95
4655	Synthesis, structure and photoresponsive properties of 4-(3-fluorobenzylideneamino)antipyrine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 43-51.	2.0	6
4656	A silver complex with ibuprofen: Synthesis, solid state characterization, DFT calculations and antibacterial assays. Journal of Molecular Structure, 2013, 1049, 1-6.	1.8	34
4657	Carbon monoxide adsorption on platinum-osmium and platinum-ruthenium-osmium mixed nanoparticles. Journal of Chemical Physics, 2013, 138, 174704.	1.2	8

#	Article	IF	Citations
4658	Synthesis, characterisation, mesomorphic investigation and temperature-dependent Raman study of a novel calamitic liquid crystal: methyl 4-(4â€²-n-alkoxybenzylideneamino)benzoate. Liquid Crystals, 2013, 40, 884-899.	0.9	22
4659	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	1.0	1,426
4660	An investigation of soluteâ€“solvent interactions in binary liquid mixtures of 3â€²-methoxyacetophenone: Using Raman spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 111, 14-23.	2.0	6
4661	Molecular structure, spectroscopic (FT-IR, FT-Raman), NBO and HOMOâ€“LUMO analyses, computation of thermodynamic functions for various temperatures of 2, 6-dichloro-3-nitrobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 130-140.	2.0	22
4662	Vibrational, electronic and quantum chemical studies of 1,2,4-benzenetricarboxylic-1,2-anhydride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 141-150.	2.0	16
4663	Mechanism Elucidation of the cisâ€“trans Isomerization of an Azole Rutheniumâ€“Nitrosyl Complex and Its Osmium Counterpart. Inorganic Chemistry, 2013, 52, 6260-6272.	1.9	26
4664	FTIR, FT-Raman, FT-NMR and quantum chemical investigations of 3-acetylcoumarin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 109, 79-89.	2.0	31
4665	Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, TD-DFT and thermodynamic analysis of 4-amino-3-hydroxy-1-naphthalenesulfonic acid by DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 107, 167-178.	2.0	32
4666	Syntheses of phenoxyalkyl esters of 3,3â€²-bis(indolyl)methanes and studies on their molecular properties from single crystal XRD and DFT techniques. Journal of Molecular Structure, 2013, 1047, 109-120.	1.8	20
4667	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. Combustion and Flame, 2013, 160, 1907-1929.	2.8	65
4668	Towards an understanding of the vibrational spectrum of the neutral Au₇cluster. Physical Chemistry Chemical Physics, 2013, 15, 1929-1943.	1.3	11
4669	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 3096-3108.	2.3	29
4670	Reaction Kinetics of Hydrogen Abstraction Reactions by Hydroperoxyl Radical from 2-Methyltetrahydrofuran and 2,5-Dimethyltetrahydrofuran. Journal of Physical Chemistry A, 2013, 117, 5028-5041.	1.1	31
4671	Theoretical structure and vibrational spectra of ciprofloxacin: Density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 102, 134-141.	2.0	5
4672	Density functional study of the intramolecular proton transfer and conformations in hydroxyaminosilanethione. Journal of Molecular Structure, 2013, 1032, 5-11.	1.8	1
4673	Structure of dimethylphenyl betaine hydrochloride studied by X-ray diffraction, DFT calculation, NMR and FTIR spectra. Journal of Molecular Structure, 2013, 1031, 49-55.	1.8	9
4674	Synthesis, characterization, and DFT study of polycyclic aromatic hydrocarbon precursors, 1,4-diiodo-2,3,5,6-tetraarylbenzene and 1,4-bis(4-bromophenyl)-2,3,5,6-tetraarylbenzene. Journal of Molecular Structure, 2013, 1032, 41-47.	1.8	4
4675	Thiosaccharine disulfide: Synthesis, crystal structure, spectroscopic characterization and theoretical study. Journal of Molecular Structure, 2013, 1032, 48-55.	1.8	1

#	Article	IF	Citations
4676	Adsorption geometry of propranolol enantiomers on silver nanoparticles. Journal of Molecular Structure, 2013, 1031, 201-206.	1.8	23
4677	Spectroscopy studies, X-ray diffraction and DFT, HF calculations of 4-allyl-5-(thiophen-2-ylmethyl)-2H-1,2,4-triazol-3(4H)-one. Journal of Molecular Structure, 2013, 1033, 243-252.	1.8	10
4678	Density functional theory study on the molecular structure and vibration spectra of fenbufen. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 119-126.	2.0	1
4679	DFT, FT-IR and Raman investigations of 1-pyrrolidino-1-cyclopentene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 22-30.	2.0	1
4680	A Comparative Quantum Mechanical Charge Field Study of Uranyl Mono- and Dicarbonate Species in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 16174-16187.	1.2	18
4681	Kinetic Modeling of Hydrogen Conversion at [Fe] Hydrogenase Active-Site Models. Journal of Physical Chemistry B, 2013, 117, 4806-4817.	1.2	24
4682	In-Situ Raman Investigation of Polysulfide Formation in Li-S Cells. Journal of the Electrochemical Society, 2013, 160, A1205-A1214.	1.3	305
4683	Accurate Modeling of Infrared Multiple Photon Dissociation Spectra: The Dynamical Role of Anharmonicities. Journal of Physical Chemistry A, 2013, 117, 3954-3959.	1.1	52
4684	Adsorption of Trimethyl Phosphite at the Ge(100)-2 Ã— 1 Surface by Nucleophilic Reaction. Journal of Physical Chemistry C, 2013, 117, 26628-26635.	1.5	10
4685	Infrared Spectroscopy of Solvation in Small Zn⁺(H₂O)_n Complexes. Journal of Physical Chemistry A, 2013, 117, 7794-7803.	1.1	46
4686	Synthesis of the Natural Product Building Block 5â€(3â€Bromophenyl)â€4â€hydroxyâ€5â€methylhexanâ€2â€one and its Chiral Characterization by Using Chiroptical Spectroscopy. ChemPhysChem, 2013, 14, 3255-3262.	1.0	2
4687	Syntheses, Spectroelectrochemical Studies, and Molecular and Electronic Structures of Ferrocenyl Ene-diynes. Organometallics, 2013, 32, 6022-6032.	1.1	21
4688	DFT study and quantitative detection by surfaceâ€enhanced Raman scattering (SERS) of ethyl carbamate. Journal of Raman Spectroscopy, 2013, 44, 1491-1496.	1.2	18
4689	Gasâ€phase interactions of organotin compounds with glycine. Journal of Mass Spectrometry, 2013, 48, 795-806.	0.7	9
4690	Design of Ionic Liquids Using Property Clustering and Decomposition Techniques. Computer Aided Chemical Engineering, 2013, 32, 955-960.	0.3	12
4691	Protonation Effect of Tyrosine in a Segment of the SRF Transcription Factor: A Combined Optical Spectroscopy, Molecular Dynamics, and Density Functional Theory Calculation Study. Journal of Physical Chemistry B, 2013, 117, 16086-16095.	1.2	9
4692	Impact of Water Molecules on the Isomerization of CH₃S(OH)CH₂ to CH₃S(O)CH₃: A Computational Investigation. Chinese Journal of Chemistry, 2013, 31, 1341-1347.	2.6	0
4693	Large Hydrogen-Bonded Pre-nucleation (HSO₄^{â€“})(H₂SO₄)_m(H₂O)_k (HSO₄^{â€“})(NH₃)(H₂SO₄)_m(H₂O) Clusters in the Earthâ€™s Atmosphere. Journal of Physical Chemistry A, 2013, 117, 133-152.	1.1	57

#	Article	IF	Citations
4694	Energetics of 2- and 3-coumaranone isomers: A combined calorimetric and computational study. Journal of Chemical Thermodynamics, 2013, 67, 210-216.	1.0	9
4695	Theoretical investigation on the geometric, spectroscopic, nonlinear optical parameter, and frontier molecular orbital of 1,3-bis(4-methoxyphenyl)prop-2-en-1-one by DFT/ab initio calculations. Canadian Journal of Chemistry, 2013, 91, 1225-1232.	0.6	3
4696	Theoretical investigation on crystal structure, detonation performance and thermal stability of a high density cage hexanitrohexaazaisowurtzitane derivative. Journal of Chemical Sciences, 2013, 125, 919-925.	0.7	7
4697	Gas-Phase Formation and Fragmentation Reactions of the Organomagnesates [RMgX2]â^'. Organometallics, 2013, 32, 2319-2328.	1.1	29
4698	Fluorescence and Phosphorescence of Single C₆₀ Molecules as Stimulated by a Scanning Tunneling Microscope. Angewandte Chemie - International Edition, 2013, 52, 4814-4817.	7.2	22
4699	Why Bindschedlerâ€™s Green Is Redder Than Michlerâ€™s Hydrol Blue. Journal of Physical Chemistry A, 2013, 117, 2455-2468.	1.1	6
4700	Analytic Molecular Hessian Calculations for CC2 and MP2 Combined with the Resolution of Identity Approximation. Journal of Chemical Theory and Computation, 2013, 9, 1469-1480.	2.3	12
4701	Collision-Induced Dissociation and Infrared Photodissociation Studies of Methane Adsorption on V₅O₁₂⁺ and V₅O₁₃⁺ Clusters. Journal of Physical Chemistry A, 2013, 117, 2961-2970.	1.1	17
4702	Effects of Collisional and Vibrational Velocity on Proton and Deuteron Transfer in the Reaction of HOD⁺ with CO. Journal of Physical Chemistry A, 2013, 117, 1083-1093.	1.1	4
4703	Simulating One-Photon Absorption and Resonance Raman Scattering Spectra Using Analytical Excited State Energy Gradients within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 5490-5503.	2.3	49
4704	Optimized Structures and Ring Strain Energies of Isoelectronic Homo- and Heterosiliranes c-AX₂SiR₂SiR₂^q (A/q = Al/1â€“, Si/0, P/1+): Unexpected Effects of Charge and Size. Organometallics, 2013, 32, 2558-2566.	1.1	7
4705	Structure and Chemistry of the Heteronuclear Oxo-Cluster [VPO₄]^{â€¢+}: A Model System for the Gas-Phase Oxidation of Small Hydrocarbons. Journal of the American Chemical Society, 2013, 135, 3711-3721.	6.6	66
4706	Interaction of Gold Acetylides with Gold(I) or Silver(I) Cations. Organometallics, 2013, 32, 7025-7033.	1.1	32
4707	Adsorption of Structural and Stereoisomers of Cyclohexanediamine at the Ge(100)-2 Ã— 1 Surface: Geometric Effects in Adsorption on a Semiconductor Surface. Journal of Physical Chemistry C, 2013, 117, 19063-19073.	1.5	13
4708	Second Hyperpolarizability of Câ€“H, Câ€“D, and Câ‰¡N Stretch Vibrations Determined from Computational Raman Activities and a Comparison with Experiments. Journal of Physical Chemistry B, 2013, 117, 15812-15818.	1.2	2
4709	Atropisomerization of di-para-substituted propyl-bridged biphenyl cyclophanes. Organic and Biomolecular Chemistry, 2013, 11, 110-118.	1.5	27
4710	Computational studies on 3,5,7,10,12,14,15,16-octanitro-3,5,7,10,12,14,15,16-octaaza-pentacyclo[7.5.1.12,8.04,13.06,11]hexadecane as potential high-energy-density compound. Structural Chemistry, 2013, 24, 139-145.	1.0	3
4711	Theoretical studies on the crystal structure, thermodynamic properties, detonation performance and thermal stability of cage-tetranitrotetraazabicyclooctane as a novel high energy density compound. Journal of Molecular Modeling, 2013, 19, 57-64.	0.8	6

#	Article	IF	Citations
4712	On-the-flyâ€ab intito calculations of anharmonic vibrational frequencies: Local-monomer theory and application to HCl clusters. Journal of Chemical Physics, 2013, 139, 164115.	1.2	23
4713	QM/MM Calculations of Vibrational Spectra. , 2013, , 2149-2154.		6
4714	Vibrational Spectroscopy Investigation Using Ab Initio and Density Functional Theory Analysis on the Structure oftert-Butyl 3a-Chloroperhydro-2,6a-epoxyoxireno[e]isoindole-5-carboxylate. Journal of Chemistry, 2013, 2013, 1-13.	0.9	0
4715	Synthesis and Anti-inflammatory Activity of Novel Furochromenes. Croatica Chemica Acta, 2013, 86, 253-264.	0.1	13
4716	Double Amino Functionalized Ag Nanoparticles as SERS Tags in Raman Diagnostic. Croatica Chemica Acta, 2013, 86, 233-244.	0.1	9
4717	A Theoretical Study on the Vibrational Spectra and Thermodynamic Properties for the Derivatives of HNS with â€“CH₃, â€“N₃, and â€“NF₂ Groups. Advanced Materials Research, 2013, 742, 202-208.	0.3	2
4718	NLO and NBO Analysis of Sarcosine-Maleic Acid by Using HF and B3LYP Calculations. Journal of Chemistry, 2013, 2013, 1-16.	0.9	27
4719	G3 Assisted Rational Design of Chemical Sensor Array Using Carbonitrile Neutral Receptors. Sensors, 2013, 13, 13835-13860.	2.1	4
4720	Thermal Restructuring of Silicaâ€Grafted TiCl_x Species and Consequences for Epoxidation Catalysis. Chemistry - A European Journal, 2013, 19, 9849-9858.	1.7	25
4721	The role of vibrations in singleâ€molecule charge transport: A case study of oligoynes with pyridine anchor groups. Physica Status Solidi (B): Basic Research, 2013, 250, 2452-2457.	0.7	17
4722	Anisotropic displacement parameters for molecular crystals from periodic Hartreeâ€“Fock and density functional theory calculations. Acta Crystallographica Section A: Foundations and Advances, 2013, 69, 309-321.	0.3	49
4723	Calculated Entropies for n-Heptane, 2-Methylhexane, 2,3-Dimethylpentane, and Radicals from the Loss of H Atoms. Advances in Physical Chemistry, 2013, 2013, 1-7.	2.0	7
4724	Calculated stabilities and structures for carbocations and singlet carbenes bearing electronâ€withdrawing groups. Journal of Physical Organic Chemistry, 2013, 26, 1023-1031.	0.9	13
4725	Remote substituent effects on gasâ€phase homolytic Feâ€“O and Feâ€“S bond energies of pâ€“C₆H₄OFe(CO)₂(Î·⁵â€“C₅H₅) and pâ€“C₆H₄SFe(CO)₂(Î·⁵â€“C₅H₅) studied using Hartreeâ€“Fock and density functional theory methods. Journal of Physical Organic Chemistry, 2013, 26, 664-674.	0.9	9
4726	Electronic states of thiophene/phenylene co-oligomers: Extreme-ultra violet excited photoelectron spectroscopy observations and density functional theory calculations. Journal of Applied Physics, 2013, 113, 083710.	1.1	14
4727	Theoretical Study on Hydrogen Bonding of Monoâ€and Dihydrated Complexes of 7â€(3â€²â€Pyridyl)indole in Excited States. Journal of the Chinese Chemical Society, 2013, 60, 618-624.	0.8	3
4728	Theoretical investigations on heat of formation, detonation performance, and pyrolysis mechanism of 1,3,5,7,9,11-hexo(nitramine)-2,4,6,8,10,12- hexaazatetracyclo[5,5,0,0,0]dodecane. Canadian Journal of Chemistry, 2013, 91, 1213-1218.	0.6	4
4729	Twoâ€dimensional stimulated ultraviolet resonance Raman spectra of tyrosine and tryptophan: a simulation study. Journal of Raman Spectroscopy, 2013, 44, 544-559.	1.2	27

#	Article	IF	Citations
4730	Fermi resonance in Ne, Ar and Kr-matrix infrared spectra of 5-bromouracil. Low Temperature Physics, 2013, 39, 546-551.	0.2	14
4731	The waterâ€“boryl radical as a proton-coupled electron transfer reagent for carbon dioxide, formic acid, and formaldehyde â€” Theoretical approach. Canadian Journal of Chemistry, 2013, 91, 155-168.	0.6	0
4732	Global warming potentials and radiative efficiencies of halocarbons and related compounds: A comprehensive review. Reviews of Geophysics, 2013, 51, 300-378.	9.0	390
4733	Analyzing the Vibrational Signatures of Thiophenol Adsorbed on Small Gold Clusters by DFT Calculations. ChemPhysChem, 2013, 14, 1633-1645.	1.0	33
4734	REGIOSELECTIVITY INVESTIGATION FOR THE PYROLYSIS OF XANTHATES: A COMPUTATIONAL STUDY. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350064.	1.8	12
4735	Computational Study of the Binding Mechanism of Complement C3b with Antigen. Bulletin of the Chemical Society of Japan, 2013, 86, 1426-1434.	2.0	0
4736	ONIOM Study of the Mechanism of Olefin Hydrogenation by the Wilkinsonâ€™s Catalyst: Reaction Paths and Energy Surfaces of trans- and cis-Forms. Bulletin of the Chemical Society of Japan, 2013, 86, 243-254.	2.0	6
4738	A New Approach to Investigate Thin Surface Layers of Polymers: Fatigue Analysis of Polycarbonate. Applied Spectroscopy, 2013, 67, 420-432.	1.2	6
4739	Refining the Interpretation of Nearâ€Infrared Band Shapes in a Polyynediyl Molecular Wire. Chemistry - A European Journal, 2013, 19, 9780-9784.	1.7	61
4740	Interaction of selected gases with zinc phthalocyanine thin films: theoretical and experimental studies. EPJ Applied Physics, 2013, 64, 10202.	0.3	8
4741	Cyclization of substitued 2-(2-fluorophenylazo)azines to azino[1,2-c]benzo[d][1,2,4]triazinium derivatives. Beilstein Journal of Organic Chemistry, 2013, 9, 1873-1880.	1.3	5
4742	Synthesis, Spectroscopic Properties and Structural Studies of Copper(II) Complexes of 2-Substituted-1,3-Diphenyl-1,3-Propanedione, Their 2,2'-Bipyridine and 1,10-Phenanthroline Adducts. International Journal of Chemistry, 2013, 6, .	0.3	4
4743	Vibrational Spectroscopic Investigation and Conformational Analysis of Methacrylamidoantipyrine: A Comparative Density Functional Study. Journal of Theoretical Chemistry, 2013, 2013, 1-10.	1.5	5
4744	The Syntheses, Molecular Structures, Spectroscopic Properties (IR, Microâ€“ Raman, NMR and UVâ€“vis) and DFT Calculations of Antioxidant 3â€“ alkylâ€“4â€“[3â€“methoxyâ€“4â€“(4â€“methylbenzoxy)benzylidenamino]â€“4,5â€“dihydroâ€“ 1Hâ€“1,2,4â€“triazolâ€“5â€“one Molecules. Letters in Organic Chemistry, 2013, 10, 395-441.	0.2	23
4745	Theoretical Investigation of Tautomerism Stability of Hydantoin in the Gas Phase and in the Solution. Oriental Journal of Chemistry, 2014, 30, 1045-1054.	0.1	9
4746	Quantum Calculation for Musk Molecules Infrared Spectra towards the Understanding of Odor. Advances in Chemistry, 2014, 2014, 1-13.	1.1	1
4747	Transfer Hydrogenation in Open-Shell Nucleotides â€” A Theoretical Survey. Molecules, 2014, 19, 21489-21505.	1.7	2
4748	Largely Reduced Grid Densities in a Vibrational Self-Consistent Field Treatment Do Not Significantly Impact the ResultingWavenumbers. Molecules, 2014, 19, 21253-21275.	1.7	12

#	Article	IF	Citations
4749	Theoretical Study on Dissociation Mechanisms of Di-ethyl Berylliums and Di-t-butyl Berylliums. Chinese Journal of Chemical Physics, 2014, 27, 168-174.	0.6	1
4751	Electronic and Optical Properties at Organic/Organic Interfaces in Organic Solar Cells. Topics in Current Chemistry, 2014, 352, 103-150.	4.0	6
4752	Theoretical study of the resonance Raman spectra for meso-tetrakis(3,5-di-tertiarybutylphenyl)-porphyrin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 707-713.	2.0	4
4753	Role of Hydrogen Abstraction Acetylene Addition Mechanisms in the Formation of Chlorinated Naphthalenes. 2. Kinetic Modeling and the Detailed Mechanism of Ring Closure. Journal of Physical Chemistry A, 2014, 118, 12205-12220.	1.1	12
4754	Theoretical investigation of the heat of formation and detonation performance on 1,1,3,5,5-pentanitro-1,5-bis(difluoramino)-3-azapentane substituted. Journal of Structural Chemistry, 2014, 55, 831-836.	0.3	2
4755	Quantum-chemical study on relationship between structure and antioxidant properties of hepatoprotective compounds occurring in Cynara scolymus and Silybum marianum. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450004.	1.8	29
4756	Modelling infrared action spectra of protonated water clusters. Molecular Simulation, 2014, 40, 176-184.	0.9	8
4757	Theoretical investigations on nonlinear optical and spectroscopic properties of 6-(3,3,4,4,4-pentafluoro-2-hydroxy-1-butenyl)-2,4-pyrimidinedione: An efficient NLO material. Russian Journal of Physical Chemistry A, 2014, 88, 2348-2358.	0.1	8
4758	Thermodynamic study on the chemical vapor deposition of boron nitride from the BCl3â€“NH3â€“H2 system. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	4
4759	Computer simulation of the structure of a sulfonated cation exchanger in the form of valinium salt. Journal of Structural Chemistry, 2014, 55, 1533-1540.	0.3	1
4760	Characterization of structure and dynamics of the solvated indium(III) ion by an extended QM/MM molecular dynamics simulation. Computational and Theoretical Chemistry, 2014, 1050, 74-82.	1.1	3
4761	Experimental and Theoretical Determination of the Antioxidant Properties of Aromatic Monoterpenes of Thymol and 2,5,6-Trifluorothymol. International Journal of Food Properties, 2014, 17, 1162-1168.	1.3	13
4762	Proton dissociation and transfer in a phosphoric acid doped imidazole system. RSC Advances, 2014, 4, 61992-62008.	1.7	10
4763	Theoretical studies on the pyrolysis of (Thion)carbonates. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450051.	1.8	7
4764	The structure and activity of potassium supported on SBA-15 molecular sieve: Density functional theory study. Journal of Theoretical and Computational Chemistry, 2014, 13, 1350076.	1.8	3
4765	Multiple sulfur isotope signatures of sulfite and thiosulfate reduction by the model dissimilatory sulfate-reducer, Desulfovibrio alaskensis str. G20. Frontiers in Microbiology, 2014, 5, 591.	1.5	26
4766	A Comparison of Theoretical and Experimental Raman Spectra of Microhydrated Sodium Glycinate. Advanced Materials Research, 2014, 934, 116-120.	0.3	0
4767	Toward precise assignment of THz spectra by DFT. , 2014, , .		1

#	Article	IF	Citations
4768	Assessing the impact of anionâ€“Ï€ effects on phenylalanine ion structures using IRMPD spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 24223-24234.	1.3	18
4769	Electronic Spectroscopy of a C7H4+ Isomer in a Neon Matrix: Methyltriacetylene Cation. Australian Journal of Chemistry, 2014, 67, 416.	0.5	1
4770	Theoretical studies of electronically excited states. , 2014, , .		1
4771	5-(Naphth-1-yl)- and 5-[(1,1â€²-biphenyl)-4-yl]isoxazole-3-carbaldehyde oximes: Synthesis, complexes with palladium, and application in catalysis. Russian Journal of General Chemistry, 2014, 84, 1782-1792.	0.3	14
4772	Theoretical Studies on the Reactions of 1,1,2,2,3,3,4â€Heptafluorocyclopentane with Hydroxyl and Hydrogen Free Radicals. Chinese Journal of Chemistry, 2014, 32, 897-908.	2.6	9
4773	Assessment of amide I spectroscopic maps for a gas-phase peptide using IR-UV double-resonance spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2014, 140, 224111.	1.2	26
4774	Efficient anharmonic vibrational spectroscopy for large molecules using local-mode coordinates. Journal of Chemical Physics, 2014, 141, 104105.	1.2	102
4775	Deexcitation Dynamics of Superhydrogenated Polycyclic Aromatic Hydrocarbon Cations after Soft-x-Ray Absorption. Physical Review Letters, 2014, 113, 053002.	2.9	47
4776	Vibrational Spectroscopy and Chemometrics for Rapid, Quantitative Analysis of Bitter Acids in Hops (Humulus lupulus). Journal of Agricultural and Food Chemistry, 2014, 62, 12521-12528.	2.4	13
4777	Diagnosis of the Redox Levels of TCNQF₄ Compounds Using Vibrational Spectroscopy. ChemPlusChem, 2014, 79, 962-972.	1.3	29
4778	¹³Câ•¹⁸O/¹⁵N Isotope Dependence of the Amide-I/II 2D IR Cross Peaks for the Fully Extended Peptides. Journal of Physical Chemistry C, 2014, 118, 29448-29457.	1.5	15
4779	Quantum Chemical, Spectroscopic, and X-Ray Diffraction Studies of N-diphenylphosphino-4-methylpiperidine Selenide (1). Molecular Crystals and Liquid Crystals, 2014, 591, 47-63.	0.4	3
4780	Azavinylidenephosphoranes: A Class of Cyclic Pushâ€“Pull Carbenes. Chemistry - A European Journal, 2014, 20, 12528-12536.	1.7	11
4781	Long-Range Distance Measurements in Proteins at Physiological Temperatures Using Saturation Recovery EPR Spectroscopy. Journal of the American Chemical Society, 2014, 136, 15356-15365.	6.6	43
4783	Oxidative Degradation of Thiaproline Derivatives in Aqueous Solutions Induced by ^{â€¢}OH Radicals. Israel Journal of Chemistry, 2014, 54, 321-332.	1.0	7
4784	Hydrogenated vacancies and hidden hydrogen in SrTiO3. Physical Review B, 2014, 89, .	1.1	36
4785	Theoretical study of an energetic material di-1H-1,3,4-triazole derivatives. Defence Technology, 2014, 10, 384-392.	2.1	7
4786	A Theoretical and Experimental Study of the Effects of Silyl Substituents in Enantioselective Reactions Catalyzed by Diphenylprolinol Silyl Ether. Chemistry - A European Journal, 2014, 20, 17077-17088.	1.7	54

#	Article	IF	Citations
4787	Theoretical prediction of nuclear magnetic shieldings and indirect spin-spin coupling constants in 1,1-, cis-, and trans-1,2-difluoroethylenes. Journal of Chemical Physics, 2014, 140, 144303.	1.2	21
4788	Theoretical study on S_H2 reaction of methyl radical with threeâ€membered ring. International Journal of Quantum Chemistry, 2014, 114, 1594-1601.	1.0	1
4789	Reaction Between CH2 and HCCN: A Theoretical Approach to Acrylonitrile Formation in the Interstellar Medium. Origins of Life and Evolution of Biospheres, 2014, 44, 143-157.	0.8	8
4790	Hartree-Fock and density functional theory study of remote substituent effects on gas-phase heterolytic Fe-O and Fe-S bond energies of p -G-C₆ H₄ OFe(CO)₂ (Î· ⁵ -C₅ H₅) and p -G-C₆ H₄ SFe(CO)₂ (Î· ⁵ -C₅) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	5
4791	Importance of cytochromes in cyclization reactions: Quantum chemical study on a model reaction of proguanil to cycloguanil. Journal of Computational Chemistry, 2014, 35, 2047-2055.	1.5	28
4792	Quantum chemical calculations of the pK a of C60H2 in DMSO, tolueneâ€"DMSO mixture, and water. Russian Chemical Bulletin, 2014, 63, 561-566.	0.4	6
4793	Polymorphs Related by an Enantiotropic Phase Transition but Having Only Orderâ€"Disorder-Level Conformational Differences in a Spiro-Conjugated Imidazolidine Ring Compound. Crystal Growth and Design, 2014, 14, 6302-6310.	1.4	6
4795	Critical interpretation of CHâ€" and OHâ€" stretching regions for infrared spectra of methanol clusters (CH3OH)n (n = 2â€"5) using self-consistent-charge density functional tight-binding molecular dynamics simulations. Journal of Chemical Physics, 2014, 141, 094303.	1.2	17
4796	Role of Hydrogen Abstraction Acetylene Addition Mechanisms in the Formation of Chlorinated Naphthalenes. 1. A Quantum Chemical Investigation. Journal of Physical Chemistry A, 2014, 118, 12192-12204.	1.1	5
4797	The Role of pH in the Mechanism of [.]OH Radical Induced Oxidation of Nicotine. Israel Journal of Chemistry, 2014, 54, 302-315.	1.0	14
4798	IR Spectroscopic Techniques to Study Isolated Biomolecules. Topics in Current Chemistry, 2014, 364, 1-42.	4.0	58
4799	Vibrational frequency scaling factors for correlation consistent basis sets and the methods CC2 and MP2 and their spin-scaled SCS and SOS variants. Journal of Chemical Physics, 2014, 141, 194106.	1.2	14
4800	Theoretical Study of the Electronic Excited States and Fluorescence Spectra of Squaraine in Solution. Journal of Solution Chemistry, 2014, 43, 1625-1643.	0.6	1
4801	Trapping in water â€" an important prerequisite for complex reactivity in astrophysical ices: the case of acetone (CH3)2CÂ=ÂO and ammonia NH3. Monthly Notices of the Royal Astronomical Society, 2014, 443, 2991-3000.	1.6	21
4802	A comparative study on the adsorption behaviors of PABA in the silver nano-particles. Journal of Molecular Structure, 2014, 1074, 660-665.	1.8	9
4803	TLCâ€SERS of mauve, the first synthetic dye. Journal of Raman Spectroscopy, 2014, 45, 1147-1152.	1.2	68
4804	Theoretical Methods for Vibrational Spectroscopy and Collision Induced Dissociation in the Gas Phase. Topics in Current Chemistry, 2014, 364, 99-151.	4.0	22
4805	Characterization Based Reverse Design of Ionic Liquids. Computer Aided Chemical Engineering, 2014, , 285-290.	0.3	1

#	Article	IF	Citations
4806	Synthesis and Characterization of Novel Re(BIAN)(CO)3Cl Derivatives Including the First Example of a Water-soluble Tricarbonyl Rhenium(I) Complex with Bis(imino)acenaphthene Ligands. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2014, 69, 691-698.	0.3	7
4807	Theoretical interpretation of the vibrational spectrum of bicyclo[1.1.0]butane in terms of an ab initio anharmonic model. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 117, 366-373.	0.2	8
4808	Quantum chemical and experimental studies on the structure and vibrational spectra of an alkaloidâ€“Corlumine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 470-480.	2.0	9
4809	Computational study of the vibrational spectroscopic studies, natural bond orbital, frontier molecular orbital and second-order non-linear optical properties of acetophenone thiosemicarbazone molecule. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 543-551.	2.0	11
4810	Experimental and theoretical study of the spectroscopic properties and the preparation of 3-benzyl-2H-pyrano[3,2-c]chromene-2,5(6H)-dione. Journal of Molecular Structure, 2014, 1065-1066, 235-240.	1.8	15
4811	Wavefunction methods for the accurate characterization of water clusters. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 199-224.	6.2	43
4812	The impact of highly correlated potential energy surfaces on the anharmonically corrected IR spectrum of acetonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 545-555.	2.0	5
4813	Phosphate adsorption on goethite and Al-rich goethite. Computational Materials Science, 2014, 85, 59-66.	1.4	29
4814	Gas-phase cleavage of the novel iminium ions [R1CH+NCHR2â†’R1CHN+CHR2]: An experimental and computational study. Journal of Molecular Structure, 2014, 1056-1057, 219-226.	1.8	1
4815	The 1-acetyl-3-methyl-4-[3-methoxy-4-(4-methylbenzoxy)benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one molecule investigated by a joint spectroscopic and quantum chemical calculations. Journal of Molecular Structure, 2014, 1056-1057, 273-284.	1.8	12
4816	Structural and spectral properties of a zinc(II) coordination polymer: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 102-108.	2.0	6
4817	Quantum-mechanical DFT calculation supported Raman spectroscopic study of some amino acids in bovine insulin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 345-351.	2.0	6
4818	Spectral and structural studies of the anti-cancer drug Flutamide by density functional theoretical method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 604-613.	2.0	25
4819	CO bonding in FeN4 complexes and the effect of the macrocycle ligand: A DFT study. Polyhedron, 2014, 67, 36-43.	1.0	11
4820	DFT calculation and vibrational spectroscopic studies of 2-(tert-butoxycarbonyl (Boc)) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 187 Td (-am 2014, 129, 74-83.	2.0	77
4821	Spectral analysis, vibrational assignments, NBO analysis, NMR, UVâ€“Vis, hyperpolarizability analysis of 2-aminofluorene by Density Functional Theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 211-221.	2.0	10
4822	Density functional theory investigations into the structure and spectroscopic properties of the Ti4+ species in Ti-MWW zeolite. Microporous and Mesoporous Materials, 2014, 195, 216-226.	2.2	32
4823	Computational Vibrational Spectroscopy of glycine in aqueous solution â€“ Fundamental considerations towards feasible methodologies. Chemical Physics, 2014, 435, 21-28.	0.9	16

#	Article	IF	Citations
4824	Structure and spectral properties of l-histidinium dipicrate dihydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 102-111.	2.0	17
4825	Configuration of wobble base pairs having pyrimidines as anticodon wobble bases: significance for codon degeneracy. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1500-1520.	2.0	10
4826	Quantitative structure-property relationship modeling of GrÃtzel solar cell dyes. Journal of Computational Chemistry, 2014, 35, 214-226.	1.5	23
4827	Synthesis, characterization and in vitro cytotoxic properties of new silver(I) complexes of two novel Schiff bases derived from thiazole and pyrazine. Polyhedron, 2014, 71, 119-132.	1.0	36
4828	Use of vibrational spectroscopy to study 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione: A combined theoretical and experimental approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 126, 280-290.	2.0	14
4829	Insight into the Gas-Phase Structure of a Copper(II) <scp>l</scp>-Histidine Complex, the Agent Used To Treat Menkes Disease. Inorganic Chemistry, 2014, 53, 2349-2351.	1.9	21
4830	Crystal and molecular structure, conformational, vibrational properties and DFT calculations of melaminium bis (hydrogen oxalate). Journal of Molecular Structure, 2014, 1067, 14-26.	1.8	10
4831	New Insights into the Nature of Observable Reaction Intermediates in Cytochrome P450 NO Reductase by Using a Combination of Spectroscopy and Quantum Mechanics/Molecular Mechanics Calculations. Chemistry - A European Journal, 2014, 20, 1602-1614.	1.7	25
4832	Charge Storage in Decyl- and 3,6,9-Trioxadecyl-Substituted Poly(dithieno[3,2-b:2,3-d]pyrrole) Electrodes. Macromolecules, 2014, 47, 79-88.	2.2	26
4833	Vibrational spectra, optical properties, NBO and HOMOâ€“LUMO analysis of L-Phenylalanine L-Phenylalaninium Perchlorate: DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 129-138.	2.0	25
4834	Synthesis, crystal structure, IR, 1H NMR and theoretical calculations of 1,2,4-triazole Schiff base. Journal of Molecular Structure, 2014, 1062, 13-20.	1.8	11
4835	Vibrational spectroscopic study, charge transfer interaction and nonlinear optical properties of l-asparaginium picrate: A density functional theoretical approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 781-789.	2.0	48
4836	Thermodynamics investigation of the gas-phase reactions in the chemical vapor deposition of silicon borides with BCl3â€“SiCl4â€“H2 precursors. Structural Chemistry, 2014, 25, 1369-1384.	1.0	3
4837	Density functional investigations on 2-naphthalenecarbonitrile dimerization within cucurbit[8]uril cavitand. Journal of Molecular Modeling, 2014, 20, 2073.	0.8	7
4838	Theoretical studies on complexes of calcium ion with amino acids. Chemical Research in Chinese Universities, 2014, 30, 125-129.	1.3	4
4839	A theoretical prediction of the molecular and electronic structures, thermodynamic properties, and stability of 1,3-diazido-2-methyl-2-nitropropane (DAMNP). Structural Chemistry, 2014, 25, 931-940.	1.0	11
4840	Study on structural and spectral properties of isobavachalcone and 4-hydroxyderricin by computational method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 126, 254-259.	2.0	5
4841	Synthesis, crystal structure and ab initio/DFT calculations of a derivative of dithiophosphonates. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 582-590.	2.0	21

#	Article	IF	Citations
4842	On the structures of 5-(4-, 3- and 2-methoxyphenylazo)-3-cyano-1-ethyl-6-hydroxy-4-methyl-2-pyridone: An experimental and theoretical study. Dyes and Pigments, 2014, 104, 160-168.	2.0	25
4843	DFT simulation, quantum chemical electronic structure, spectroscopic and structureâ€“activity investigations of 2-benzothiazole acetonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 22-36.	2.0	12
4844	3-Pyridazinylnitrenes and 2-Pyrimidinylnitrenes. Journal of Organic Chemistry, 2014, 79, 1758-1770.	1.7	11
4845	Molecular orbital studies (hardness, chemical potential and electrophilicity), vibrational investigation and theoretical NBO analysis of 4-4â€²-(1H-1,2,4-triazol-1-yl methylene) dibenzonitrile based on abinitio and DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 237-251.	2.0	114
4846	Exploring the structureâ€“activity relations of N-carbethoxyphthalimide by combining FTIR, FT-Raman and NMR spectroscopy with DFT electronic structure method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 473-488.	2.0	19
4847	Molecular structure, vibrational spectra and nonlinear optical properties of 2,5-dimethylanilinium chloride monohydrate: A density functional theory approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 127, 275-285.	2.0	39
4848	Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, 1H, 13C NMR) investigations of O-desmethyltramadol hydrochloride an active metabolite in tramadol â€“ An analgesic drug. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 315-330.	2.0	11
4849	Structureâ€“activity relations of 2-(methylthio)benzimidazole by FTIR, FT-Raman, NMR, DFT and conceptual DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 951-965.	2.0	28
4850	A new look into the quantum chemical and spectroscopic investigations of 5-chloro-1-methyl-4-nitroimidazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 160-174.	2.0	4
4851	The role of substituents in the molecular and crystal structure of 1-(adamantane-1-carbonyl)-3-(mono)- and 3,3-(di) substituted thioureas. Journal of Molecular Structure, 2014, 1065-1066, 150-159.	1.8	22
4852	FT-Raman and FTIR-ATR spectroscopies and DFT calculations of triterpene acetyl aleuritolic acid. Journal of Molecular Structure, 2014, 1058, 221-227.	1.8	13
4853	Ionized <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si96.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si97.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> in aqueous environment: Ab initio QM. Computational and Theoretical Chemistry, 2014, 1034, 85-93.	1.1	3
4854	Complexations of alkali/alkaline earth metal cations with gaseous glutamic acid. Computational and Theoretical Chemistry, 2014, 1039, 1-10.	1.1	9
4855	Inclusion complexes of cypermethrin and permethrin with monochlorotriazinyl-beta-cyclodextrin: A combined spectroscopy, TG/DSC and DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 576-586.	2.0	22
4856	Molecular structure and vibrational analysis on (E)-1-(3-methyl-2,6-diphenyl piperidin-4-ylidene) semicarbazide. Journal of Molecular Structure, 2014, 1058, 41-50.	1.8	31
4857	Theoretical studies on the pyrolysis of thiocarbonates. Computational and Theoretical Chemistry, 2014, 1030, 67-73.	1.1	20
4858	Decay of Iron(V) Nitride Complexes By a Nï£¿N Bondâ€Coupling Reaction in Solution: A Combined Spectroscopic and Theoretical Analysis. Angewandte Chemie - International Edition, 2014, 53, 8727-8731.	7.2	31
4859	Hydrazinolysis of 3-R-[1,2,4]Triazino[2,3-c]quinazolin-2-ones. Synthetic and Theoretical Aspects. Journal of Physical Chemistry A, 2014, 118, 1895-1905.	1.1	18

#	Article	IF	Citations
4860	A comparative study of selected disperse azo dye derivatives based on spectroscopic (FT-IR, NMR and) Tj ETQq0 0 0 rgBT /Overlock 10 T Spectroscopy, 2014, 122, 682-689.	2.0	24
4861	CVD precursors for transition metal oxide nanostructures: molecular properties, surface behavior and temperature effects. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 251-259.	0.8	24
4862	Explanation through density functional theory of the unanticipated loss of CO₂and differences in mass fragmentation profiles of ritonavir and its rCYP3A4-mediated metabolites. Journal of Mass Spectrometry, 2014, 49, 452-467.	0.7	0
4863	Synthesis, vibrational, NMR, quantum chemical and structure-activity relation studies of 2-hydroxy-4-methoxyacetophenone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 164-177.	2.0	82
4864	Possibility of the Existence of Donorâ€“Acceptor Interactions in Bis(azole)amines: An Electronic Structure Analysis. Journal of Organic Chemistry, 2014, 79, 4852-4862.	1.7	25
4866	Influence of Supramolecular Interactions on Electron-Transfer Photochromism of the Crystalline Adducts of 4,4â€²-Bipyridine and Carboxylic Acids. Crystal Growth and Design, 2014, 14, 2527-2531.	1.4	50
4867	Terahertz and FTIR spectroscopy of â€˜Bisphenol Aâ€™. Journal of Molecular Structure, 2014, 1059, 255-259.	1.8	16
4868	Vibrational spectroscopy and density functional theory study of 4-mercaptophenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 698-703.	2.0	14
4869	Oxidative Addition to Palladium(0) Diphosphine Complexes: Observations of Mechanistic Complexity with Iodobenzene as Reactant. Chemistry - A European Journal, 2014, 20, 1116-1125.	1.7	31
4870	Crystal structure and DFT calculations of 5-(4-Chlorophenyl)-1-(6-methoxypyridazin-3-yl)-1H-pyrazole-3-carboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 555-562.	2.0	16
4871	Photoinduced intermolecular electron transfer and off-resonance Raman characteristics of Rhodamine 101/N,N-diethylaniline. Chemical Physics, 2014, 429, 12-19.	0.9	13
4872	Carbon Monoxide Adsorption Coverage Study on Platinum and Ruthenium Surfaces. Journal of Physical Chemistry C, 2014, 118, 11711-11722.	1.5	35
4873	DFT study on the organocatalytic carbonylâ€“olefin metathesis. Computational and Theoretical Chemistry, 2014, 1027, 179-185.	1.1	3
4874	Vibrational and Electronic Spectral Study on 3,5-Dihydro-4H-Imidazol-4-One Derivatives Containing Organo-Selenium. Spectroscopy Letters, 2014, 47, 690-703.	0.5	0
4875	Computational studies of molecular charge transfer complexes of heterocyclic 4-methylepyridine-2-azomethine-p-benzene derivatives with picric acid and m-dinitrobenzene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 25-31.	2.0	12
4876	FTIR spectra and density functional theory P.E.D. assignments of oxiranes in Ar matrix at 12K. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 558-567.	2.0	9
4877	Study on molecular structure, spectroscopic investigation (IR, Raman and NMR), vibrational assignments and HOMOâ€“LUMO analysis of L-sodium folinate using DFT: A combined experimental and quantum chemical approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 106-118.	2.0	41
4878	Conformational analysis and vibrational study of daidzein by using FT-IR and FT-Raman spectroscopies and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 405-415.	2.0	37

#	Article	IF	Citations
4879	DFT analysis of P-nitrobenzotrifluoride â€“ A combined study of experimental (FT-IR and FT-Raman) and theoretical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 641-649.	2.0	3
4880	Structure and vibrational spectra of copper(II) 2-pyridylmethanolate tetrahydrate. Chemical Papers, 2014, 68, .	1.0	2
4881	Hybrid MP2/MP4 potential surfaces in VSCF calculations of IR spectra: Applications for organic molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 2-11.	2.0	8
4882	Computational modeling of single- versus double-anchoring modes in di-branched organic sensitizers on TiO₂ surfaces: structural and electronic properties. Physical Chemistry Chemical Physics, 2014, 16, 4709-4719.	1.3	28
4883	Synthesis, DFT and antimicrobial activity assays in vitro for novel cis/trans-but-2-enedioic acid esters. Journal of Molecular Structure, 2014, 1063, 226-234.	1.8	10
4884	A comparative study of the electronic structure and spectra of tetraoxa[8]circulene and octathio[8]circulene. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 116, 33-46.	0.2	26
4885	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 126-136.	2.0	14
4886	Nitrene-Carbene-Carbene Rearrangement. Photolysis and Thermolysis of Tetrazolo[5,1-a]phthalazine with Formation of 1-Phthalazinylnitrene, o-Cyanophenylcarbene, and Phenylcyanocarbene. Journal of Organic Chemistry, 2014, 79, 307-313.	1.7	8
4887	Direct Observation of Multiple Tautomers of Oxythiamine and their Recognition by the Thiamine Pyrophosphate Riboswitch. ACS Chemical Biology, 2014, 9, 227-236.	1.6	27
4888	Importance of weak interactions and conformational equilibrium in N -butyl- N -methylpiperidinium bis(trifluromethanesulfonyl) imide room temperature ionic liquids: Vibrational and theoretical studies. Vibrational Spectroscopy, 2014, 75, 107-117.	1.2	23
4889	Dehalogenation of Arenes via S_N2 Reactions at Bromine: Competition with Nucleophilic Aromatic Substitution.. Journal of Organic Chemistry, 2014, 79, 11020-11028.	1.7	14
4890	Monitoring of Reaction Intermediates in the Gas Phase: Ruthenium-Catalyzed Câ€“C Coupling. Organometallics, 2014, 33, 6868-6878.	1.1	22
4891	Experimental and Theoretical Spectroscopic Study of 3-Aryl-2-Phenyl-3-Phenylaminopropanoic Acids. Journal of Applied Spectroscopy, 2014, 81, 577-582.	0.3	0
4892	Diradicals acting through diamagnetic phenylene vinylene bridges: Raman spectroscopy as a probe to characterize spin delocalization. Journal of Chemical Physics, 2014, 140, 164903.	1.2	6
4893	Structure and Dynamics of the Uranyl Tricarbonate Complex in Aqueous Solution: Insights from Quantum Mechanical Charge Field Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 12938-12951.	1.2	30
4894	Molecular structure, spectroscopic properties (FT-IR, Micro-Raman, and UV-vis), and DFT calculations of minaprine. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 117, 82-95.	0.2	4
4895	Terahertz Chiroptical Spectroscopy of an Î±-Helical Polypeptide: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 12837-12843.	1.2	27
4896			

#	Article	IF	Citations
4897	Temperature-dependent reaction between trimethylaluminum and poly(methyl methacrylate) during sequential vapor infiltration: experimental and ab initio analysis. Journal of Materials Chemistry C, 2014, 2, 9416-9424.	2.7	54
4898	SERS spectroscopic evidence for the integrity of surface-deposited self-assembled coordination cages. Physical Chemistry Chemical Physics, 2014, 16, 21930-21935.	1.3	6
4899	Raman Spectroscopy of Conformational Rearrangements at Low Temperatures. Springer Theses, 2014, , .	0.0	4
4900	Unbranched n-Alkanes. Springer Theses, 2014, , 37-117.	0.0	2
4901	Formaldehyde chemistry in cometary ices: the case of HOCH₂OH formation. Physical Chemistry Chemical Physics, 2014, 16, 24200-24208.	1.3	21
4902	Mechanistic Contrasts between Manganese and Rhenium Bipyridine Electrocatalysts for the Reduction of Carbon Dioxide. Journal of the American Chemical Society, 2014, 136, 16285-16298.	6.6	269
4903	The reactions of Cr(CO)₆, Fe(CO)₅, and Ni(CO)₄ with O₂ yield viable oxoâ€metal carbonyls. Journal of Computational Chemistry, 2014, 35, 998-1009.	1.5	6
4904	Thermochemistry of C₇H₁₆ to C₁₀H₂₂ Alkane Isomers: Primary, Secondary, and Tertiary Câ€“H Bond Dissociation Energies and Effects of Branching. Journal of Physical Chemistry A, 2014, 118, 9364-9379.	1.1	44
4905	Coordinating Tectons: Bimetallic Complexes from Bipyridyl Terminated Group 8 Alkynyl Complexes. Organometallics, 2014, 33, 4911-4922.	1.1	20
4906	Understanding the mechanism of the Povarov reaction. A DFT study. RSC Advances, 2014, 4, 25268.	1.7	54
4907	Biomolecular structure manipulation using tailored electromagnetic radiation: a proof of concept on a simplified model of the active site of bacterial DNA topoisomerase. Physical Chemistry Chemical Physics, 2014, 16, 21768-21777.	1.3	3
4908	Macromolecular Entropy Can Be Accurately Computed from Force. Journal of Chemical Theory and Computation, 2014, 10, 4777-4781.	2.3	15
4909	Actinoid(III) Hydrationâ€”First Principle Gibbs Energies of Hydration Using High Level Correlation Methods. Journal of Chemical Theory and Computation, 2014, 10, 5593-5598.	2.3	30
4910	Synthesis and Characterization of 12-Pyridinium Derivatives of the [closo-1-CB₁₁H₁₂]^â Anion. Inorganic Chemistry, 2014, 53, 12617-12626.	1.9	26
4911	Strength by Joining Methods: Combining Synthesis with NMR, IR, and Vibrational Circular Dichroism Spectroscopy for the Determination of the Relative Configuration in Hemicalide. Chemistry - A European Journal, 2014, 20, 17385-17394.	1.7	23
4912	Theoretical study of the vibrational frequencies of carbon disulfide. International Journal of Quantum Chemistry, 2014, 114, 429-435.	1.0	3
4913	Î²-Phenyl quenching of 9-phenylphenalenones: a novel photocyclisation reaction with biological implications. Physical Chemistry Chemical Physics, 2014, 16, 18813-18820.	1.3	12
4914	Study of the synthesis mechanism of 4-amino-3,5-dimethyl pyrazole by fibre optic in-line FT-IR spectroscopy combined with independent component analysis. Analytical Methods, 2014, 6, 4305-4311.	1.3	13

#	Article	IF	Citations
4915	On the kinetics and reaction mechanisms of boronic acid in interaction with diols for non-enzymatic glucose monitoring applications: a hybrid DFT study. RSC Advances, 2014, 4, 10505.	1.7	19
4916	Vibrational dynamics of the salicylideneaniline molecule in the solid phase and the confined state. Physical Chemistry Chemical Physics, 2014, 16, 7562.	1.3	7
4917	Competitive reaction pathways in vibrationally induced photodissociation of H₂SO₄. Physical Chemistry Chemical Physics, 2014, 16, 18533.	1.3	17
4918	Metallo phosphonate catalyzed benzoin couplings: the influence of the counterion. New Journal of Chemistry, 2014, 38, 1040.	1.4	2
4919	Infrared Photodissociation Spectroscopy of Microhydrated Nitrateâ€“Nitric Acid Clusters NO₃^{â€“}(HNO₃)_m(H₂O)_n. Journal of Physical Chemistry A, 2014, 118, 7613-7622.	1.1	34
4920	The Solventâ€“Gelator Interaction as the Origin of Different Diffusivity Behavior of Diols in Gels Formed with Sugar-Based Low-Molecular-Mass Gelator. Journal of Physical Chemistry B, 2014, 118, 4005-4015.	1.2	18
4921	Gas-phase acid-base properties of homocysteine, homoserine, 5-mercaptonorvaline, and 5-hydroxynorvaline from the extended kinetic method. International Journal of Mass Spectrometry, 2014, 369, 71-80.	0.7	8
4922	Atomistic Insight into Orthoborate-Based Ionic Liquids: Force Field Development and Evaluation. Journal of Physical Chemistry B, 2014, 118, 8711-8723.	1.2	57
4923	Computational evaluation of tris(carbene)borate donor properties in {NiNO}10complexes. Dalton Transactions, 2014, 43, 14689-14695.	1.6	9
4924	Theoretical prediction of structural, vibrational and NMR parameters of plastic optical fiber (POF) material precursors. Cis and trans perhydro- and perfluoro-2-methylene-4,5-dimethyl-1,3-dioxolanes. Journal of Molecular Graphics and Modelling, 2014, 52, 36-45.	1.3	5
4925	Cupric Yersiniabactin Is a Virulence-Associated Superoxide Dismutase Mimic. ACS Chemical Biology, 2014, 9, 551-561.	1.6	91
4926	Effects of Relative Humidity on the Surface and Bulk Structures of Linear Polyethylenimine Thin Films. Journal of Physical Chemistry C, 2014, 118, 17686-17698.	1.5	10
4927	Approximate First-Principles Anharmonic Calculations of Polyatomic Spectra Using MP2 and B3LYP Potentials: Comparisons with Experiment. Journal of Physical Chemistry A, 2014, 118, 6730-6739.	1.1	32
4928	Catalytic Effect of Water, Formic Acid, or Sulfuric Acid on the Reaction of Formaldehyde with OH Radicals. Journal of Physical Chemistry A, 2014, 118, 4797-4807.	1.1	82
4929	Formation of a New Benzeneâ€“Ethane Co-Crystalline Structure Under Cryogenic Conditions. Journal of Physical Chemistry A, 2014, 118, 4087-4094.	1.1	23
4930	Computational Study of the Effects of Steric Hindrance on Amide Bond Cleavage. Journal of Physical Chemistry A, 2014, 118, 8664-8675.	1.1	8
4931	FT-Raman and FTIR spectra of photoactive aminobenzazole derivatives in the solid state: A combined experimental and theoretical study. Materials Chemistry and Physics, 2014, 148, 833-840.	2.0	16
4932	Dynamics and Thermodynamics of Crystalline Polymorphs. 3. Î³-Glycine, Analysis of Variable-Temperature Atomic Displacement Parameters, and Comparison of Polymorph Stabilities. Journal of Physical Chemistry A, 2014, 118, 9951-9959.	1.1	17

#	Article	IF	Citations
4933	Ozone Dissociation to Oxygen Affected by Criegee Intermediate. Journal of Physical Chemistry A, 2014, 118, 1644-1650.	1.1	19
4934	Thermal Decomposition of Propargyl Alcohol: Single Pulse Shock Tube Experimental and ab Initio Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 5927-5938.	1.1	10
4935	Catalytic behavior of hydrogen radicals in the thermal decomposition of crystalline furoxan: DFT-based molecular dynamics simulations. RSC Advances, 2014, 4, 34454.	1.7	22
4936	Reactivities of Substituted Î±-Phenyl-N-tert-butyl Nitrones. Journal of Organic Chemistry, 2014, 79, 6615-6626.	1.7	21
4937	Investigation of the Active Sites of Rhodium Sulfide for Hydrogen Evolution/Oxidation Using Carbon Monoxide as a Probe. Langmuir, 2014, 30, 5662-5668.	1.6	7
4938	Bromination and Accompanying Rearrangement of the Polycyclic Oxetane 2,4-Oxytwistane. Journal of Organic Chemistry, 2014, 79, 8786-8799.	1.7	8
4939	A Combined Computational and Spectroelectrochemical Study of Platinum-Bridged Bis-Triarylamine Systems. Inorganic Chemistry, 2014, 53, 1544-1554.	1.9	43
4940	Direct Spectroscopic Observation of Closed-Shell Singlet, Open-Shell Singlet, and Triplet p-Biphenylyloxenium Ion. Journal of the American Chemical Society, 2014, 136, 12364-12370.	6.6	19
4941	Thermodynamic properties of the methyl esters of p-hydroxy and p-methoxy benzoic acids. Journal of Chemical Thermodynamics, 2014, 78, 43-57.	1.0	23
4942	Reactivity of polychlorinated biphenyls in nucleophilic and electrophilic substitutions. Journal of Hazardous Materials, 2014, 278, 491-499.	6.5	22
4943	Synthesis, spectroscopic characterization and density functional studies of a bis-benzimidazole derivative and of its complexes with palladium(II) halides. Comptes Rendus Chimie, 2014, 17, 905-912.	0.2	9
4944	Accuracy of density functionals in the description of dispersion interactions and IR spectra of phosphates and phosphorylated compounds. Journal of Molecular Modeling, 2014, 20, 2426.	0.8	9
4945	Synthesis, Structure, and Reactivity of Diazene Adducts: Isolation of isoâ€Diazene Stabilized as a Borane Adduct. Chemistry - A European Journal, 2014, 20, 11800-11811.	1.7	25
4946	Surface Structures of Amine-Bearing Siloxane Self-Assembled Monolayers: Influence of Conformation on Methylene Vibrational Frequencies. Journal of Physical Chemistry C, 2014, 118, 15804-15815.	1.5	2
4947	Singlet Exciton Diffusion in Organic Crystals Based on Marcus Transfer Rates. Journal of Chemical Theory and Computation, 2014, 10, 1242-1255.	2.3	56
4948	Raman Spectroscopy, X-ray Diffraction, and Hydrogenation Thermochemistry of N,N,N,N-Tetramethylcyclotriborazane under Pressure. Journal of Physical Chemistry C, 2014, 118, 9871-9879.	1.5	1
4949	Theoretical studies of vibrational spectra of [N(CH₃)₄]₂ZnCl_{4âˆ’y}Br_ycompounds withy= 0, 2 and 4. Phase Transitions, 2014, 87, 613-628.	1.6	16
4950	Methyl-Perfluoroheptene-Ethers (CH₃OC₇F₁₃): Measured OH Radical Reaction Rate Coefficients for Several Isomers and Enantiomers and Their Atmospheric Lifetimes and Global Warming Potentials. Environmental Science & Technology, 2014, 48, 4954-4962.	4.6	6

#	Article	IF	Citations
4951	Reactivity in the nucleophilic aromatic substitution reactions of pyridinium ions. Organic and Biomolecular Chemistry, 2014, 12, 6175-6180.	1.5	8
4952	A Semi-homodesmotic Approach for Estimating Ring Strain Energies (RSEs) of Highly Substituted Cyclopropanes That Minimizes Use of Acyclic References and Cancels Steric Interactions: RSEs for c-C₃R₆ that Make Sense. Journal of Physical Chemistry A, 2014, 118, 6050-6059.	1.1	16
4953	Proton affinity and molecular basicity of m - and p -substituted benzamides in gas phase and in solution: A theoretical study. Chemical Physics Letters, 2014, 610-611, 321-330.	1.2	30
4954	Analytical Harmonic Vibrational Frequencies for the Green Fluorescent Protein Computed with ONIOM: Chromophore Mode Character and Its Response to Environment. Journal of Chemical Theory and Computation, 2014, 10, 751-766.	2.3	24
4955	Role of Gold(I) Î±-Oxo Carbenes in the Oxidation Reactions of Alkynes Catalyzed by Gold(I) Complexes. Journal of the American Chemical Society, 2014, 136, 11513-11523.	6.6	80
4956	Simulations of Raman Spectra Using the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2014, 10, 3689-3698.	2.3	33
4957	An integrated experimental and theoretical investigation of the structural and spectroscopic properties of two nickel(II) isothiosemicarbazone complexes. Journal of Coordination Chemistry, 2014, 67, 1392-1404.	0.8	5
4958	Nitroâ€Substituted Bishomocubanes: Synthesis, Characterization, and Application as Energetic Materials. Chemistry - an Asian Journal, 2014, 9, 3533-3541.	1.7	29
4959	Exploration of minima on the C 7 H 7 + $_{oldsymbol {7}} ext{H}_{oldsymbol {7}}^{oldsymbol {+} }$ surface: Structural, stability- and charge-related considerations. Journal of Chemical Sciences, 2014, 126, 1181-1195.	0.7	6
4960	Photochemical Dihydrogen Production Using an Analogue of the Active Site of [NiFe] Hydrogenase. Inorganic Chemistry, 2014, 53, 4430-4439.	1.9	26
4961	Re(I) Complexes of Substituted dppz: A Computational and Spectroscopic Study. Inorganic Chemistry, 2014, 53, 3126-3140.	1.9	26
4962	Hydrogen from Formic Acid through Its Selective Disproportionation over Sodium Germanateâ€”A Nonâ€Transitionâ€Metal Catalysis System. Angewandte Chemie - International Edition, 2014, 53, 11275-11279.	7.2	11
4963	DFT studies on a high-energy density cage compound 1, 3, 5, 7, 9, 11-hexo(N(CH₃)NO₂)-2, 4, 6, 8, 10, 12-hexaazatetracyclo[5, 5, 0, 0, 0] dodecane. Molecular Physics, 2014, 112, 1040-1046.	0.8	1
4964	Synthesis, characterization, microbiological evaluation, genotoxicity and synergism tests of new nano silver complexes with sulfamoxole. Journal of Inorganic Biochemistry, 2014, 141, 58-69.	1.5	31
4965	Radical Model of Arsenic(III) Toxicity: Theoretical and EPR Spin Trapping Studies. Chemical Research in Toxicology, 2014, 27, 765-774.	1.7	30
4966	The mechanistic study of the hydroxyl radical reaction with trans-2-chlorovinyldichloroarsine. Journal of Molecular Modeling, 2014, 20, 2335.	0.8	4
4967	Bioinspired Hydrogenase Models: The Mixed-Valence Triiron Complex [Fe₃(CO)₇(Î¼-edt)₂] and Phosphine Derivatives [Fe₃(CO)_{7â€“x}(PPh₃)_x(Î¼-edt)₂] (x = 1, 2) and [Fe₃(CO)₅(Î²-diphosphine)(Î¼-edt)₂] as Proton Reduction Catalysts. Organometallics, 2014, 33, 1356-1366.	1.1	22
4968	Does cation break the cyano bond? A critical evaluation of nitrile-cation interaction. Journal of Molecular Modeling, 2014, 20, 2219.	0.8	2

#	Article	IF	Citations
4969	Coreâ€“valence correlation effects on IR calculations: the BF3 and BCl3 cases. Journal of Molecular Modeling, 2014, 20, 2333.	0.8	2
4970	Charge-sensitive vibrational modes in the (EDT-TTF-OX)2AsF6 chiral molecular conductors. Open Physics, 2014, 12, .	0.8	1
4971	Catalytic Formation of Ammonia from Molecular Dinitrogen by Use of Dinitrogen-Bridged Dimolybdenumâ€“Dinitrogen Complexes Bearing PNP-Pincer Ligands: Remarkable Effect of Substituent at PNP-Pincer Ligand. Journal of the American Chemical Society, 2014, 136, 9719-9731.	6.6	202
4972	Surface-enhanced Raman scattering and DFT investigation of 1,5-diphenylcarbazide and its metal complexes with Ca(II), Mn(II), Fe(III) and Cu(II). Journal of Molecular Structure, 2014, 1073, 10-17.	1.8	5
4973	Structure and Dynamics of Octamethyl-POSS Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 5579-5592.	1.5	27
4974	Influence of metal to ligand molar ratios on the supramolecular structure formation of Cu(II) with diaminopropane and iodide: Synthesis, structure, spectroscopic and DFT studies. Journal of Molecular Structure, 2014, 1062, 158-166.	1.8	7
4975	Infrared Photodissociation Spectroscopy of Oxygen-Rich Fe(O₂)_n⁺ (n = 3â€“5) Cation Complexes. Journal of Physical Chemistry A, 2014, 118, 4519-4526.	1.1	10
4976	Mesomorphic, micro-Raman and DFT studies of new calamitic liquid crystals; methyl 4-[4-(4-alkoxy) Tj ETQq1 1 0.784314 rgBT /Overlock Spectroscopy, 2014, 128, 248-256.	2.0	25
4977	Prediction of Experimentally Unavailable Product Branching Ratios for Biofuel Combustion: The Role of Anharmonicity in the Reaction of Isobutanol with OH. Journal of the American Chemical Society, 2014, 136, 5150-5160.	6.6	69
4978	Standard molar enthalpy of formation of methoxyacetophenone isomers. Journal of Chemical Thermodynamics, 2014, 74, 22-31.	1.0	11
4979	Transition State Analysis of Enantioselective BrÃ¸nsted Base Catalysis by Chiral Cyclopropenimines. Journal of the American Chemical Society, 2014, 136, 10700-10707.	6.6	35
4980	Thermochemical study of the dicyanoimidazole isomers. Structural Chemistry, 2014, 25, 775-783.	1.0	3
4981	Vibrational investigation of 1-cyclopentylpiperazine: A combined experimental and theoretical study. Science China: Physics, Mechanics and Astronomy, 2014, 57, 1654-1661.	2.0	9
4982	Structural Investigation of Protonated Azidothymidine and Protonated Dimer. Journal of the American Society for Mass Spectrometry, 2014, 25, 176-185.	1.2	2
4983	The Î±-Effect and Competing Mechanisms: The Gas-Phase Reactions of Microsolvated Anions with Methyl Formate. Journal of the American Society for Mass Spectrometry, 2014, 25, 159-168.	1.2	18
4984	The Role of Methoxy Group in the Nazarov Cyclization of 1,5-bis-(2-Methoxyphenyl)-1,4-Pentadien-3-one in the Gas Phase and Condensed Phase. Journal of the American Society for Mass Spectrometry, 2014, 25, 398-409.	1.2	5
4985	Studying the Chemistry of Cationized Triacylglycerols Using Electrospray Ionization Mass Spectrometry and Density Functional Theory Computations. Journal of the American Society for Mass Spectrometry, 2014, 25, 1421-1440.	1.2	16
4986	Mechanistic Study on Electron Capture Dissociation of the Oligosaccharide-Mg²⁺ Complex. Journal of the American Society for Mass Spectrometry, 2014, 25, 1451-1460.	1.2	26

#	Article	IF	Citations
4987	Pushing the limits in accurate vibrational structure calculations: anharmonic frequencies of lithium fluoride clusters (LiF)_n, n = 2â€“10. Physical Chemistry Chemical Physics, 2014, 16, 16426.	1.3	20
4988	Density Functional Theory Study of Selective Deacylation of Aromatic Acetate in the Presence of Aliphatic Acetate under Ammonium Acetate Mediated Conditions. Journal of Organic Chemistry, 2014, 79, 6135-6142.	1.7	5
4989	Dynamic Effects on the Charge Transport in an Organic Near-Infrared Absorber Material. Journal of Physical Chemistry C, 2014, 118, 6537-6547.	1.5	15
4990	Molecular structure, NLO, MEP, NBO analysis and spectroscopic characterization of 2,5-dimethylanilinium dihydrogen phosphate with experimental (FT-IR and FT-Raman) techniques and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 856-866.	2.0	26
4991	Experimental and Theoretical Studies into the Formation of C4â€“C6Products in Partially Chlorinated Hydrocarbon Pyrolysis Systems: A Probabilistic Approach to Congener-Specific Yield Predictions. Journal of Physical Chemistry A, 2014, 118, 8644-8663.	1.1	8
4992	Experimental Characterization of Unimolecular Water Dissociative Adsorption on Î±-Alumina. Journal of Physical Chemistry C, 2014, 118, 13623-13630.	1.5	34
4993	Gas-Phase Enthalpies of Formation and Enthalpies of Sublimation of Amino Acids Based on Isodesmic Reaction Calculations. Journal of Physical Chemistry A, 2014, 118, 3490-3502.	1.1	45
4994	Self-Association Behavior of aNovelNonproteinogenic Î²-Strand-Mimicin an Organic Solvent. Journal of Physical Chemistry B, 2014, 118, 9199-9208.	1.2	5
4995	Infrared Spectra of CX₃â€“AuCl and CX₂â€“AuCl₂ Generated in Reactions of Laser-Ablated Gold Atoms with Chlorofluoromethanes and Carbon Tetrachloride. Organometallics, 2014, 33, 4315-4322.	1.1	10
4996	Synthesis, characterization, and DFT studies of a new chiral ionic liquid from (S)-1-phenylethylamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 778-784.	2.0	9
4997	Atomistic Modeling of Vibrational Action Spectra in Polyatomic Molecules: Nuclear Quantum Effects. Journal of Physical Chemistry A, 2014, 118, 5427-5436.	1.1	11
4998	Competition between carboxylic and phenolic groups for the preferred sites at the periphery of graphene â€“ A DFT study. Carbon, 2014, 80, 405-418.	5.4	24
4999	Combined Spectroscopic and Quantum Chemical Study of [trans-Ru(Câ‰¡CC₆H₄R¹-4)₂(dppe)₂]ⁿ⁺ and [trans-Ru(Câ‰¡CC₆H₄R¹-4)(Câ‰¡CC₆H₄R²-4)(n = 0, 1) Complexes: Interpretations beyond the Lowest Energy Conformer Paradigm. Organometallics, 2014, 33, 4947-4963.	1.1	66
5000	Oâ€“H anharmonic vibrational motions in Clâ¯â‹¯(CH3OH)1â¯2 ionic clusters. Combined IRPD experiments and AIMD simulations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 12-17.	2.0	14
5001	Crystal structure, spectroscopic investigations and quantum chemical calculational studies of N-diphenylphosphino-4-methylpiperidine sulfide. Journal of Molecular Structure, 2014, 1063, 170-177.	1.8	2
5002	Raman spectroscopy of carbon nanohoops. Carbon, 2014, 67, 203-213.	5.4	70
5003	Balancing the Interactions of Ions, Water, and DNA in the Drude Polarizable Force Field. Journal of Physical Chemistry B, 2014, 118, 6742-6757.	1.2	74
5004	Thermochemical Properties and Bond Dissociation Enthalpies of 3- to 5-Member Ring Cyclic Ether Hydroperoxides, Alcohols, and Peroxy Radicals: Cyclic Ether Radical + 3O2 Reaction Thermochemistry. Journal of Physical Chemistry A, 2014, 118, 3147-3167.	1.1	20

#	Article	IF	Citations
5005	Theoretical study of the structure, IR and NMR of the bis-peroxo-oxovanadate species containing-histidine peptides. Inorganica Chimica Acta, 2014, 420, 149-158.	1.2	9
5006	Do phenolic and carboxylic groups coexist at the tips of oxidized single-wall carbon nanotubes (o-SWNTs)?. Carbon, 2014, 73, 194-205.	5.4	10
5007	Anharmonic partition functions for polyatomic thermochemistry. Journal of Chemical Thermodynamics, 2014, 73, 183-189.	1.0	11
5008	Crystal structure, DFT and HF calculations and radical scavenging activities of (E)-4,6-dibromo-3-methoxy-2-[(3-methoxyphenylimino)methyl]phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 319-327.	2.0	10
5009	Reproducible quantification of ethanol in gasoline via a customized mobile near-infrared spectrometer. Analytica Chimica Acta, 2014, 826, 61-68.	2.6	70
5010	A new platinum complex with tryptophan: Synthesis, structural characterization, DFT studies and biological assays in vitro over human tumorigenic cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 209-215.	2.0	10
5011	Spectroscopic properties and orientation of molecules in Langmuirâ€“Blodgett layers of selected functionalized fullerenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 204-209.	2.0	6
5012	Spectral and structural studies of dimethylphenyl betaine hydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 844-851.	2.0	16
5013	Structural, vibrational and thermal studies of a new nonlinear optical crystal tetrapropylammonium dihydrogenmonoarsenate bis arsenic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 131, 274-281.	2.0	16
5014	Spectroscopic and density functional theory studies of trans-3-(trans-4-imidazolyl)acrylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 466-477.	2.0	5
5015	Ab initio/DFT calculations of butyl ammonium salt of O,Oâ€²-dibornyl dithiophosphate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 421-428.	2.0	13
5016	FT-IR spectroscopy combined with DFT calculation to explore solvent effects of vinyl acetate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 126, 122-128.	2.0	10
5017	Chalcogen analogues of nicotine lactam studied by NMR, FTIR, DFT and X-ray methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 773-780.	2.0	6
5018	Changing the regioselectivity and asynchronicity of the possible concerted [2+2] and [4+2] cycloadditions of ketene and halogenated ketenes with cyclopentadiene: a DFT survey. Tetrahedron, 2014, 70, 708-719.	1.0	5
5019	Characteristics of selenate in aqueous solution â€“ An ab initio QMCF-MD study. Chemical Physics Letters, 2014, 595-596, 226-229.	1.2	5
5020	Spectroscopic and structural investigation of 2,5-dicarboxy-1-methylpyridinium inner salt. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 121, 586-595.	2.0	1
5021	Theoretical studies on the dissociation reactions of chloromethyl peroxynitrate. Chemical Physics Letters, 2014, 595-596, 121-126.	1.2	3
5022	Synthesis, FTIR and FT-Raman spectral analysis and structureâ€“activity relations of N-(4-bromophenyl)-2,2-dichloroacetamide by DFT studies. Journal of Molecular Structure, 2014, 1064, 15-26.	1.8	8

#	Article	IF	Citations
5023	Regioselectivity of the intramolecular nucleophilic attack in [RCHâ^'NCHC6H4Y]: A mass spectrometric and computational study. Journal of Molecular Structure, 2014, 1063, 8-15.	1.8	0
5024	Experimental and theoretical investigation of pâ€“n alkoxy benzoic acid based liquid crystals â€“ A DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 511-523.	2.0	18
5025	Theoretical constraints on the effects of pH, salinity, and temperature on clumped isotope signatures of dissolved inorganic carbon species and precipitating carbonate minerals. Geochimica Et Cosmochimica Acta, 2014, 125, 610-652.	1.6	123
5026	Effects of the basis set and of the exchangeâ€“correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 34-41.	2.0	4
5027	A comparative DFT study on the differences between normal modes of polyethylene and polyethylene glycol via B3LYP Hamiltonian and the Hartreeâ€“Fock method in multiple bases. Optik, 2014, 125, 228-231.	1.4	8
5028	Reprint of: Energetics of 2- and 3-coumaranone isomers: A combined calorimetric and computational study. Journal of Chemical Thermodynamics, 2014, 73, 283-289.	1.0	3
5029	Mixedâ€Valence Ruthenium Complexes Rotating through a Conformational Robinâ€“Day Continuum. Chemistry - A European Journal, 2014, 20, 6895-6908.	1.7	76
5030	Physicochemical characterization of nimodipineâ€“polyethylene glycol solid dispersion systems. Drug Development and Industrial Pharmacy, 2014, 40, 886-895.	0.9	10
5031	Nitrile Imines and Nitrile Ylides: Rearrangements of Benzonitrile N-Methylimine and Benzonitrile Dimethylmethylide to Azabutadienes, Carbodiimides, and Ketenimines. Chemical Activation in Thermolysis of Azirenes, Tetrazoles, Oxazolones, Isoxazolones, and Oxadiazolones. Journal of Organic Chemistry, 2014, 79, 1247-1253.	1.7	30
5032	Thermochemistry, Reaction Paths, and Kinetics on the tert-Isooctane Radical Reaction with O₂. Journal of Physical Chemistry A, 2014, 118, 4631-4646.	1.1	25
5035	Influence of Amino Acid Stereocenters on the Formation of Bicyclic N,O-Acetals. Journal of Organic Chemistry, 2014, 79, 2556-2563.	1.7	5
5036	Vibrational spectra (FT-IR and FT-Raman), molecular structure, natural bond orbital, and TD-DFT analysis of l-Asparagine Monohydrate by Density Functional Theory approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 190-200.	2.0	14
5037	Efficient vibrational analysis for unrestricted Hartreeâ€“Fock based on the fragment molecular orbital method. Chemical Physics Letters, 2014, 603, 67-74.	1.2	21
5038	Molecular geometry, conformational, vibrational spectroscopic, molecular orbital and Mulliken charge analysis of 2-acetoxybenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 329-336.	2.0	60
5039	Molecular structure, quantum mechanical calculation and radical scavenging activities of (E)-4,6-dibromo-2-[(3,5-dimethylphenylimino)methyl]-3-methoxyphenol and (E)-4,6-dibromo-2-[(2,6-dimethylphenylimino)methyl]-3-methoxyphenol compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 357-366.	2.0	17
5040	Studies on molecular structure, vibrational spectra and molecular docking analysis of 3-Methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl 4-aminobenzoate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 591-603.	2.0	9
5041	Natural bond orbital analysis, electronic structure and vibrational spectral analysis of N-(4-hydroxyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Biomolecular Spectroscopy, 2014, 130, 621-633.	2.0	17
5042	Studies of the molecular geometry, vibrational spectra, Frontier molecular orbital, nonlinear optical and thermodynamics properties of Aceclofenac by quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 239-251.	2.0	22

#	Article	IF	Citations
5043	Detection of thiabendazole applied on citrus fruits and bananas using surface enhanced Raman scattering. Food Chemistry, 2014, 145, 814-820.	4.2	94
5044	SiO2@Au nanoshells-based SERS method for detection of sunset yellow and chrysoidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 355-360.	2.0	35
5045	Molecular structure and vibrational bands and 13C chemical shift assignments of both enmein-type diterpenoids by DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 449-458.	2.0	9
5046	Abâ€ˆinitio molecular dynamics with noisy forces: Validating the quantum Monte Carlo approach with benchmark calculations of molecular vibrational properties. Journal of Chemical Physics, 2014, 141, 194112.	1.2	26
5047	Computational Study on the Mechanism of the Electron-Transfer-Induced Repair of the (6â€“4) Tâ€“T Photoproduct of DNA by Photolyase: Possibility of a Radical Cation Pathway. Bulletin of the Chemical Society of Japan, 2014, 87, 390-399.	2.0	5
5049	Gasâ€Phase Peptide Structures Unraveled by Farâ€IR Spectroscopy: Combining IRâ€UV Ionâ€Dip Experiments with Bornâ€“Oppenheimer Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2014, 53, 3663-3666.	7.2	46
5050	Structures and vibrational frequencies of CO adsorbed on transition metals from calculations using the vdW-DF2 functional. Computational and Theoretical Chemistry, 2015, 1069, 147-154.	1.1	16
5051	Spectroscopic characterization, X-ray structure and DFT studies on 4-[3-(2,5-dimethylphenyl)-3-methylcyclobutyl]-N-methylthiazol-2-amine. Journal of Structural Chemistry, 2015, 56, 1342-1352.	0.3	3
5052	Vibrational coherence transfer in an electronically decoupled molecular dyad. Scientific Reports, 2015, 5, 9368.	1.6	14
5053	Dissociation Mechanism of the 3-Hydroxypyridine Radical Cation: A Computational Study. European Journal of Mass Spectrometry, 2015, 21, 161-169.	0.5	0
5054	Vibrational properties of organic donor-acceptor molecular crystals: Anthracene-pyromellitic-dianhydride (PMDA) as a case study. Journal of Chemical Physics, 2015, 143, 224503.	1.2	14
5055	Adsorption and Vibrational Study of Folic Acid on Gold Nanopillar Structures Using Surface-Enhanced Raman Scattering Spectroscopy. Nanomaterials and Nanotechnology, 2015, 5, 29.	1.2	33
5056	Geometry optimization, HOMO and LUMO energy, molecular electrostatic potential, NMR, FT-IR and FT-Raman analyzes on 4-nitrophenol. EPJ Applied Physics, 2015, 69, 10202.	0.3	6
5057	A complete map of the ion chemistry of the naphthalene radical cation? DFT and RRKM modeling of a complex potential energy surface. Journal of Chemical Physics, 2015, 143, 104305.	1.2	46
5058	Solvation structure and dynamics of Na+ in liquid ammonia studied by ONIOM-XS MD simulations. Chemical Physics, 2015, 463, 88-94.	0.9	5
5059	The molecular designs and properties of asymmetric heterocycles (HBrBN3) n (n = 1-4). Journal of Structural Chemistry, 2015, 56, 1468-1473.	0.3	2
5060	Evaluation of Hybrid Theoretical Approaches for Structural Determination of a Glycine-Linked Cisplatin Derivative via Infrared Multiple Photon Dissociation (IRMPD) Action Spectroscopy. Journal of Physical Chemistry A, 2015, 119, 10980-10987.	1.1	35
5061	Can 2â€acylpyrroles form an intramolecular hydrogen bond?. Journal of Physical Organic Chemistry, 2015, 28, 652-662.	0.9	3

#	Article	IF	Citations
5062	Dynamics of proton exchange in a model phosphonic acid-functionalized polymer. International Journal of Quantum Chemistry, 2015, 115, 1161-1174.	1.0	2
5063	Origins of regioselectivity in radical arylation of aniline: A computational study. International Journal of Quantum Chemistry, 2015, 115, 1658-1667.	1.0	8
5064	Why Inverted Small Molecule Solar Cells Outperform Their Noninverted Counterparts. Advanced Functional Materials, 2015, 25, 6511-6518.	7.8	3
5065	Atomistic Modeling of IR Action Spectra Under Circularly Polarized Electromagnetic Fields: Toward Action VCD Spectra. Chirality, 2015, 27, 253-261.	1.3	3
5066	Asymmetric Nitrocyclopropanation of Î±â€Substituted Î±,Î²â€Enals Catalyzed by Diphenylprolinol Silyl Ether for the Construction of Allâ€Carbon Quaternary ÂStereogenic Centers. European Journal of Organic Chemistry, 2015, 2015, 5747-5754.	1.2	12
5067	Raman spectra of hydrocarbons formed in carbon nanotubes - a theoretical study. Physica Status Solidi (B): Basic Research, 2015, 252, 2541-2545.	0.7	4
5068	IR Spectra and DFT Calculations of ÂMâ€“Î·²â€(NC)â€“CH₃, CH₃â€“MNC, and CH₂=M(H)NC Prepared by Reactions of Laserâ€Ablated Hf and Ti Atoms with AcetoÂnitrile. European Journal of Inorganic Chemistry, 2015, 2015, 4379-4387.	1.0	10
5069	Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. Journal of Computational Chemistry, 2015, 36, 2158-2167.	1.5	10
5070	Surfaceâ€enhanced Raman Spectroscopic Studies of Ellagic Acid in Silver Colloids. Bulletin of the Korean Chemical Society, 2015, 36, 1637-1644.	1.0	9
5071	Rutheniumâ€Grafted Vinylhelicenes: Chiroptical Properties and Redox Switching. Chemistry - A European Journal, 2015, 21, 17100-17115.	1.7	43
5072	Computational Studies on Intramolecular Cycloadditions of Azidoenynes and Azidobutenenitriles to Give 6Hâ€Pyrrolo[1,2â€c][1,2,3]triazoles and 5Hâ€Pyrrolo[1,2â€d]tetrazoles. Helvetica Chimica Acta, 2015, 98, 1018-1027.	1.0	3
5073	New Singlet Oxygen Donors Based on Naphthalenes: Synthesis, Physical Chemical Data, and Improved Stability. Chemistry - A European Journal, 2015, 21, 8569-8577.	1.7	43
5074	Reactivity of an Allâ€Ferrous Ironâ€“Nitrogen Heterocubane under Reductive and Oxidative Conditions. Chemistry - A European Journal, 2015, 21, 15797-15805.	1.7	4
5075	Sevenâ€Coordinate Luminophores: Brilliant Luminescence of Lanthanide Complexes with C_{3v} Geometrical Structures. European Journal of Inorganic Chemistry, 2015, 2015, 4769-4774.	1.0	60
5076	FT-IR and FT-Raman Spectral Investigation and DFT Computations of Pharmaceutical Important Molecule: Ethyl 2-(4-Benzoyl-2,5- Dimethylphenoxy) Acetate. Pharmaceutica Analytica Acta, 2015, 07, .	0.2	2
5077	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. , 2015, , 169-201.		0
5078	Assessment of Functionals for First-Principle Studies of the Structural and Electronic Properties ofÎ´-Bi2O3. Advances in Condensed Matter Physics, 2015, 2015, 1-9.	0.4	1
5079	TDDFT Study on Excited-State Hydrogen Bonding of 2â€²-Deoxyguanosine in H2O Solution. Chinese Journal of Chemical Physics, 2015, 28, 721-726.	0.6	1

#	Article	IF	Citations
5080	Ab Initio Anharmonic Analysis of Vibrational Spectra of Uracil Using the Numerical-Analytic Implementation of Operator Van Vleck Perturbation Theory. Journal of Physical Chemistry A, 2015, 119, 6723-6737.	1.1	29
5081	Microwave-assisted synthesis and mesomorphic investigations ofp-substituted aroylhydrazones and their nickel(II) and copper(II) complexes. Liquid Crystals, 2015, 42, 222-232.	0.9	10
5082	Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method. Journal of Chemical Physics, 2015, 142, 124101.	1.2	12
5083	Development of force field parameters for cyclopentane-modified peptide nucleic acids. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	3
5084	Opening of an icosahedral boron framework: A combined infrared spectroscopic and computational study. Chemical Physics Letters, 2015, 625, 48-52.	1.2	22
5085	Crystallography and computational electronic structure investigations on 14-(3, 4,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 542	1.8	11
5086	Synthesis and investigation of the properties of novel azocalix[4]arenes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 151-162.	2.0	6
5087	Thermodynamics of H₂O Splitting and H₂ Formation at the Cu(110)â€“Water Interface. Journal of Physical Chemistry C, 2015, 119, 14102-14113.	1.5	31
5088	Atomic-Level Structural and Electronic Properties of Hybrid Inorganicâ€“Organic ZnO:Hydroquinone Superlattices Fabricated by ALD/MLD. Journal of Physical Chemistry C, 2015, 119, 13105-13114.	1.5	75
5089	Carbonyl group coordination preferences in square-planar NiII and PdII complexes of pentadentate ligands by electron-withdrawing/donating substituents. Inorganica Chimica Acta, 2015, 433, 3-12.	1.2	1
5090	Theoretical study of the structure, spectroscopic properties and anti-cancer activity of tetrahydrochromeno[4,3-b]quinolines. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550052.	1.8	3
5091	Theoretical investigation on the nitrogen-rich energetic compound 5-nitro-2-nitratomethyl-1,2,3,4-tetrazole. Journal of Structural Chemistry, 2015, 56, 836-844.	0.3	1
5092	Activation enthalpies and entropies of the atropisomerization of substituted butyl-bridged biphenyls. Physical Chemistry Chemical Physics, 2015, 17, 11165-11173.	1.3	9
5093	First principles Raman study of boron and nitrogen doped planar T-graphene clusters. Materials Research Express, 2015, 2, 095603.	0.8	18
5094	Quadratic Corrections to Harmonic Vibrational Frequencies Outperform Linear Models. Journal of Physical Chemistry A, 2015, 119, 13107-13112.	1.1	12
5095	Sulfosuccinate and Sulfocarballylate Surfactants As Charge Control Additives in Nonpolar Solvents. Langmuir, 2015, 31, 13690-13699.	1.6	6
5096	The regioselective pyrolysis of (trithio)carbonate: A computational study. Russian Journal of General Chemistry, 2015, 85, 2399-2407.	0.3	4
5097	Theoretical studies of the structures and properties of (Cl2InN3) n (n = 1â€“6) clusters. Russian Journal of Physical Chemistry A, 2015, 89, 1863-1871.	0.1	2

#	Article	IF	Citations
5098	Numerical differentiation method to calculate molecular properties at ground and excited states â€“ Application to Julolidinemalononitrile. Chemical Physics Letters, 2015, 634, 249-254.	1.2	3
5099	Dynamics of ultrathin gold layers on vitreous silica probed by density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 27488-27495.	1.3	7
5100	Effects of volumetric expansion in molecular crystals: A quantum mechanical investigation on aspirin and paracetamol most stable polymorphs. Chemical Physics Letters, 2015, 621, 109-116.	1.2	4
5101	Theoretical Study of Intermolecular Chain Transfer to Polymer Reactions of Alkyl Acrylates. Industrial & Engineering Chemistry Research, 2015, 54, 4148-4165.	1.8	20
5102	Estimation of spectroscopic constants of isotopologues: Dependence of the scaling factors on isotopic mass. Computational and Theoretical Chemistry, 2015, 1054, 46-54.	1.1	0
5103	Current Status of Protein Force Fields for Molecular Dynamics Simulations. Methods in Molecular Biology, 2015, 1215, 47-71.	0.4	139
5104	Enthalpy of formation of CL-20. Computational and Theoretical Chemistry, 2015, 1057, 54-59.	1.1	22
5105	Materials Meets Concepts in Moleculeâ€Based Electronics. Advanced Functional Materials, 2015, 25, 1933-1954.	7.8	47
5106	Synthesis, molecular structure, spectroscopic investigations and computational studies of (E)-1-(4-(4-(diethylamino)-2-hydroxybenzylideneamino)phenyl)ethanone. Structural Chemistry, 2015, 26, 1095-1113.	1.0	8
5107	The Association of Two â€œFrustratedâ€•Lewis Pairs by Stateâ€ofâ€theâ€Art Quantum Chemical Methods. Israel Journal of Chemistry, 2015, 55, 235-242.	1.0	23
5108	Solid-state characterization of sertraline baseâ€“Î²-cyclodextrin inclusion complex. Journal of Pharmaceutical and Biomedical Analysis, 2015, 107, 265-272.	1.4	16
5109	Top cited articles in thermodynamic research. Journal of Engineering Thermophysics, 2015, 24, 68-85.	0.6	59
5110	Thermodynamic study of the chemical vapor deposition in the SiCl3CH3â€“NH3â€“H2 system. Chemical Physics Letters, 2015, 623, 29-36.	1.2	3
5111	Near edge X-ray absorption mass spectrometry on coronene. Journal of Chemical Physics, 2015, 142, 024308.	1.2	15
5112	DFT study of structural, vibrational and electronic properties of polyaniline pernigraniline model compounds. Journal of Computational Science, 2015, 10, 195-208.	1.5	17
5113	Investigation of the Role of Protonation of Benzophenone and Its Derivatives in Acidic Aqueous Solutions Using Time-Resolved Resonance Raman Spectroscopy: How Are Ketyl Radicals Formed in Aqueous Solutions?. Journal of Physical Chemistry B, 2015, 119, 2241-2252.	1.2	11
5114	Prediction Uncertainty of Density Functional Approximations for Properties of Crystals with Cubic Symmetry. Journal of Physical Chemistry A, 2015, 119, 5288-5304.	1.1	78
5115	Theoretical Investigation of Vibrational Sum-Frequency Generation Signatures of Functionalized Hâ€“Si(111). Journal of Physical Chemistry C, 2015, 119, 3180-3191.	1.5	9

#	Article	IF	Citations
5116	New High Pressure Crystal Structures of 2,2-Dimethylbutane and 2,3-Dimethylaniline: Combined X-ray, Raman, and Theoretical Studies. Crystal Growth and Design, 2015, 15, 45-52.	1.4	1
5117	Plagioclase Dissolution during CO₂â€“SO₂ Cosequestration: Effects of Sulfate. Environmental Science & Technology, 2015, 49, 1946-1954.	4.6	23
5118	Raman-Active Modes of Even-Numbered Cycloparaphenylenes: Comparisons between Experiments and Density Functional Theory (DFT) Calculations with Group Theory Arguments. Journal of Physical Chemistry C, 2015, 119, 2879-2887.	1.5	19
5119	Hydroxymethyl Radical Self-Recombination in High-Temperature Water. Journal of Physical Chemistry A, 2015, 119, 1830-1837.	1.1	5
5120	Experimental and theoretical studies of (E)-2-(2-hydroxystyryl)-6-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-1,2,4-triazin-3(2H)-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 141, 307-315.	2.0	11
5121	Intermolecular proton transfer in cyclic carbonate synthesis from epoxide and carbon dioxide catalyzed by azaphosphatranes: a DFT mechanistic study. RSC Advances, 2015, 5, 12382-12386.	1.7	21
5122	Combined spectroscopic and DFT studies on 6-bromo-4-chloro-3-formyl coumarin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 139, 505-514.	2.0	19
5123	Explosive properties of nanosized diacetone diperoxide and its nitro derivatives: a DFT study. Monatshefte FÃ¼r Chemie, 2015, 146, 1401-1408.	0.9	3
5124	Synthesis, characterization and DFT studies of two new silver(I) complexes with 3,4-lutidine. Journal of Molecular Structure, 2015, 1085, 126-136.	1.8	7
5125	Crystal Structure and Vibrational Spectra of 3-Chloro-4-Phenyl-6-(Morpholine-4-yl)-Pyridazine by Hartree-Fock and Density Functional Methods. Molecular Crystals and Liquid Crystals, 2015, 606, 216-236.	0.4	2
5126	Towards the computations of accurate spectroscopic parameters and vibrational spectra for organic compounds. Molecular Physics, 2015, 113, 1661-1673.	0.8	16
5127	Comment on â€œThe role of electrostatic induction in secondary isotope effects on acidityâ€•by E. A. Halevi, New J. Chem., 2014, 38, 3840. New Journal of Chemistry, 2015, 39, 1517-1521.	1.4	5
5128	Robust Ethylenedioxythiopheneâ€“Vinylene Oligomers from Fragile Thiopheneâ€“Vinylene Cores: Synthesis and Optical, Chemical and Electrochemical Properties of Multicharged Shapes. Chemistry - A European Journal, 2015, 21, 1713-1725.	1.7	13
5129	Theoretical study of the complexes of tyrosine and tryptophan with biologically important metal cations in aqueous solutions. Computational and Theoretical Chemistry, 2015, 1057, 7-14.	1.1	6
5130	First Principle Calculations of the Electronic and Vibrational Properties of the 3-(1,1-Dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole Molecule. Journal of Physical Chemistry A, 2015, 119, 1347-1358.	1.1	17
5131	Experimental and theoretical spectroscopic studies, HOMOâ€“LUMO, NBO analyses and thioneâ€“thiol tautomerism of a new hybrid of 1,3,4-oxadiazole-thione with quinazolin-4-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 145, 270-279.	2.0	53
5132	Application of spectroscopic methods for identification (FT-IR, Raman spectroscopy) and determination (UV, EPR) of quercetin-3-O-rutinoside. Experimental and DFT based approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 140, 132-139.	2.0	33
5133	Theoretical studies on the AnO₂ⁿ⁺ (An = U, Np; n = 1, 2) complexes with di-(2-ethylhexyl)phosphoric acid. Dalton Transactions, 2015, 44, 3227-3236.	1.6	31

#	Article	IF	Citations
5134	Theoretical analysis of vibrational modes in uranyl aquo chloro complexes. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
5135	3-Iodobenzaldehyde: XRD, FT-IR, Raman and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 145, 90-97.	2.0	4
5136	Characterization of Meldrumâ€™s acid derivative 5-(5-Ethyl-1,3,4-thiadiazol-2-ylamino)methylene-2,2-dimethyl-1,3-dioxane-4,6-dione by Raman and FT-IR spectroscopy and DFT calculations. Journal of Molecular Structure, 2015, 1091, 37-42.	1.8	20
5137	Spectroscopy studies, crystal structure and DFT calculations of 4-4{E-[(2-Fluorophenyl)imino]methyl}-2-methoxyphenol. Optics and Spectroscopy (English Translation) Tj ETQq1 1 0.784314 rgBT /Ov		
5138	Identification of the best DFT functionals for a reliable prediction of lignin vibrational properties. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	6
5139	Preparation of candidate reference materials for the determination of phosphorus containing flame retardants in styrene-based polymers. Analytical and Bioanalytical Chemistry, 2015, 407, 3023-3034.	1.9	4
5140	Computational and spectroscopic characterization of key intermediates of the Selective Catalytic Reduction cycle of NO on zeolite-supported Cu catalyst. Inorganica Chimica Acta, 2015, 430, 132-143.	1.2	16
5141	Tautomeric equilibrium in trifluoroacetaldehyde arylhydrazones. Tetrahedron, 2015, 71, 2349-2356.	1.0	17
5142	Exploring aliphatic nitro azides for plasticizers: a combined DFT and MD investigation. RSC Advances, 2015, 5, 12843-12848.	1.7	3
5143	Gas-phase acid-base properties of 1-aminocycloalkane-1-carboxylic acids from the extended kinetic method. International Journal of Mass Spectrometry, 2015, 378, 59-68.	0.7	4
5144	Infrared signature of micro-hydration in the organophosphate Sarin: an ab initio study. Journal of Molecular Modeling, 2015, 21, 182.	0.8	4
5145	Theoretical and experimental studies on the atmospheric degradation of 2-bromo-3,3,3-trifluoropropene. Physical Chemistry Chemical Physics, 2015, 17, 20543-20550.	1.3	11
5146	Nonlinear effects in infrared action spectroscopy of silicon and vanadium oxide clusters: experiment and kinetic modeling. Physical Chemistry Chemical Physics, 2015, 17, 25956-25967.	1.3	17
5147	Experimental and computational energetic study of 1-R-2-phenylindole (R = H, CH3, C2H5). Journal of Chemical Thermodynamics, 2015, 85, 129-140.	1.0	9
5148	FT-IR, FT-Raman, UV, NMR spectra and molecular structure investigation of (E)-2-(3-chloropyrazin-2-yl)-1-(3-ethyl-2, 6-diphenyl piperidin-4-ylidene) hydrazine: A combined experimental and theoretical study. Journal of Molecular Structure, 2015, 1100, 137-144.	1.8	4
5149	First-Principles Thermochemistry for the Thermal Decomposition of Titanium Tetraisopropoxide. Journal of Physical Chemistry A, 2015, 119, 8376-8387.	1.1	31
5150	Binding of Alkenes and Ionic Liquids to Bâ€“H-Functionalized Boron Nanoparticles: Creation of Particles with Controlled Dispersibility and Minimal Surface Oxidation. ACS Applied Materials & Interfaces, 2015, 7, 9991-10003.	4.0	29
5151	(R)-(â^')-2-Pyrrolidinemethanol: A combined experimental and DFT vibrational analysis of monomers, dimers and hydrogen bonding. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 860-868.	2.0	5

#	Article	IF	Citations
5152	A simple way to predict vibrational zero point energy of organophosphorus (III) compounds. Computational and Theoretical Chemistry, 2015, 1068, 13-20.	1.1	5
5153	Vibrational spectra and DFT calculations of sonderianin diterpene. Journal of Molecular Structure, 2015, 1099, 226-231.	1.8	8
5154	Theoretical study on the activity of hydrogen atom of imidazolium ring in ionic liquids. Computational and Theoretical Chemistry, 2015, 1067, 7-12.	1.1	2
5155	NMR, FT-IR, Raman and UVâ€“Vis spectroscopic investigation and DFT study of 6-Bromo-3-Pyridinyl Boronic Acid. Journal of Molecular Structure, 2015, 1099, 625-632.	1.8	15
5156	Synthesis, electronic structure investigation of 3-pentyl-2,6-di(furan-2-yl)piperidin-4-one by FT-IR, FT-Raman and UVâ€“Visible spectral studies and ab initio/DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 773-784.	2.0	15
5157	A Comparative Study of [CaEDTA]^{2â€“} and [MgEDTA]^{2â€“}: Structural and Dynamical Insights from Quantum Mechanical Charge Field Molecular Dynamics. Journal of Physical Chemistry B, 2015, 119, 8613-8622.	1.2	6
5158	Structural, spectral, thermodynamical, NLO, HOMO, LUMO and NBO analysis of fluconazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 974-991.	2.0	44
5159	Synthesis, computational and spectroscopic analysis on (E)-(4-(2-(benzo[d]thiazol-2-yl)hydrazono)-3-methyl-2,6-diphenylpiperidine-1-yl)(phenyl)methanone using DFT approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 480-489.	2.0	7
5160	Evans hole and non linear optical activity in Bis(melaminium) sulphate dihydrate: A vibrational spectral study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 151, 292-301.	2.0	3
5161	Correlating Photoacidity to Hydrogen-Bond Structure by Using the Local Oâ€“H Stretching Probe in Hydrogen-Bonded Complexes of Aromatic Alcohols. Journal of Physical Chemistry A, 2015, 119, 4800-4812.	1.1	26
5162	Synthesis, structural, spectral (FT-IR, FT-Ra, and UVâ€“Vis), thermal, and density functional studies on p-methylaniline complexes of Mn(II), Co(II), and Ni(II) bromides. Journal of Molecular Structure, 2015, 1100, 475-485.	1.8	7
5163	Raman, SERS, and DFT of Mauve Dye: Adsorption on Ag Nanoparticles. Journal of Physical Chemistry C, 2015, 119, 14297-14303.	1.5	37
5164	Molecular Design and Property Prediction for a Series of Novel Dicyclic Cyclotrimethylene Trinitramines (RDX) Derivatized as High Energy Density Materials. Journal of Physical Chemistry A, 2015, 119, 8250-8255.	1.1	35
5165	Raman spectroscopy studies of phosphorus dendrimers with phenoxy and deuterophenoxy terminal groups. Vibrational Spectroscopy, 2015, 80, 17-23.	1.2	1
5166	A DFT study of the role of the Lewis acid catalysts in the [3 + 2] cycloaddition reaction of the electrophilic nitrone isomer of methyl glyoxylate oxime with nucleophilic cyclopentene. RSC Advances, 2015, 5, 64098-64105.	1.7	22
5167	Metal selectivity by the virulence-associated yersiniabactin metallophore system. Metallomics, 2015, 7, 1011-1022.	1.0	57
5168	Synthesis, spectral characterization and DFT analysis for the validation of 2, 6 diaryl -piperidin-4-ones as potential sunscreens and UV filters. Journal of Molecular Structure, 2015, 1099, 560-566.	1.8	7
5169	Small copper-doped silicon clusters CuSin (nÂ=Â4â€“10) and their anions: structures, thermochemistry, and electron affinities. Journal of Molecular Modeling, 2015, 21, 155.	0.8	11

#	Article	IF	Citations
5170	The effect of density functional dispersion correction (DFT-D3) on lignans. Computational and Theoretical Chemistry, 2015, 1067, 60-63.	1.1	6
5171	Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand [OC^tBu₂Ph]. Inorganic Chemistry, 2015, 54, 5624-5633.	1.9	32
5172	Dispersion Corrections Improve the Accuracy of Both Noncovalent and Covalent Interactions Energies Predicted by a Density-Functional Theory Approximation. Journal of Physical Chemistry A, 2015, 119, 6703-6713.	1.1	27
5173	Hydrogen from Formic Acid via Its Selective Disproportionation over Nanodomain-Modified Zeolites. ACS Catalysis, 2015, 5, 4353-4362.	5.5	16
5174	Simple descriptors for assessing the outcome of aza-Dielsâ€“Alder reactions. RSC Advances, 2015, 5, 50729-50740.	1.7	3
5175	Peculiarities of formation of hydroxonium ion and its small clusters. Russian Journal of General Chemistry, 2015, 85, 1005-1018.	0.3	0
5176	Quantifying N-heterocyclic carbenes as umpolung catalysts in the benzoin reaction: balance between nucleophilicity and electrophilicity. New Journal of Chemistry, 2015, 39, 4508-4518.	1.4	26
5177	Vibrational analysis, NBO analysis, NMR, UVâ€“VIS, hyperpolarizability analysis of Trimethadione by density functional theory. Journal of Molecular Structure, 2015, 1099, 633-643.	1.8	8
5178	Substituent influence on the structural, vibrational and electronic properties of 2,5-dihydrothiophene-1,1-dioxide by experimental and DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 641-651.	2.0	5
5179	Elucidating Pharmacological Mechanisms of Natural Medicines by Biclustering Analysis of the Gene Expression Profile: A Case Study on Curcumin and Si-Wu-Tang. International Journal of Molecular Sciences, 2015, 16, 510-520.	1.8	13
5180	Potential energy surfaces for the HBr+ + CO2 â†' Br + HOCO+ reaction in the HBr+â€‰2Î3/2 and 2Î1/2 spin-orbit states. Journal of Chemical Physics, 2015, 142, 104302.	1.2	6
5181	A hybrid density functional study on the effects of pressure on paracetamol and aspirin polymorphs. Computational and Theoretical Chemistry, 2015, 1062, 90-98.	1.1	6
5182	Vibrational spectroscopy and density functional theory study of 4-mercaptobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 148, 369-374.	2.0	45
5183	Spectroscopic and quantum chemical analysis of a natural product â€“ Hayatin hydrochloride. Journal of Molecular Structure, 2015, 1093, 101-112.	1.8	3
5184	Quantum chemical characterization of the CF2(OH)CF2OONO2 and CF3CF2OONO2 peroxynitrates and related radicals. Computational and Theoretical Chemistry, 2015, 1062, 65-73.	1.1	3
5185	Synthesis, spectroscopic (FT-IR, FT-Raman, UV and NMR) and computational studies on 3t-pentyl-2r,6c-diphenylpiperidin-4-one semicarbazone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 148, 189-202.	2.0	20
5186	Prototypical metalâ€“oxo bonds: the reactions of Cr(PF3)6, Fe(PF3)5, and Ni(PF3)4 with oxygen. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	0
5187	Density functional theory (DFT) prediction of structural and spectroscopic parameters of cytosine using harmonic and anharmonic approximations. Structural Chemistry, 2015, 26, 1083-1093.	1.0	33

#	Article	IF	Citations
5188	Vibrational spectrum and electronic structure of C60-fullerene in an external electric field. European Physical Journal D, 2015, 69, 1.	0.6	13
5189	Multivariate characterization, modeling, and design of ionic liquid molecules. Computers and Chemical Engineering, 2015, 81, 310-322.	2.0	14
5190	On Copper(I) Fluorides, the Cuprophilic Interaction, the Preparation of Copper Nitride at Room Temperature, and the Formation Mechanism at Elevated Temperatures. Chemistry - A European Journal, 2015, 21, 3290-3303.	1.7	30
5191	Quantum-chemical studies of the structure and performance properties of 5-(1,2,4-triazol-C-yl)tetrazol-1-ols. Chemistry of Heterocyclic Compounds, 2015, 51, 153-158.	0.6	4
5192	Hydrothermal synthesis of novel cobaltâ€“organic framework, involving in-situ ligand transformation, DFT calculation, spectroscopic and thermal studies. Inorganica Chimica Acta, 2015, 432, 267-274.	1.2	3
5193	Theoretical calculations of a compound formed by Fe+3 and tris(catechol). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 592-599.	2.0	15
5194	(2E)-1-(5-Chlorothiophen-2-yl)-3-{4-[(E)-2-phenylethenyl]phenyl}prop-2-en-1-one: Synthesis, XRD, FT-IR, Raman and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 149, 385-395.	2.0	3
5195	Advances in theory and their application within the field of zeolite chemistry. Chemical Society Reviews, 2015, 44, 7044-7111.	18.7	405
5196	Spectroscopic and theoretical studies of bis(dimethylphenyl betaine) hydrochloride monohydrate. Vibrational Spectroscopy, 2015, 79, 16-23.	1.2	8
5197	Theoretical study of the structureâ€“properties relationship in new class of 2,5-di(2-thienyl)pyrrole compounds. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 1174-1183.	2.0	18
5198	Using the Alkynyl-Substituted Rhenium(I) Complex (4,4â€²-Bisphenyl-Ethynyl-2,2â€²-Bipyridyl)Re(CO)3Cl as Catalyst for CO2 Reductionâ€”Synthesis, Characterization, and Application. Electrocatalysis, 2015, 6, 185-197.	1.5	22
5199	Surface enhanced Raman scattering, natural bond orbitals and Mulliken atomic charge distribution in the normal modes of diethyldithiocarbamate cadmium (II) complex, [Cd(DDTC)2]. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 192-203.	2.0	9
5200	Crystal structure, spectroscopy, and theoretical calculations of two bis(benzimidazolyl)butane derivatives. Journal of Structural Chemistry, 2015, 56, 42-51.	0.3	0
5201	Characterization of compounds derived from copper-oxamate and imidazolium by X-ray absorption and vibrational spectroscopies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 142, 303-310.	2.0	9
5202	Combined experimental (FT-IR, UVâ€“visible spectra, NMR) and theoretical studies on the molecular structure, vibrational spectra, HOMO, LUMO, MESP surfaces, reactivity descriptor and molecular docking of Phomarin. Journal of Molecular Structure, 2015, 1096, 94-101.	1.8	44
5203	Beyond Local Group Modes in Vibrational Sum Frequency Generation. Journal of Physical Chemistry A, 2015, 119, 3407-3414.	1.1	18
5204	Resveratrol-based benzoselenophenes with an enhanced antioxidant and chain breaking capacity. Organic and Biomolecular Chemistry, 2015, 13, 5757-5764.	1.5	46
5205	Vibrational spectra, NLO analysis, and HOMOâ€“LUMO studies of 2-chloro-6-fluorobenzoic acid and 3,4-dichlorobenzoic acid by density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 147, 235-244.	2.0	5

#	Article	IF	Citations
5206	FT-IR and Raman spectroscopic and DFT studies of anti-cancer active molecule N-{(meta-ferrocenyl) Benzoyl} â€“ l -Alanine â€“ Glycine ethyl ester. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 145, 523-530.	2.0	10
5207	Proton dissociation and transfer in hydrated phosphoric acid clusters. International Journal of Quantum Chemistry, 2015, 115, 486-501.	1.0	5
5208	Using computational chemistry to design Ru photosensitizers with directional charge transfer. Coordination Chemistry Reviews, 2015, 304-305, 146-165.	9.5	55
5209	X-ray, tautomeric preference, vibrational spectra, and density functional studies on benzoxazole and benzoxazoline derivatives. Vibrational Spectroscopy, 2015, 81, 1-12.	1.2	6
5210	Structural and spectral properties of tartrato complexes of vanadium(V) from quantum chemical calculations. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	0
5211	Structure and energetics of graphene oxide isomers: ab initio thermodynamic analysis. Nanoscale, 2015, 7, 17055-17062.	2.8	17
5212	Synthesis and structural study on (1E,2E,1â€²E,2â€²E)-3,3â€²-bis[(4-bromophenyl)-3,3â€²-(4-methy-1,2-phenylene) Tj ETQq0 0 0 rgBT / Spectroscopy (English Translation of Optika I Spektroskopiya), 2015, 118, 865-881.	0.2	8
5213	Geometric description and electronic properties of the principal photosynthetic pigments of higher plants: a DFT study. Journal of Molecular Modeling, 2015, 21, 256.	0.8	3
5214	Zero-Cost Estimation of Zero-Point Energies. Journal of Physical Chemistry A, 2015, 119, 10229-10240.	1.1	10
5215	Anion-effects on electrochemical properties of ionic liquid electrolytes for rechargeable aluminum batteries. Journal of Materials Chemistry A, 2015, 3, 22677-22686.	5.2	165
5216	Vibrational scaling factors for transition metal carbonyls. Chemical Physics Letters, 2015, 640, 175-179.	1.2	59
5217	The [closo-B12H11-1-lAr]â^' zwitterion as a precursor to monosubstituted derivatives of [closo-B12H12]2â^'. Journal of Organometallic Chemistry, 2015, 798, 70-79.	0.8	18
5218	Ferutinin as a Ca²⁺complexone: lipid bilayers, conductometry, FT-IR, NMR studies and DFT-B3LYP calculations. Dalton Transactions, 2015, 44, 16506-16515.	1.6	8
5219	Calculating singlet excited states: Comparison with fast time-resolved infrared spectroscopy of coumarins. Journal of Chemical Physics, 2015, 142, 154119.	1.2	14
5220	Diruthenium Complexes with Bridging Diethynyl Polyaromatic Ligands: Synthesis, Spectroelectrochemistry, and Theoretical Calculations. Organometallics, 2015, 34, 3967-3978.	1.1	49
5221	Probing structural features of self-assembled violanthrone-79 using two dimensional infrared spectroscopy. Journal of Chemical Physics, 2015, 142, 212435.	1.2	18
5222	Competing Mechanisms, Substituent Effects, and Regioselectivities of Nickel-Catalyzed [2 + 2 + 2] Cycloaddition between Carboryne and Alkynes: A DFT Study. Journal of Organic Chemistry, 2015, 80, 9108-9117.	1.7	16
5223	Water Adsorption on Free Cobalt Cluster Cations. Journal of Physical Chemistry A, 2015, 119, 10828-10837.	1.1	24

#	Article	IF	Citations
5224	First-Principles Prediction of Enthalpies of Formation for Polycyclic Aromatic Hydrocarbons and Derivatives. Journal of Physical Chemistry A, 2015, 119, 11329-11365.	1.1	38
5225	Antioxidant Activity of Magnolol and Honokiol: Kinetic and Mechanistic Investigations of Their Reaction with Peroxyl Radicals. Journal of Organic Chemistry, 2015, 80, 10651-10659.	1.7	89
5226	Delicate Distinction between OH Groups on Proton-Exchanged H-Chabazite and H-SAPO-34 Molecular Sieves. Journal of Physical Chemistry C, 2015, 119, 24046-24055.	1.5	21
5227	Structures and vibrational spectra of Ti-MWW zeolite upon adsorption of H2O and NH3: A density functional theory study. Chinese Journal of Catalysis, 2015, 36, 1733-1741.	6.9	5
5228	Intermolecular Reactions of a Foiled Carbene with Carbonyl Compounds: The Effects of Trishomocyclopropyl Stabilization. Journal of Organic Chemistry, 2015, 80, 11877-11887.	1.7	4
5229	Estimating Ring Strain Energies of Highly Substituted Cyclohexanes with the Semi-homodesmotic Approach: Why Substantial Ring Strain Exists for Nominally Tetrahedral Ring Carbon Atoms. Journal of Organic Chemistry, 2015, 80, 10234-10243.	1.7	6
5230	Vibrational assignments, spectroscopic investigation (FT-IR and FT-Raman), NBO, MEP, HOMOâ€'LUMO analysis and intermolecular hydrogen bonding interactions of 7-fluoroisatin, 7-bromoisatin and 1-methylisatin â€' A comparative study. Journal of Molecular Structure, 2015, 1101, 189-211.	1.8	25
5231	Bond Energies and Thermochemical Properties of Ring-Opened Diradicals and Carbenes of exo-Tricyclo[5.2.1.0^{2,6}]decane. Journal of Physical Chemistry A, 2015, 119, 9857-9878.	1.1	15
5232	Multiple-Timestep ab Initio Molecular Dynamics Using an Atomic Basis Set Partitioning. Journal of Physical Chemistry A, 2015, 119, 12119-12130.	1.1	17
5233	The effect of (H2O)n (n=1â€"2) or H2S on the hydrogen abstraction reaction of H2S by OH radicals in the atmosphere. Computational and Theoretical Chemistry, 2015, 1069, 77-85.	1.1	25
5234	Raman and SERS study of N-acetyl-5-methoxytryptamine, melatoninâ€"The influence of the different molecular fragments on the SERS effect. Vibrational Spectroscopy, 2015, 80, 70-78.	1.2	14
5235	Theoretical studies on the reactions of the simplest Criegee intermediate CH2OO with CH3CHO. Computational and Theoretical Chemistry, 2015, 1074, 142-149.	1.1	14
5236	Quantum calculations of acidity constants of hydro[60]fullerenes in DMSO. Tetrahedron Letters, 2015, 56, 6008-6011.	0.7	3
5237	Toxicity Originating from Thiophene Containing Drugs: Exploring the Mechanism using Quantum Chemical Methods. Chemical Research in Toxicology, 2015, 28, 2364-2376.	1.7	35
5238	High Temperature Chemistry of Chlorinated Acenaphthylene. 3C Bay Acetylene Additions and Annealing by Five-Membered Ring Shifts. Journal of Physical Chemistry A, 2015, 119, 12767-12780.	1.1	2
5239	Non-classical CHâ‹¯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. RSC Advances, 2015, 5, 99299-99311.	1.7	36
5240	Calculation of the vibrational frequencies of carbon clusters and fullerenes with empirical potentials. Physical Chemistry Chemical Physics, 2015, 17, 3898-3908.	1.3	12
5241	Effects of Aromaticity in Cations and Their Functional Groups on the Low-Frequency Spectra and Physical Properties of Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 9173-9187.	1.2	42

#	Article	IF	Citations
5242	Vibrational spectroscopic and DFT calculation studies of 2-amino-7-bromo-5-oxo-[1]benzopyrano [2,3-b]pyridine-3 carbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 252-263.	2.0	44
5243	Substituent effect on Nâ€“H bond dissociation enthalpies of carbamates: a theoretical study. Canadian Journal of Chemistry, 2015, 93, 279-288.	0.6	3
5244	Theoretical study of dibenzotetraaza[14]annulene complexes with first row transition metals. Computational and Theoretical Chemistry, 2015, 1054, 93-99.	1.1	15
5245	Molecular structure, spectral investigation (1H NMR, 13C NMR, UVâ€“Visible, FT-IR, FT-Raman), NBO, intramolecular hydrogen bonding, chemical reactivity and first hyperpolarizability analysis of formononetin [7-hydroxy-3(4-methoxyphenyl)chromone]: A quantum chemical study. Journal of Molecular Structure, 2015, 1084, 55-73.	1.8	36
5246	11,11-Dimethyl-1,6-methano[10]annuleneâ€”An Annulene with an Ultralong CC Bond or a Fluxional Molecule?. Journal of Physical Chemistry A, 2015, 119, 1666-1682.	1.1	41
5247	Quantum chemical calculations and interpretation of electronic transitions and spectroscopic characteristics belonging to 1-(3-Mesityl-3-methylcyclobutyl)-2-(naphthalene-1-yloxy)ethanone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 899-912.	2.0	0
5248	Adsorption of 2-propanol on MgO surface: A combined experimental and theoretical study. Applied Surface Science, 2015, 327, 268-276.	3.1	14
5249	Lithium(I) in liquid ammonia: A quantum mechanical charge field (QMCF) molecular dynamics simulation study. Chemical Physics Letters, 2015, 619, 158-162.	1.2	19
5250	Spectroscopic, structural and theoretical investigation of bis(4-trimethylammoniumbenzoate) hydroiodide hydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1149-1156.	2.0	5
5251	Structural, spectroscopic and theoretical studies of dimethylphenyl betaine complex with two molecules of 2,6-dichloro-4-nitro-phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1216-1226.	2.0	10
5252	The spectroscopic (FT-IR, FT-Raman, l3C, 1H NMR and UV) and NBO analyses of 4-bromo-1-(ethoxycarbonyl)piperidine-4-carboxylic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 1-12.	2.0	23
5253	Thermodynamic study on the chemical vapor deposition of silicon nitride from the SiCl4â€“NH3â€“H2 system. Computational and Theoretical Chemistry, 2015, 1051, 93-103.	1.1	3
5254	Study on conformational stability, molecular structure, vibrational spectra, NBO, TD-DFT, HOMO and LUMO analysis of 3,5-dinitrosalicylic acid by DFT techniques. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1107-1118.	2.0	35
5255	Vibrational spectroscopic investigations of 4,4-dimethyl-2-oxazoline: A density functional theory approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1530-1542.	2.0	8
5256	Cu-catalyzed arylation of the amino group in the indazole ring: regioselective synthesis of pyrazolo-carbazoles. Organic and Biomolecular Chemistry, 2015, 13, 1481-1491.	1.5	21
5257	Synthesis and redox properties of mono-, di- and tri-metallic platinum-ethynyl complexes based on the trans-Pt(C6H4N{C6H4OCH3-4}2)(C CR)(PPh3)2 motif. Polyhedron, 2015, 86, 31-42.	1.0	6
5258	DFT investigations of the ground and excited state geometries of the benzothiazine and benzisothiazol based anticancer drugs. Journal of Saudi Chemical Society, 2015, 19, 318-321.	2.4	19
5259	Experimental and theoretical studies on IR, Raman, and UVâ€“Vis spectra of quinoline-7-carboxaldehyde. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 81-89.	2.0	26

#	Article	IF	Citations
5260	FTIR, Raman and NMR spectroscopic and DFT theoretical studies on poly(N-vinylimidazole). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 267-275.	2.0	51
5261	Syntheses, structural elucidation, thermal properties, theoretical quantum chemical studies (DFT) and biological studies of barbituricâ€“hydrazone complexes. Journal of Saudi Chemical Society, 2015, 19, 217-226.	2.4	14
5262	N-bromosuccinimide (NBS)-promoted, three-component synthesis of Î±,Î²-unsaturated isoxazol-5(4H)-ones, and spectroscopic investigation and computational study of 3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4H)-one. Research on Chemical Intermediates, 2015, 41, 7739-7773.	1.3	47
5263	Bimetallic zinc complex â€“ active species in coupling of terminal alkynes with aldehydes via nucleophilic addition/Oppenauer oxidation. Chemical Communications, 2015, 51, 576-579.	2.2	39
5264	Synthesis, conformational, spectroscopic and chemical reactivity analysis of 2-cyano-3-(1H-pyrrol-2-yl)acrylohydrazide using experimental and quantum chemical approaches. Journal of Molecular Structure, 2015, 1082, 118-130.	1.8	13
5265	Vibrational spectroscopy and density functional theory study of ninhydrin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1642-1648.	2.0	5
5266	Polarizable Empirical Force Field for Hexopyranose Monosaccharides Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2015, 119, 637-652.	1.2	67
5267	The gas-phase reactions of localized and delocalized carbanions with aryl halides: Competition between attack on the Ï€-system and the periphery. International Journal of Mass Spectrometry, 2015, 378, 31-37.	0.7	4
5268	Spectroscopic (FT-IR, FT-Raman) and quantum mechanical studies of 3t-pentyl-2r,6c-diphenylpiperidin-4-one thiosemicarbazone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 782-792.	2.0	33
5269	Temperature-responsive ionic liquid extraction and separation of the aromatic sulfur compounds. Fuel, 2015, 140, 590-596.	3.4	100
5270	Re-print of â€œGas-phase acidâ€“base properties of homocysteine, homoserine, 5-mercaptonorvaline and 5-hydroxynorvaline from the extended kinetic methodâ€: International Journal of Mass Spectrometry, 2015, 377, 73-83.	0.7	0
5271	FT-IR and FT-Raman spectra, molecular structure and first-order molecular hyperpolarizabilities of a potential antihistaminic drug, cyproheptadine HCl. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 350-360.	2.0	14
5272	Vibrational spectroscopy and density functional theory study of 3-[4,5-dimethyl-2-thiazolyl]-2,5-diphenyl-2H-tetrazolium bromide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 1-6.	2.0	4
5273	Structural and vibrational spectral investigations of melaminium glutarate monohydrate by FTIR, FT-Raman and DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 540-550.	2.0	12
5274	Conformational, structural, vibrational, electronic and quantum chemical investigations of cis-2-methoxycinnamic acid. Journal of Molecular Structure, 2015, 1080, 122-136.	1.8	6
5275	Thermoanalytical study of linkage isomerism in coordination compounds. Part 5: A DSC and DFT study on the linkage isomerization of the dinitrito and dinitro isomers of cis-tetraamminecobalt(III) complexes. Polyhedron, 2015, 85, 412-428.	1.0	6
5276	Molecular structure and vibrational analysis of Trifluoperazine by FT-IR, FT-Raman and UVâ€“Vis spectroscopies combined with DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 1184-1193.	2.0	19
5277	Design, synthesis, biological evaluation and toxicity studies of N,N-disubstituted biguanides as quorum sensing inhibitors. Medicinal Chemistry Research, 2015, 24, 1974-1987.	1.1	17

#	Article	IF	Citations
5278	Structural, vibrational, NLO, MEP, NBO analysis and DFT calculation of bis 2,5-dimethylanilinium sulfate. Journal of Molecular Structure, 2015, 1080, 176-187.	1.8	40
5279	Twisted intramolecular charge transfer and its contribution to the NLO activity of Diglycine Picrate: A vibrational spectroscopic study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 720-731.	2.0	2
5280	Molecular structure, vibrational spectral assignments, HOMOâ€“LUMO, MESP, Mulliken analysis and thermodynamic properties of 2,6-xylenol and 2,5-dimethyl cyclohexanol based on DFT calculation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 490-502.	2.0	24
5281	Spectroscopic and molecular structure investigations of 9-vinylcarbazole by DFT and ab initio method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 690-699.	2.0	10
5282	X-ray diffraction, spectroscopic characterization and quantum chemical calculations by DFT and HF of novel 2-hydroxy-12-(4-hydroxyphenyl)-9,9-dimethyl-9,10-dihydro-8 H -benzo[a]xanthen-11(12 H)-one. Journal of Molecular Structure, 2015, 1079, 21-34.	1.8	8
5283	Frequency and Zero-Point Vibrational Energy Scale Factors for Double-Hybrid Density Functionals (and Other Selected Methods): Can Anharmonic Force Fields Be Avoided?. Journal of Physical Chemistry A, 2015, 119, 1701-1714.	1.1	441
5284	Synthesis and Structural Characterization of 2-Hydroxy-5- (Phenyldiazenyl) Benzaldehyde Oxime - A Theoretical Approach. Journal of Theoretical and Computational Science, 2016, 03, .	0.1	0
5285	Infrared Spectral Investigations and Ab Initio Computations of Pharmacological Drug Goniofufurone Monoacetate. Pharmaceutica Analytica Acta, 2016, 7, .	0.2	0
5286	Tautomeric Study of Neutral, Protonated and Deprotonated Isorhodanine Based on High Level Density Functional Theory. Oriental Journal of Chemistry, 2016, 32, 2371-2381.	0.1	5
5287	Reverse Design of Ionic Liquids for the Absorption of CO2. Computer Aided Chemical Engineering, 2016, 38, 1117-1122.	0.3	1
5288	A Study of the Far Infrared Spectrum of N-Acetyl-D-Glucosamine Using THz-TDS, FTIR, and Semiempirical Quantum Chemistry Methods. Journal of Spectroscopy, 2016, 2016, 1-7.	0.6	4
5289	Spectroscopic Investigations, DFT Calculations, and Molecular Docking Studies of the Anticonvulsant (2E)-2-[3-(1H-Imidazol-1-yl)-1-phenylpropylidene]-N-(4-methylphenyl)hydrazinecarboxamide. Journal of Spectroscopy, 2016, 2016, 1-10.	0.6	4
5290	The Influence of Molecular Structure Modifications on Vibrational Properties of Some Beta Blockers: A Combined Raman and DFT Study. Journal of Spectroscopy, 2016, 2016, 1-9.	0.6	11
5291	Computational Isotope Geochemistry. Annual Reports in Computational Chemistry, 2016, 12, 117-156.	0.9	1
5292	Structural Properties and Biological Prediction of ({[(1E)-3-(1H-Imidazol-1-yl)-1-phenylpropylidene]) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.1	29
5293	Vibrational Frequencies andÂIntensities. , 2016, , 247-289.		4
5294	Comparative Theoretical Studies on Several Energetic Substituted Dioxin-imidazole Derivatives. Chinese Journal of Chemical Physics, 2016, 29, 349-357.	0.6	1
5295	Time-Resolved Infrared (TRIR) Studies of Oxycarbonylnitrenes. Journal of Organic Chemistry, 2016, 81, 6320-6328.	1.7	16

#	Article	IF	Citations
5296	Synthesis, spectroscopic characterization and DFT calculations on N-(Phenylsulfonyl)-l-asparagine (NPLAS): A potential nonlinear optical material. Optik, 2016, 127, 8782-8794.	1.4	3
5297	Vibrational spectroscopy for milk fat quantification: line shape analysis of the Raman and infrared spectra. Journal of Raman Spectroscopy, 2016, 47, 692-698.	1.2	19
5298	Formation of Oxazoles from Elusive Gold(I) Î±â€Oxocarbenes: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 9827-9834.	1.7	33
5299	Combined spectroscopic and quantum chemical studies of ezetimibe. Journal of Molecular Structure, 2016, 1125, 193-203.	1.8	12
5300	A computational chemist's guide to accurate thermochemistry for organic molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 292-310.	6.2	185
5301	Conformations of Prolylâ€“Peptide Bonds in the Bradykinin 1â€“5 Fragment in Solution and in the Gas Phase. Journal of the American Chemical Society, 2016, 138, 9224-9233.	6.6	57
5302	Temperature-dependent Raman spectroscopic studies of microstructure present in dipotassium molybdate crystals and their melts. Journal of Raman Spectroscopy, 2016, 47, 1259-1265.	1.2	17
5303	Molecular docking, TG/DTA, molecular structure, harmonic vibrational frequencies, natural bond orbital and TD-DFT analysis of diphenyl carbonate by DFT approach. Journal of Molecular Structure, 2016, 1125, 204-216.	1.8	26
5304	Analysis of furfural dissolved in transformer oil based on confocal laser Raman spectroscopy. IEEE Transactions on Dielectrics and Electrical Insulation, 2016, 23, 915-921.	1.8	60
5305	Computational (DFT and MP2) and spectral interpretations, normal coordinate analysis, force constants and barriers to internal rotations of Trimethylacetonitrile. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650034.	1.8	2
5306	Celebrating Our 120th Anniversary. Journal of Physical Chemistry B, 2016, 120, 12417-12419.	1.2	1
5307	Celebrating Our 120th Anniversary. Journal of Physical Chemistry Letters, 2016, 7, 4977-4979.	2.1	0
5308	Competitive 1,2-C Atom Shifts in the Strained Carbene Spiro[3.3]hept-1-ylidene Explained by Distinct Ring-Puckered Conformers. Journal of Organic Chemistry, 2016, 81, 12388-12400.	1.7	12
5309	Search for the structures, stabilities, IR spectra, and thermodynamic properties of the asymmetric clusters (HClBN3) n (n = 1â€“6). Russian Journal of Physical Chemistry A, 2016, 90, 2541-2549.	0.1	2
5310	The investigation of structure and IR spectra for hydrated potassium ion clusters K+(H2O)n=1â€“16 by density functional theory*. European Physical Journal D, 2016, 70, 1.	0.6	9
5311	Vibrational smearing of the electron density as function of the strength and directionality of interatomic interactions: nonvalent interactions of a nitro group within an island-type crystal [Fe(NO)2(SC6H4NO2)]2. Russian Chemical Bulletin, 2016, 65, 1473-1487.	0.4	8
5312	Analysis of methyl formate dissolved in transformer oil by laser Raman spectroscopy. , 2016, , .		2
5313	Modeling collision energy transfer in APCI/CID mass spectra of PAHs using thermal-like post-collision internal energy distributions. Journal of Chemical Physics, 2016, 145, 164311.	1.2	3

#	Article	IF	Citations
5314	Analysis of acetic acid dissolved in transformer oil based on laser Raman spectroscopy. , 2016, , .		5
5315	Hydrolytic Glycosidic Bond Cleavage in RNA Nucleosides: Effects of the 2â€²-Hydroxy Group and Acidâ€“Base Catalysis. Journal of Physical Chemistry B, 2016, 120, 12795-12806.	1.2	12
5316	Theoretical study of the decomposition pathways and products of C5- perfluorinated ketone (C5 PFK). AIP Advances, 2016, 6, .	0.6	50
5317	Analytic second derivatives from auxiliary density perturbation theory. Journal of Chemical Physics, 2016, 145, 224103.	1.2	17
5318	Celebrating Our 120th Anniversary. Journal of Physical Chemistry A, 2016, 120, 9679-9681.	1.1	3
5319	Celebrating Our 120th Anniversary. Journal of Physical Chemistry C, 2016, 120, 27731-27733.	1.5	0
5320	Transition from Molecular Vibrations to Phonons in Atomically Precise Cadmium Selenide Quantum Dots. Journal of the American Chemical Society, 2016, 138, 16754-16763.	6.6	36
5321	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. Journal of Chemical Physics, 2016, 145, .	1.2	60
5322	A theoretical study of the spectroscopic properties of B2H6 and of a series of B<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mtext>H</mml:mtext><mml:mi>y</mml:mi><mml:mrow><mml:mi>z</mml:mi><mml:mi><</mml:mi></mml:mrow></mml:msubsup></mml:mrow></mml:math> species (xÂ=Â1â^'12, yÂ=Â3â^'14, zÂ=Â0â^'2): From BH3 to B12<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mtext>H</mml:mtext></mml:msubsup></mml:mrow></mml:math>. International Journal of Hydrogen En	3.8	31
5323	Early Oxidation Processes on the Greigite Fe₃S₄(001) Surface by Water: A Density Functional Theory Study. Journal of Physical Chemistry C, 2016, 120, 8616-8629.	1.5	32
5324	Characteristic infrared intensities of carbonyl stretching vibrations. Physical Chemistry Chemical Physics, 2016, 18, 17575-17585.	1.3	17
5325	A Metal and Base-Free Chemoselective Primary Amination of Boronic Acids Using Cyanamidyl/Arylcyanamidyl Radical as Aminating Species: Synthesis and Mechanistic Studies by Density Functional Theory. Journal of Organic Chemistry, 2016, 81, 5120-5127.	1.7	26
5326	Experimental and DFT computational studies of L-alanine cadmium chloride crystals. International Journal of Computational Materials Science and Engineering, 2016, 05, 1630001.	0.5	0
5327	Thermodynamics of Anharmonic Systems: Uncoupled Mode Approximations for Molecules. Journal of Chemical Theory and Computation, 2016, 12, 2861-2870.	2.3	38
5328	Chlorine Para-Substitution of 1-Phenylethanol: Resonant Photoionization Spectroscopy and Quantum Chemical Calculations of Hydrated and Diastereomeric Complexes. Journal of Physical Chemistry A, 2016, 120, 5023-5031.	1.1	1
5329	Phosphine-Based Z-Selective Ruthenium Olefin Metathesis Catalysts. Organometallics, 2016, 35, 1825-1837.	1.1	30
5330	Electrochemical and Spin-Trapping Properties of para-substituted Î±-Phenyl-N-tert-butyl Nitrones. Electrochimica Acta, 2016, 193, 231-239.	2.6	15
5331	Vibrational spectra, DFT calculations, conformational stabilities and assignments of the fundamentals of the 1-butylpiperazine. Journal of Molecular Structure, 2016, 1122, 324-330.	1.8	10

#	Article	IF	Citations
5332	Structure, spectroscopy and DFT calculations of 1,2-di(3-hydroxymethylpyridinium)ethane dibromide. Journal of Molecular Structure, 2016, 1120, 341-350.	1.8	4
5333	Vapor pressures, thermodynamic stability, and fluorescence properties of three 2,6-alkyl naphthalenes. Chemosphere, 2016, 146, 173-181.	4.2	8
5334	Quantum Mechanical and Molecular Dynamics Studies of the Reaction Mechanism of the Nucleophilic Substitution at the Si Atom. Journal of Physical Chemistry A, 2016, 120, 2636-2646.	1.1	6
5335	Density functional efficiency in the calculations of vibrational frequencies and molecular structures of Î²-diketones. Journal of Structural Chemistry, 2016, 57, 65-75.	0.3	2
5336	DFT studies on the structural and vibrational properties of polyenes. Journal of Molecular Modeling, 2016, 22, 101.	0.8	21
5337	Morphology and molecular arrangement of perylene-3,4,9,10-(n-pentylester) in thin layers obtained by zone-casting. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 165, 15-20.	2.0	1
5338	A reduced dimensionality model of torsional vibrations in star molecules. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 77, 131-137.	1.3	0
5339	Synthesis, crystal structures, spectroscopic analysis and DFT calculations of 2-ethoxy-1-naphtaldehyde and (E)-N-((2-ethoxynaphthalen-1-yl)methylene)-3-methylaniline. Journal of Molecular Structure, 2016, 1118, 194-202.	1.8	11
5340	Mechanism for Ag (I)-catalyzed decarboxylative chlorination: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
5341	Infrared Spectrum of Toluene: Comparison of Anharmonic Isolated-Molecule Calculations and Experiments in Liquid Phase and in a Ne Matrix. Journal of Physical Chemistry A, 2016, 120, 3380-3389.	1.1	16
5342	Long-Lived Charge Transfer Excited States in HBC-Polypyridyl Complex Hybrids. Inorganic Chemistry, 2016, 55, 4710-4719.	1.9	19
5343	[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study. Computational and Theoretical Chemistry, 2016, 1087, 36-47.	1.1	2
5344	Theoretical studies and spectroscopic characterization of novel 4-methyl-5-((5-phenyl-1,3,4-oxadiazol-2-yl)thio)benzene-1,2-diol. Journal of Molecular Structure, 2016, 1119, 18-24.	1.8	70
5345	Structural analysis of bioinspired nano materials with synchrotron far IR spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 11467-11473.	1.3	7
5346	Structure, IR and Raman spectra of phosphotrihydrazide studied by DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 166, 19-24.	2.0	8
5347	Uncatalyzed thermal gas phase aziridination of alkenes by organic azides. Part I: Mechanisms with discrete nitrene species. Journal of Chemical Sciences, 2016, 128, 681-693.	0.7	4
5348	Spectroscopic and theoretical study of the charge transfer interaction effect on the vibrational modes and nonlinear optical properties in l-asparaginium nitrate crystal. Journal of Molecular Structure, 2016, 1120, 79-85.	1.8	7
5349	Theoretical design of bicyclo[2.2.1]heptane derivatives for high-energy density compounds with low impact sensitivity. Computational and Theoretical Chemistry, 2016, 1095, 54-64.	1.1	10

#	Article	IF	Citations
5350	Predicting Infrared Spectra of Nerve Agents Using Density Functional Theory. Journal of Applied Spectroscopy, 2016, 83, 673-681.	0.3	4
5351	Theoretical calculation of oxygen equilibrium isotope fractionation factors involving various NO molecules, OH, and H2O and its implications for isotope variations in atmospheric nitrate. Geochimica Et Cosmochimica Acta, 2016, 191, 89-101.	1.6	94
5352	Implementation of Molecular Gradients for Local Hybrid Density Functionals Using Seminumerical Integration Techniques. Journal of Chemical Theory and Computation, 2016, 12, 4254-4262.	2.3	33
5353	A DFT study of the mechanism and the regioselectivity of [3 + 2] cycloaddition reactions of nitrile oxides with Î±,Î²-acetylenic aldehyde. Molecular Physics, 2016, 114, 3193-3200.	0.8	4
5354	Prediction of equilibrium distributions of isotopologues for methane, ethane and propane using density functional theory. Geochimica Et Cosmochimica Acta, 2016, 190, 1-12.	1.6	42
5355	Atmospheric pressure plasma treatment study for 2-((4-Hydroxyphenyl)Diazenil)Benzene-1,3,5-Triol molecule. Journal of Molecular Liquids, 2016, 222, 1128-1138.	2.3	2
5356	Infrared Spectroscopy of NaCl(CH₃OH)_n Complexes in Helium Nanodroplets. Journal of Physical Chemistry A, 2016, 120, 8085-8092.	1.1	17
5357	Temperature-Induced Neutral-Ionic Phase Transition in the (EDT-TTF-I₂)₂TCNQF Mixed-Stack Charge-Transfer Salt. Journal of Physical Chemistry C, 2016, 120, 23740-23747.	1.5	4
5358	Intramolecular Reactions of Tethered Furanâ€Based Bis(p â€quinodimethanes). European Journal of Organic Chemistry, 2016, 2016, 5559-5568.	1.2	5
5359	Surface chemistry of carbon dioxide revisited. Surface Science Reports, 2016, 71, 595-671.	3.8	132
5360	Variable-temperature X-ray diffraction study of structural parameters of NH---S hydrogen bonds in triethylammonium and pyridinium silanethiolates. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 763-770.	0.5	3
5361	Effect of Bridge Alteration on Ground- and Excited-State Properties of Ruthenium(II) Complexes with Electron-Donor-Substituted Dipyrido[3,2-a:2â€²,3â€²-c]phenazine Ligands. Inorganic Chemistry, 2016, 55, 11170-11184.	1.9	37
5362	Rational Control of Conformational Distributions and Mixedâ€Valence Characteristics in Diruthenium Complexes. Chemistry - A European Journal, 2016, 22, 16138-16146.	1.7	38
5363	Fractional molecular charge studied via molecular vibrational properties. Specific aspects in Jahnâ€“Teller active molecular species. RSC Advances, 2016, 6, 93715-93721.	1.7	8
5364	Silicon Tetrahydroborate and Silylene Dihydroborate with Interelement Bâ€“Hâ€“Si and Bâ•Si Bonds. Organometallics, 2016, 35, 3272-3280.	1.1	13
5365	Generation of C7H7+ cations with isomerization reactions. Computational and Theoretical Chemistry, 2016, 1091, 150-164.	1.1	9
5366	Gas-phase study of metal complexes with redox-active ligands. International Journal of Mass Spectrometry, 2016, 407, 92-100.	0.7	14
5369	Origins of the Relative Stabilities of Anhydrous and Hydrated <scp>d</scp>-Mannitol Crystals. Journal of Physical Chemistry A, 2016, 120, 6629-6636.	1.1	15

#	Article	IF	Citations
5370	Vibrational and electronic profiles, molecular docking and biological prediction of 5-methoxy-1-[(5-methoxy- 1H-indol-2-yl)methyl]-1H-indole: Experimental and theoretical investigations. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650046.	1.8	0
5371	Vibrational zero point energy of organophosphorus(V) compounds. Vibrational Spectroscopy, 2016, 86, 173-180.	1.2	2
5372	C₂H₄ adsorption on Cu(210), revisited: bonding nature and coverage effects. Physical Chemistry Chemical Physics, 2016, 18, 23621-23627.	1.3	6
5373	Raman Line Imaging of Poly(Îµ-caprolactone)/Carbon Dioxide Solutions at High Pressures: A Combined Experimental and Computational Study for Interpreting Intermolecular Interactions and Free-Volume Effects. Journal of Physical Chemistry B, 2016, 120, 9115-9131.	1.2	7
5374	Size dependent magnetic and optical properties in diamond shaped graphene quantum dots: A DFT study. Journal of Physics and Chemistry of Solids, 2016, 99, 34-42.	1.9	46
5375	Gas phase vibrational spectroscopy of the protonated water pentamer: the role of isomers and nuclear quantum effects. Physical Chemistry Chemical Physics, 2016, 18, 26743-26754.	1.3	53
5376	Hydrogen sulfide removal from hydrocarbon gas mixtures by diethanolamine (computer simulation). Petroleum Chemistry, 2016, 56, 616-622.	0.4	4
5377	Disproportional proton tautomers of pipecolic acid and 2,6-dichloro-4-nitrophenol in a 2:3 complex. Chemical Physics, 2016, 477, 88-95.	0.9	6
5378	Effect of Hydrogen Bonds on the Vibrational Relaxation and Orientational Relaxation Dynamics of HN₃ and N₃^{â€“} in Solutions. Journal of Physical Chemistry B, 2016, 120, 9723-9731.	1.2	3
5379	Synthesis, characterization, and third-order nonlinear optical properties of a new neolignane analogue. RSC Advances, 2016, 6, 79215-79227.	1.7	31
5380	Matrix Infrared Spectra and Quantum Chemical Calculations of Ti, Zr, and Hf Dihydride Phosphinidene and Arsinidene Molecules. Inorganic Chemistry, 2016, 55, 8786-8793.	1.9	26
5381	Calculation of Raman parameters of real-size zigzag (n, 0) single-walled carbon nanotubes using finite-size models. Physical Chemistry Chemical Physics, 2016, 18, 25058-25069.	1.3	13
5382	Differential Permeability of Proton Isotopes through Graphene and Graphene Analogue Monolayer. Journal of Physical Chemistry Letters, 2016, 7, 3395-3400.	2.1	40
5383	Quantitative First-Principles Kinetic Modeling of the Aza-Michael Addition to Acrylates in Polar Aprotic Solvents. Journal of Organic Chemistry, 2016, 81, 12291-12302.	1.7	31
5384	Generation, Characterization, and Reactions of Thionium Ions Based on the Indirect Cation Pool Method. Bulletin of the Chemical Society of Japan, 2016, 89, 61-66.	2.0	12
5385	Vibrational Signatures of Electronic Properties in Oxidized Water: Unraveling the Anomalous Spectrum of the Water Dimer Cation. Journal of the American Chemical Society, 2016, 138, 11936-11945.	6.6	22
5386	The computational prediction of Raman and ROA spectra of charged histidine tautomers in aqueous solution. Physical Chemistry Chemical Physics, 2016, 18, 27377-27389.	1.3	4
5387	Multiâ€Pathway Consequent Chemoselectivities of CpRuCl(PPh₃)₂/Melâ€Catalysed Norbornadiene Alkyne Cycloadditions. Chemistry - A European Journal, 2016, 22, 15396-15403.	1.7	6

#	Article	IF	Citations
5388	Sterically (un)encumbered mer-tridentate N-heterocyclic carbene complexes of titanium(<scp>iv</scp>) for the copolymerization of cyclohexene oxide with CO₂. Dalton Transactions, 2016, 45, 14734-14744.	1.6	31
5389	Tunable Design of Gold(III)â€“Doxorubicin Complexâ€“PEGylated Nanocarrier. The Golden Doxorubicin for Oncological Applications. ACS Applied Materials & Interfaces, 2016, 8, 19946-19957.	4.0	49
5390	Experimental and theoretical studies on a novel helical architecture driven by hydrogen and halogen bonding interactions. Journal of Chemical Sciences, 2016, 128, 1895-1904.	0.7	1
5391	Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea. RSC Advances, 2016, 6, 111997-112015.	1.7	46
5392	Substituent Effects on the Photodeprotection Reactions of Selected Ketoprofen Derivatives in Phosphate Buffered Aqueous Solutions. Scientific Reports, 2016, 6, 21606.	1.6	1
5393	Theoretical investigation on two different mechanisms of fulleropyrrolidine formation. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	2
5395	The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites. Journal of Molecular Modeling, 2016, 22, 270.	0.8	12
5396	Dynamics of proton transfer in imidazole hydrogen-bond chains. RSC Advances, 2016, 6, 99391-99403.	1.7	7
5397	A computational study on the thermal decomposition of di(tri)thiocarbonates. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650061.	1.8	4
5398	- Controlling the Moleculeâ€“Electrode Contact in Single-Molecule Devices. , 2016, , 132-169.		1
5399	Synthesis, Structure, and Anticancer Activity of Areneâ€“Ruthenium(II) Complexes with Acylpyrazolones Bearing Aliphatic Groups in the Acyl Moiety. Inorganic Chemistry, 2016, 55, 11770-11781.	1.9	59
5400	Substituent effects on gasâ€phase homolytic Feâ€“O and Feâ€“S bond energies of mâ€Câ€₆H₄OFe(CO)₂(Î·⁵â€C₅H₅) and mâ€Câ€₆H₄SFe(CO)₂(Î·⁵â€C₅H₅) studied using Hartreeâ€“Fock and density functional theory methods. Journal of Physical Organic Chemistry, 2016, 29, 172-184.	0.9	5
5401	Extraordinarily Strong Interlayer Interaction in 2D Layered PtS₂. Advanced Materials, 2016, 28, 2399-2407.	11.1	415
5402	NIR-Raman spectrum and DFT calculations of okadaic acid DSP marine biotoxin microprobe. Journal of Raman Spectroscopy, 2016, 47, 636-642.	1.2	7
5403	Thermal reaction of the ionic liquid 1,2-dimethyl-(3-aminoethyl) imidazolium tetrafluoroborate: a kinetic and theoretical study. Journal of Molecular Modeling, 2016, 22, 138.	0.8	6
5404	Structural and vibrational study of graphene oxide via coronene based models: theoretical and experimental results. Materials Research Express, 2016, 3, 055020.	0.8	18
5405	Theoretical and thermogravimetric study on the thermo-oxidative decomposition of Quinolin-65 as an asphaltene model molecule. RSC Advances, 2016, 6, 54418-54430.	1.7	20
5406	Unraveling the real structures of solution-based and surface-bound poly(3-hexylthiophene) (P3HT) oligomers: a combined theoretical and experimental study. RSC Advances, 2016, 6, 56174-56182.	1.7	21

#	Article	IF	Citations
5407	Molecular modelling of tantalum penta-halides during hydrolysis and oxidation reactions. Computational and Theoretical Chemistry, 2016, 1090, 112-119.	1.1	12
5408	A Laser Flash Photolysis Study of Azo-Compound Formation from Aryl Nitrenes at Room Temperature. Journal of Physical Chemistry A, 2016, 120, 4267-4276.	1.1	6
5409	Design and selection of triazole-based compounds with high energetic properties and stabilities. Journal of Chemical Sciences, 2016, 128, 1223-1236.	0.7	6
5410	Transition State Structure of RNA Depurination by Saporin L3. ACS Chemical Biology, 2016, 11, 1383-1390.	1.6	6
5411	Force dependence of the infrared spectra of polypropylene calculated with density functional theory. Polymer Degradation and Stability, 2016, 128, 294-299.	2.7	9
5412	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of Î±-Pinene on Silica. Journal of Physical Chemistry C, 2016, 120, 12578-12589.	1.5	29
5413	Vibrational spectroscopic and DFT calculation studies of a new organicâ€“inorganic compound of bis (4-acetylanilinium) tetrachlorocadmiate (II). Physica E: Low-Dimensional Systems and Nanostructures, 2016, 84, 1-9.	1.3	7
5414	A combined experimental and theoretical approach to study SmC â†' NcybC phase transition in a four-ring bent-core liquid crystal. New Journal of Chemistry, 2016, 40, 6834-6847.	1.4	11
5415	Raman modeâ€selective spectroscopic imaging of coenzyme and enzyme redox states. Journal of Raman Spectroscopy, 2016, 47, 801-807.	1.2	9
5416	Modeling red coral (Corallium rubrum) and African snail (Helixia aspersa) shell pigments: Raman spectroscopy versus DFT studies. Journal of Raman Spectroscopy, 2016, 47, 908-916.	1.2	10
5417	Hydrogenase Enzymes and Their Synthetic Models: The Role of Metal Hydrides. Chemical Reviews, 2016, 116, 8693-8749.	23.0	473
5418	Vibrational Signatures of Conformer-Specific Intramolecular Interactions in Protonated Tryptophan. Journal of Physical Chemistry A, 2016, 120, 5598-5608.	1.1	32
5419	Energetic Properties of Rocket Propellants Evaluated through the Computational Determination of Heats of Formation of Nitrogenâ€Rich Compounds. Chemistry - an Asian Journal, 2016, 11, 730-744.	1.7	6
5420	Does the mâ€Nitrotoluene Cation Isomerize to the oâ€•and pâ€Isomers before Dissociation?. Bulletin of the Korean Chemical Society, 2016, 37, 977-980.	1.0	0
5421	Synthesis, spectroscopic and theoretical studies of (R/S)-piperidinium-3-carboxylic acid 2,6-dichloro-4-nitrophenolate. Vibrational Spectroscopy, 2016, 83, 46-56.	1.2	6
5422	Vibrational anharmonicity of small gold and silver clusters using the VSCF method. Physical Chemistry Chemical Physics, 2016, 18, 529-549.	1.3	10
5423	Carbon monoxide protonation in condensed phases and bonding to surface superacidic BrÃ¸nsted centers. Physical Chemistry Chemical Physics, 2016, 18, 4871-4880.	1.3	16
5424	Mechanism and enantioselectivity in Î±-alkylation of carbonyl compounds via photoredox organocatalysis: A DFT study. Computational and Theoretical Chemistry, 2016, 1078, 113-122.	1.1	5

#	Article	IF	Citations
5425	Isotope Effects Reveal the Mechanism of Enamine Formation in <scp>l</scp>-Proline-Catalyzed Î±-Amination of Aldehydes. Journal of the American Chemical Society, 2016, 138, 1756-1759.	6.6	27
5426	Fluorescence-suppressed time-resolved Raman spectroscopy of pharmaceuticals using complementary metal-oxide semiconductor (CMOS) single-photon avalanche diode (SPAD) detector. Analytical and Bioanalytical Chemistry, 2016, 408, 761-774.	1.9	40
5427	Stereochemical analysis of (+)-limonene using theoretical and experimental NMR and chiroptical data. Journal of Molecular Structure, 2016, 1106, 141-153.	1.8	13
5428	Molecular structure, NMR, UVâ€“Visible, vibrational spectroscopic and HOMO, LUMO analysis of (E)-1-(2,) Tj ETQq1 1 0.784314 rgBT /O hydrazine by DFT method. Journal of Molecular Structure, 2016, 1106, 277-285.	1.8	14
5429	Characterisation of 1,3-diammonium propylselenate monohydrate by XRD, FT-IR, FT-Raman, DSC and DFT studies. Journal of Molecular Structure, 2016, 1107, 220-230.	1.8	11
5430	Structure analysis and spectroscopic characterization of 2-Fluoro-3-Methylpyridine-5-Boronic Acid with experimental (FT-IR, Raman, NMR and XRD) techniques and quantum chemical calculations. Journal of Molecular Structure, 2016, 1108, 103-111.	1.8	14
5431	Asymmetric oxidation of vinyl- and ethynyl terthiophene ligands in triruthenium complexes. Dalton Transactions, 2016, 45, 768-782.	1.6	19
5432	Vibrational spectroscopic, molecular docking and density functional theory studies on 2-acetylamino-5-bromo-6-methylpyridine. European Journal of Pharmaceutical Sciences, 2016, 82, 115-125.	1.9	63
5433	Luminescent Cages: Pendant Emissive Units on [Pd₂L₄]⁴⁺ â€œClickâ€• Cages. Inorganic Chemistry, 2016, 55, 3440-3447.	1.9	52
5434	Gasâ€Phase Studies of Formamidopyrimidine Glycosylase (Fpg) Substrates. Chemistry - A European Journal, 2016, 22, 3881-3890.	1.7	9
5435	Additive <scp>CHARMM</scp> force field for naturally occurring modified ribonucleotides. Journal of Computational Chemistry, 2016, 37, 896-912.	1.5	63
5436	Hydration of ion exchangers: Thermodynamics and quantum chemistry calculations. III. The state of the proton and water molecules in hydrogen form of sulfostyrene ion exchangers. Reactive and Functional Polymers, 2016, 102, 156-164.	2.0	6
5437	Combined experimental and theoretical studies on 4-(2-hydroxy-3-morpholin-4-yl-propoxy)-chromen-2-one. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650017.	1.8	0
5438	Spectroscopic studies of the 1:1 complex of piperidine-4-carboxylic acid (isonipecotic acid) with 2,6-dichloro-4-nitrophenol. Vibrational Spectroscopy, 2016, 85, 35-42.	1.2	8
5439	Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. Journal of Physical Chemistry B, 2016, 120, 1919-1927.	1.2	17
5440	[N(CH3)3H]2CuCl4: Ab initio calculations and characterization of phase transitions by Raman spectroscopy. Journal of Molecular Structure, 2016, 1114, 161-170.	1.8	9
5441	Vapor Pressures of Four Methyl Esters of Substituted Benzoic Acids. The Intermolecular Hydrogen Bond OHÂ·Â·Â·O. Journal of Chemical & Engineering Data, 2016, 61, 1012-1020.	1.0	16
5442	Functionally substituted isoxazoles and isothiazoles: Synthesis, palladium(II) complexes and their catalytic activity. Russian Journal of General Chemistry, 2016, 86, 68-81.	0.3	22

#	Article	IF	Citations
5443	Layered double hydroxide and sulindac coiled and scrolled nanoassemblies for storage and drug release. RSC Advances, 2016, 6, 16419-16436.	1.7	45
5444	A theoretical study of the regio- and stereoselectivities of non-polar 1,3-dipolar cycloaddition reaction betweenC-diethoxyphosphoryl-N-methylnitrone andN-(2-fluorophenyl)acrylamide. Molecular Physics, 2016, 114, 663-670.	0.8	9
5445	A study of hydrogen bonded vibrational spectra of (R)-(+)-Methylsuccinic acid, as aided by DFT dimer analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 160, 19-25.	2.0	6
5446	Predicting the structure and vibrational frequencies of ethylene using harmonic and anharmonic approaches at the Kohnâ€“Sham complete basis set limit. Journal of Molecular Modeling, 2016, 22, 42.	0.8	21
5447	Synthesis, click reaction, molecular structure, spectroscopic and DFT computational studies on 3-(2,6-bis(trifluoromethyl)phenoxy)-6-(prop-2-yn-1-yloxy)phthalonitrile. Journal of Molecular Structure, 2016, 1113, 88-98.	1.8	10
5448	Crystal structure, phase transitions, and IR spectroscopic investigations of a new sulfate templated by diethylene triammonium. Phosphorus, Sulfur and Silicon and the Related Elements, 2016, 191, 765-771.	0.8	1
5449	Thermodynamic properties of alkyl 1 H -indole carboxylate derivatives: A combined experimental and computational study. Journal of Chemical Thermodynamics, 2016, 97, 70-82.	1.0	7
5450	Spectroscopic and quantum chemical studies of molecular geometry, frontier molecular orbital, NLO, NBO analysis of 7-chloro-1 methyl-5-phenyl-1,5-dihydro-benzo[1,4]diazepine-2,4-dione. Optik, 2016, 127, 5055-5064.	1.4	5
5451	Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. Journal of Chemical Theory and Computation, 2016, 12, 1905-1918.	2.3	20
5452	First-Principles Study of the Structural, Electronic, Dynamic, and Mechanical Properties of HOPG and Diamond: Influence of Exchangeâ€“Correlation Functionals and Dispersion Interactions. Journal of Physical Chemistry C, 2016, 120, 5083-5100.	1.5	23
5453	Formation of Hexamethylenetetramine (HMT) from HCHO and NH3 â€“ Relevance to Prebiotic Chemistry and B3LYP Consideration. Origins of Life and Evolution of Biospheres, 2016, 46, 223-231.	0.8	6
5454	Structure of the complex of dimethylphenyl betaine with dichloroacetic acid studied by X-ray diffraction, DFT calculations, infrared and Raman spectra. Vibrational Spectroscopy, 2016, 84, 92-100.	1.2	15
5455	Insights into the mechanism of silver-catalyzed decarboxylative fluorination. Computational and Theoretical Chemistry, 2016, 1082, 11-20.	1.1	26
5456	Molecular structures, charge distributions, and vibrational analyses of the tetracoordinate Cu(II), Zn(II), Cd(II), and Hg(II) bromide complexes of p-toluidine investigated by density functional theory in comparison with experiments. Journal of Molecular Structure, 2016, 1116, 292-302.	1.8	7
5457	FT-Raman, FT-IR spectroscopic and DFT studies of hexaphenoxycyclotriphosphazene. Journal of Molecular Structure, 2016, 1115, 124-135.	1.8	4
5458	Thermal desorption of molecular oxygen from SnO 2 (110) surface: Insights from first-principles calculations. Journal of Physics and Chemistry of Solids, 2016, 89, 15-22.	1.9	14
5459	Syntheses, spectroscopic investigation and electronic properties of two sulfonamide derivatives: A combined experimental and quantum chemical approach. Journal of Molecular Structure, 2016, 1108, 496-507.	1.8	26
5460	Interlayer electronic hybridization leads to exceptional thickness-dependent vibrational properties in few-layer black phosphorus. Nanoscale, 2016, 8, 2740-2750.	2.8	153

#	Article	IF	Citations
5461	Cyclopentadienone Oxidation Reaction Kinetics and Thermochemistry for the Alcohols, Hydroperoxides, and Vinylic, Alkoxy, and Alkylperoxy Radicals. Journal of Physical Chemistry A, 2016, 120, 433-451.	1.1	12
5462	Analytic calculations of anharmonic infrared and Raman vibrational spectra. Physical Chemistry Chemical Physics, 2016, 18, 4201-4215.	1.3	27
5463	A DFT analysis of the molecular structure, vibrational spectra and other molecular properties of 5-nitrouracil and comparison with uracil. Journal of Molecular Structure, 2016, 1106, 300-315.	1.8	9
5464	Vibrational spectroscopic, structural and quantum chemical studies on N-phenyl-3-pyridinecarboxamide. Journal of Molecular Structure, 2016, 1107, 254-265.	1.8	15
5465	Basis set dependence using DFT/B3LYP calculations to model the Raman spectrum of thymine. Journal of Bioinformatics and Computational Biology, 2016, 14, 1650002.	0.3	17
5466	Ferrocenyl-substituted dinuclear Cu(II) complex: Synthesis, spectroscopy, electrochemistry, DFT calculations and catecholase activity. Journal of Molecular Structure, 2016, 1106, 331-342.	1.8	5
5467	Weak hydrogen bonding interaction Sâ€“HÂ·Â·Â·OC studied by FT-IR spectroscopy and DFT calculations. Journal of Molecular Structure, 2016, 1103, 217-223.	1.8	21
5468	Solvation of coumarin6 studied by vibrational spectroscopy and density functional theory. Journal of Molecular Structure, 2016, 1106, 170-180.	1.8	2
5469	Synthesis, characterization and DFT studies of diethyl 4-hydroxy-6-nitro-4H-chromene-2,3-dicarboxylate. Journal of Molecular Structure, 2016, 1105, 118-127.	1.8	12
5470	Molecular structure, vibrational spectral assignments (FT-IR and FT-Raman), UV-Vis, NMR, NBO, HOMO-LUMO and NLO properties ofÂ3t-pentyl-2r,6c-diphenylpiperidin-4-one picrate based on DFT calculations. Journal of Molecular Structure, 2016, 1105, 225-237.	1.8	31
5471	Delivery system for mefenamic acid based on the nanocarrier layered double hydroxide: Physicochemical characterization and evaluation of anti-inflammatory and antinociceptive potential. Materials Science and Engineering C, 2016, 58, 629-638.	3.8	42
5472	Infrared, Raman and NMR spectral analysis, vibrational assignments, normal coordinate analysis, and quantum mechanical calculations of 2-Amino-5-ethyl-1,3,4-thiadiazole. Journal of Molecular Structure, 2016, 1103, 70-81.	1.8	11
5473	A theoretical study on the structure of thiazolidine-2,4-dione and its 5-substituted derivatives in the gas phase. Implications for the thiazolidine-2,4-dione -water complex. Arabian Journal of Chemistry, 2016, 9, 616-625.	2.3	16
5474	Mechanistic Study on Electronic Excitation Dissociation of the Cellobiose-Na⁺ Complex. Journal of the American Society for Mass Spectrometry, 2016, 27, 319-328.	1.2	24
5475	The influence of the halogen atoms and acetyl group on vapour pressures and related properties of the p -haloacetophenones. Journal of Chemical Thermodynamics, 2016, 92, 118-125.	1.0	16
5476	Synthesis, crystal structure, biological activity and theoretical calculations of novel isoxazole derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 226-232.	2.0	16
5477	Tautomeric conversion, vibrational spectra, and density functional studies on peripheral sulfur derivatives of benzothiazole and benzothiazoline isomers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 181-191.	2.0	6
5478	Symmetry, Conjugated System, and N-oxides in 2,4,6-Trinitro-1,3,5-triazine-1,3,5-trioxides: A New Design Concept for Energetic Oxidizers. Journal of Energetic Materials, 2017, 35, 63-76.	1.0	0

#	Article	IF	Citations
5479	Density functional theory study of substituent effects on gasâ€phase heterolytic Feâ€“O and Feâ€“S bond energies of mâ€Câ€₆H₄OFe(CO)₂(Î·⁵â€C₅H₅) and mâ€Câ€₆H₄SFe(CO)₂(Î·⁵â€C₅H₅). Journal of Physical Organic Chemistry, 2017, 30, e3582.	0.9	3
5480	Giant Anisotropic Raman Response of Encapsulated Ultrathin Black Phosphorus by Uniaxial Strain. Advanced Functional Materials, 2017, 27, 1600986.	7.8	100
5481	Thiol-Michael addition in polar aprotic solvents: nucleophilic initiation or base catalysis?. Polymer Chemistry, 2017, 8, 1341-1352.	1.9	22
5482	Mechanistic study on silver-catalyzed direct amination of unactivated C H bond. Journal of Organometallic Chemistry, 2017, 832, 1-8.	0.8	7
5483	Isostructural zinc and cadmium silanethiolates with bridging biimidazole co-ligands â€“ Enhanced luminescence of zinc complex. Inorganica Chimica Acta, 2017, 459, 22-28.	1.2	5
5484	Molecular Doping of a High Mobility Diketopyrrolopyrroleâ€“Dithienylthieno[3,2-b]thiophene Donorâ€“Acceptor Copolymer with F6TCNNQ. Macromolecules, 2017, 50, 914-926.	2.2	66
5485	Molecular structure and spectral properties of 4-(1-pyridinium)-butyrate dihydrate and its hydrobromide. Vibrational Spectroscopy, 2017, 88, 40-48.	1.2	4
5486	What is the effect of carbon nanotube shape on desalination process? A simulation approach. Desalination, 2017, 407, 103-115.	4.0	36
5487	Absorption Tails of Donor:C₆₀ Blends Provide Insight into Thermally Activated Charge-Transfer Processes and Polaron Relaxation. Journal of the American Chemical Society, 2017, 139, 1699-1704.	6.6	73
5488	Conformational landscape, stability, potential energy curves and vibrations of 1,2,3,4 tetrahydroquinoline. Journal of Molecular Structure, 2017, 1136, 80-89.	1.8	11
5489	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754.	23.0	181
5490	Spectroscopic properties of diketopyrrolopyrrole derivatives with long alkyl chains. Journal of Luminescence, 2017, 185, 219-227.	1.5	13
5491	A new PET and FRET-based molecular logic circuit mimicking the three-state logic gate. Dyes and Pigments, 2017, 140, 460-468.	2.0	13
5492	Structural, vibrational (FTIR and FT-Raman), NMR, UVâ€“vis spectral analysis, and DFT study of 2-(6-oxo-2-thioxotetrahydropyrimidin-4(1H)-ylidene) hydrazine carboxamide. Canadian Journal of Chemistry, 2017, 95, 580-589.	0.6	1
5493	Development of Predictive Models of the Kinetics of a Hydrogen Abstraction Reaction Combining Quantum-Mechanical Calculations and Experimental Data. Industrial & Engineering Chemistry Research, 2017, 56, 815-831.	1.8	8
5494	On-line attenuated total reflection infrared (ATR-IR) spectroscopy combined with advanced chemometrics for investigating the synthesis process of 3,5-diamino-1,2,4-triazole. Journal of the Iranian Chemical Society, 2017, 14, 915-923.	1.2	2
5495	Trimethylamine-N-oxide: its hydration structure, surface activity, and biological function, viewed by vibrational spectroscopy and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 6909-6920.	1.3	39
5496	Formation of E-cyanomethamine in a nitrile rich environment. Research in Astronomy and Astrophysics, 2017, 17, 1.	0.7	9

#	Article	IF	Citations
5497	Experimental and theoretical investigation on conformational and spectroscopic properties of dimethyl dithiodiglycolate, [CH 3 OC(O)CH 2 S] 2. Journal of Molecular Structure, 2017, 1137, 524-529.	1.8	1
5498	Molecular structure, FT IR, NMR, UV, NBO and HOMOâ€“LUMO of 1-(3-(dimethylamino)propyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile by DFT/B3LYP and PBEPBE methods with LanL2DZ and 6-311 ++G(d,2p) basis sets. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 180, 51-66.	2.0	46
5499	Synthesis, characterization, and DFT study of some transition metal complexes with Schiff base derived from 2-acetylthiophene and l-methionine. Research on Chemical Intermediates, 2017, 43, 4585-4610.	1.3	6
5500	Detection of surface-linked polychlorinated biphenyls using surface-enhanced Raman scattering spectroscopy. Vibrational Spectroscopy, 2017, 90, 1-6.	1.2	12
5501	Thorium and Uranium Hydride Phosphorus and Arsenic Bearing Molecules with Single and Double Actinide-Pnictogen and Bridged Agostic Hydrogen Bonds. Inorganic Chemistry, 2017, 56, 2949-2957.	1.9	11
5502	Theoretical study of the spectroscopic and nonlinear optical properties of trans- and cis-4-hydroxyazobenzene. Journal of Molecular Modeling, 2017, 23, 79.	0.8	8
5503	Infrared Spectra of Hexa-peri-hexabenzocoronene Cations: HBC⁺ and HBC²⁺. Astrophysical Journal, 2017, 836, 28.	1.6	18
5504	Experimental and theoretical IR study of methyl thioglycolate, CH 3 OC(O)CH 2 SH, in different phases: Evidence of a dimer formation. Journal of Molecular Structure, 2017, 1139, 160-165.	1.8	4
5505	Harmonic Vibrational Frequencies: Approximate Global Scaling Factors for TPSS, M06, and M11 Functional Families Using Several Common Basis Sets. Journal of Physical Chemistry A, 2017, 121, 2265-2273.	1.1	141
5506	Fingerprints of Through-Bond and Through-Space Exciton and Charge Ï€-Electron Delocalization in Linearly Extended [2.2]Paracyclophanes. Journal of the American Chemical Society, 2017, 139, 3095-3105.	6.6	34
5507	Structural investigation of the cocrystal formed between 5-fluorocytosine and fumaric acid based on vibrational spectroscopic technique. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 178, 251-257.	2.0	24
5508	Fourier-transform infrared spectroscopy (FTIR) analysis of triclinic and hexagonal birnessites. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 178, 32-46.	2.0	40
5509	Identification of Al₁₃ on the Colloid Surface Using Surface-Enhanced Raman Spectroscopy. Environmental Science & Technology, 2017, 51, 2899-2906.	4.6	13
5510	Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates. Journal of Computer-Aided Molecular Design, 2017, 31, 349-363.	1.3	16
5511	Vibrational Frequencies of Fractionally Charged Molecular Species: Benchmarking DFT Results against ab Initio Calculations. Journal of Physical Chemistry A, 2017, 121, 2282-2287.	1.1	4
5512	Synthesis, tautomeric stability, spectroscopy and computational study of a potential molecular switch of (Z)-4-(phenylamino)pent-3-en-2-one. Molecular Physics, 2017, 115, 795-808.	0.8	12
5513	Identifying Atomic Scale Structure in Undoped/Doped Semicrystalline P3HT Using Inelastic Neutron Scattering. Macromolecules, 2017, 50, 2424-2435.	2.2	52
5514	Structural and vibrational analyses of new potential anticancer drug 2-(phenylmethyl)-2-azaspiro[5.11]heptadecane-1,3,7-trione. Journal of Molecular Structure, 2017, 1137, 97-108.	1.8	2

#	Article	IF	Citations
5515	Computational study of the vibrational spectroscopy properties of boron-hydrogen compounds: Mg(B3H8)2, CB9H10â˜ and CB11H12â˜. International Journal of Hydrogen Energy, 2017, 42, 22496-22501.	3.8	12
5516	Spectroscopic and computational investigation of the structure and pharmacological activity of 1-benzylimidazole. Journal of Taibah University for Science, 2017, 11, 975-996.	1.1	14
5517	Experimental and quantum chemical studies on the structure and vibrational spectra of cearoin (a) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.4	1
5518	Calculation of IR-spectra of structural fragments of lignins. EPJ Web of Conferences, 2017, 132, 03011.	0.1	1
5519	Does a Nitrogen Lone Pair Lead to Two Centeredâ€“Three Electron (2câ€“3e) Interactions in Pyridyl Radical Isomers?. Journal of Physical Chemistry A, 2017, 121, 3781-3791.	1.1	9
5520	Adsorption of Nitrate and Bicarbonate on Fe-(Hydr)oxide. Inorganic Chemistry, 2017, 56, 5455-5464.	1.9	22
5521	Solvation Enhances the Distinction between Carboxylated Armchair and Zigzag Single-Wall Carbon Nanotubes (SWNT-COOH). Journal of Physical Chemistry C, 2017, 121, 9516-9527.	1.5	2
5522	Synthesis, crystal structure, DFT calculation and DNA binding studies of new water-soluble derivatives of dppz. Journal of Molecular Structure, 2017, 1145, 141-151.	1.8	5
5523	Synthesis, spectroscopic characterization, biological activity and theoretical studies of (E)-N3-(2-chlorobenzylidene)-H-1,2,4-triazole-3,5-diamine. Journal of Molecular Structure, 2017, 1144, 324-337.	1.8	12
5524	The open-cubane oxoâ€“oxyl coupling mechanism dominates photosynthetic oxygen evolution: a comprehensive DFT investigation on Oâ€“O bond formation in the S4state. Physical Chemistry Chemical Physics, 2017, 19, 13909-13923.	1.3	31
5525	Conformational Analysis, Structural and Vibrational Investigations of transâ€“2â€“Chlorocinnamic Acid and transâ€“4â€–Chlorocinnamic Acid. Springer Proceedings in Physics, 2017, , 563-598.	0.1	0
5526	Vibrational analysis of dibenzo-18-crown-6. Effect of dispersion correction on the calculated vibrational spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 23-29.	2.0	1
5527	Chirality of the trisubstituted nitrogen center â€“ XRD, dynamic NMR, and DFT investigation of 1,2-dihydrobenzo[e][1,2,4]triazine derivatives. Tetrahedron, 2017, 73, 3823-3830.	1.0	7
5528	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
5529	Structural, spectral analysis of ambroxol using DFT methods. Journal of Molecular Structure, 2017, 1144, 379-388.	1.8	16
5530	Thermochemistry of Hydroxyl and Hydroperoxide Substituted Furan, Methylfuran, and Methoxyfuran. Journal of Physical Chemistry A, 2017, 121, 4523-4544.	1.1	19
5531	Spectroscopic and molecular docking studies on N , N -di- tert -butoxycarbonyl (Boc)-2-amino pyridine: A potential bioactive agent for lung cancer treatment. Journal of Molecular Structure, 2017, 1143, 415-423.	1.8	41
5532	Studies of Carbon Monoxide Release from Ruthenium(II) Bipyridine Carbonyl Complexes upon UV-Light Exposure. Inorganic Chemistry, 2017, 56, 5941-5952.	1.9	28

#	Article	IF	Citations
5533	Coordinating Tectons. Experimental and Computational Infrared Data as Tools To Identify Conformational Isomers and Explore Electronic Structures of 4-Ethynyl-2,2â€²-bipyridine Complexes. Organometallics, 2017, 36, 1946-1961.	1.1	14
5534	Polymorphs of Neutral Red, a Redox-Mediating Phenazine in Biological Systems. Australian Journal of Chemistry, 2017, 70, 1032.	0.5	4
5535	NMR, FT-IR spectroscopic studies and molecular docking study of 4-acetoxyphenethyl acrylate. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750025.	1.8	0
5536	DFT calculations of the tautomerization and NLO properties of 5-amino-7-(pyrrolidin-1-yl)-2,4,4-trimethyl-1,4-dihydro-1,6-naphthyridine-8-carbonitrile (APNC). Journal of Molecular Structure, 2017, 1143, 397-404.	1.8	23
5537	Conformations and interactions in pasiniazid: A spectroscopic and computational characterization. Journal of Molecular Structure, 2017, 1133, 179-186.	1.8	3
5538	Site-selective substitution of gold atoms in the Au24(SR)20 nanocluster by silver. Journal of Colloid and Interface Science, 2017, 505, 1202-1207.	5.0	24
5539	Why Low Valent Lead(II) Hydride Complex Would be a Better Catalyst for CO₂ Activation than Its 14 Group Analogues?. Journal of Physical Chemistry C, 2017, 121, 12127-12135.	1.5	9
5540	Molecular â€œsurgeryâ€•on a 23-gold-atom nanoparticle. Science Advances, 2017, 3, e1603193.	4.7	121
5541	Spectra-structure correlations of saturated and unsaturated medium-chain fatty acids. Near-infrared and anharmonic DFT study of hexanoic acid and sorbic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 35-44.	2.0	38
5542	Characterization of forced degradation products of torasemide through MS tools and explanation of unusual losses observed during mass fragmentation of drug and degradation products through density functional theory. Journal of Pharmaceutical and Biomedical Analysis, 2017, 145, 209-218.	1.4	9
5543	Synthesis, characterization and theoretical study in gaseous and solid phases of the imine 4-Acetyl-N-(4-methoxybenzylidene)aniline. Journal of Molecular Structure, 2017, 1147, 300-309.	1.8	2
5544	A Strategy for the Synthesis of 1,2-Dichlorotetrafluorocyclobutene from Hexachlorobutadiene and Its Reaction Pathway. Industrial & Engineering Chemistry Research, 2017, 56, 7623-7630.	1.8	9
5545	Crystal structure, vibrational spectra and DFT studies of hydrogen bonded 1,2,4â€“triazolium hydrogenselenate. Journal of Molecular Structure, 2017, 1145, 211-221.	1.8	6
5546	The vibrational properties of the bee-killer imidacloprid insecticide: A molecular description. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 185, 245-255.	2.0	20
5547	Nanoclusters of Cyanuric Acid. Journal of Chemical Sciences, 2017, 129, 873-881.	0.7	1
5548	Comparative study of the structural and spectral properties of tetraaza- and tetraoxaannelated tetracirculenes. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2017, 122, 523-540.	0.2	6
5549	Solid-state cocrystal formation between acyclovir and fumaric acid: Terahertz and Raman vibrational spectroscopic studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 186, 29-36.	2.0	19
5550	Spectroscopic and quantum chemical studies of interaction between the alginic acid and Fe 3 O 4 nanoparticles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 182, 1-7.	2.0	4

#	Article	IF	Citations
5551	Energetic Effect of the Carboxylic Acid Functional Group in Indole Derivatives. Journal of Physical Chemistry A, 2017, 121, 2980-2989.	1.1	5
5552	Vibrational frequency fluctuations of ionic vibrational probe in water: Theoretical study with molecular dynamics simulation. Chemical Physics Letters, 2017, 683, 547-552.	1.2	4
5553	Doppler-limited high-resolution spectrum and VPT2 assisted assignment of the C-H stretch of CH2Br2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 181, 180-191.	2.0	6
5554	Proton conducting system (ImH 2) 2 SeO 4 Â·2H 2 O investigated with vibrational spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 180, 224-233.	2.0	10
5555	Raman Spectroscopic Signature Markers of Dopamineâ€“Human Dopamine Transporter Interaction in Living Cells. ACS Chemical Neuroscience, 2017, 8, 1510-1518.	1.7	27
5556	Cî€€/Bâ€“N substitution in five membered heterocycles. A computational analysis. New Journal of Chemistry, 2017, 41, 3619-3633.	1.4	11
5557	Density functional theory analysis and molecular docking evaluation of 1-(2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td (5-dichloro-4- Journal of Molecular Structure, 2017, 1141, 335-345.	1.8	10
5558	Improved Infrared Spectra Prediction by DFT from a New Experimental Database. Chemistry - A European Journal, 2017, 23, 8414-8423.	1.7	50
5559	Density Functional Theory Investigations on Vibrational Spectra, Molecular Structure, and Properties of the L-Serine, L-Cysteine, and L-Aspartic Acid Molecules. Journal of the Chinese Chemical Society, 2017, 64, 503-521.	0.8	2
5560	Synthesis, crystal structure analysis and DFT studies of 3a,8a-Dihydroxy-2-thioxo-2,3,3a,8a-tetrahydroindeno[1,2- d]imidazol-8(1 H)-one. Journal of Molecular Structure, 2017, 1139, 282-293.	1.8	8
5561	Comparative studies on molecular structure, vibrational spectra and hyperpolarizabilies of NLO chromophore Ethyl 4-Dimethylaminobenzoate. Journal of Molecular Structure, 2017, 1141, 400-416.	1.8	5
5562	Spectroscopic (FT-IR, FT-Raman, UV, 1H and 13C NMR) profiling and computational studies on methyl 5-methoxy-1H-indole-2-carboxylate: A potential precursor to biologically active molecules. Journal of Molecular Structure, 2017, 1133, 199-210.	1.8	19
5563	Theoretical Calculation of Boron Isotopic Separation Factors in Ion-Exchange Chromatography. Journal of Chemical & Engineering Data, 2017, 62, 525-531.	1.0	6
5564	Theoretical design and characterisation on the fluorinated nitrophenyl azidotriazoles. Molecular Simulation, 2017, 43, 183-188.	0.9	2
5565	Vibrational spectroscopic, molecular docking and quantum chemical studies on 6-aminonicotinamide. Journal of Molecular Structure, 2017, 1134, 143-156.	1.8	23
5566	Investigation of 9-(2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-en-1-yl)-3,3-dimethyl-2,3,4,9-tetrahydro-1H-xanthen-1-one: Crystal structure, AIM and NBO analysis. Journal of Molecular Structure, 2017, 1133, 510-518.	1.8	23
5567	Band alignment in organic light emitting diodes - On the track of thickness dependent onset voltage shifts. Organic Electronics, 2017, 41, 79-90.	1.4	6
5568	Structural insights, protein-ligand interactions and spectroscopic characterization of isoformononetin. Journal of Molecular Structure, 2017, 1133, 479-491.	1.8	3

#	Article	IF	Citations
5569	Comparison of different hybrid DFT methods on structural, spectroscopic, electronic and NLO parameters for a potential NLO material. Computational and Theoretical Chemistry, 2017, 1100, 34-45.	1.1	46
5570	Efficient and Accurate Bornâ€“Oppenheimer Molecular Dynamics for Large Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5479-5485.	2.3	16
5571	Biotransformation of Isoniazid by Cytochromes P450: Analyzing the Molecular Mechanism using Density Functional Theory. Chemical Research in Toxicology, 2017, 30, 2060-2073.	1.7	11
5572	Matrix Infrared Spectra of Insertion and Metallacyclopropane Complexes [CH₃CH₂â€“MH and (CH₂)₂â€“MH₂] Prepared in Reactions of Laser-Ablated Group 3 Metal Atoms with Ethane. Journal of Physical Chemistry A, 2017, 121, 8583-8595.	1.1	1
5573	Electronic Structures of Divinylchalcogenopheneâ€Bridged Biruthenium Complexes: Exploring Trends from O to Te. European Journal of Inorganic Chemistry, 2017, 2017, 5015-5026.	1.0	12
5574	Photodissociation kinetics of the isobutanal radical cation: a combined experimental and theoretical study. RSC Advances, 2017, 7, 47689-47694.	1.7	3
5575	Characterization of the Fâ^'-water and Clâ^'-water hydrogen bonds in aqueous solution: From â€œinteriorâ€• (I) to â€œsurfaceâ€•(S) states. Journal of Molecular Liquids, 2017, 248, 271-277.	2.3	7
5576	Salt-induced thermochromism of a conjugated polyelectrolyte. Physical Chemistry Chemical Physics, 2017, 19, 28853-28866.	1.3	12
5577	A novel dihydrocoumarin under experimental and theoretical characterization. Journal of Molecular Modeling, 2017, 23, 315.	0.8	5
5578	Thermoanalytical Study of Linkage Isomerism in Coordination Compounds. Part 7. A DSC and DFT Investigation of Solid-state Linkage Isomerization in Bis(thiocyanato)-bipyridineplatinum(II) Complex. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1131-1138.	0.6	3
5579	Why can a gold salt react as a base?. Organic and Biomolecular Chemistry, 2017, 15, 7841-7852.	1.5	6
5580	Computational study on the mechanism and kinetics for reaction of CH 3 SH + H with water vapor. Computational and Theoretical Chemistry, 2017, 1117, 235-240.	1.1	4
5581	The solid state structure and environmental polarization effect of a novel asymmetric azine. New Journal of Chemistry, 2017, 41, 11361-11371.	1.4	22
5582	Study of molecular structure, chemical reactivity and H-bonding interactions in the cocrystal of nitrofurantoin with urea. New Journal of Chemistry, 2017, 41, 11069-11078.	1.4	24
5583	Kinetically Trapped Liquid-State Conformers of a Sodiated Model Peptide Observed in the Gas Phase. Journal of Physical Chemistry A, 2017, 121, 6838-6844.	1.1	5
5584	TD-DFT, NBO analyses, electronic and NLO properties of hydrogen-bonded undecyloxy benzoic acid with suberic acid mesogen. Molecular Crystals and Liquid Crystals, 2017, 650, 65-79.	0.4	4
5585	Bonding and Electronic Properties of Linear Diethynyl Oligothienoacene-Bridged Diruthenium Complexes and Their Oxidized Forms. Inorganic Chemistry, 2017, 56, 11074-11086.	1.9	30
5586	Insight into the theoretical and experimental studies of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone N(4)-methyl-N(4)- phenylthiosemicarbazone - A potential NLO material. Journal of Molecular Structure, 2017, 1150, 135-145.	1.8	22

#	Article	IF	Citations
5587	4-Methyl-1H-Indazole-5-Boronic acid: Crystal structure, vibrational spectra and DFT simulations. Journal of Molecular Structure, 2017, 1150, 299-306.	1.8	8
5588	Surface chemistry of MgO/SiO₂ catalyst during the ethanol catalytic conversion to 1,3-butadiene: in-situ DRIFTS and DFT study. Catalysis Science and Technology, 2017, 7, 4648-4668.	2.1	58
5589	The parameter uncertainty inflation fallacy. Journal of Chemical Physics, 2017, 147, 104102.	1.2	29
5590	Liquid Quinones for Solventâ€Free Redox Flow Batteries. Advanced Materials, 2017, 29, 1606592.	11.1	41
5591	Binding and electrophilic activation of ethylene by zinc(II), cadmium(II), and mercury(II) complexes: A theoretical investigation. Journal of Organometallic Chemistry, 2017, 851, 122-135.	0.8	3
5592	Reaction Paths and Chemical Activation Reactions of 2-Methyl-5-Furanyl Radical with ³O₂. Journal of Physical Chemistry A, 2017, 121, 7309-7323.	1.1	3
5593	A theoretical quantum chemical study of alanine formation in interstellar medium. European Physical Journal D, 2017, 71, 1.	0.6	9
5594	Experimental and quantum chemical study of biosynthetic lignin models â€" dehydropolymers. Russian Chemical Bulletin, 2017, 66, 643-647.	0.4	5
5595	Influence of the nature of solvent and substituents on the oxidation potential of 2,2,6,6-tetramethylpiperidine 1-oxyl derivatives. Russian Chemical Bulletin, 2017, 66, 683-689.	0.4	12
5596	Observation and Characterization of CH3CH2â€“MH, (CH2)2â€“MH2, CH2â•CHâ€“MH3, and CH3â€“Câ‰¡MH3â€“ Produced by Reactions of Group 5 Metal Atoms with Ethane. Journal of Physical Chemistry A, 2017, 121, 6766-6777.	1.1	2
5597	Anharmonic vibrational and electronic spectral study of 2-amino-4-hydroxy-6â€“methylpyrimidine: A combined experimental (FTIR, FT-Raman, UVâ€“Vis) and theoretical (DFT, MP2) approach. Journal of Molecular Structure, 2017, 1148, 89-100.	1.8	16
5598	Synthesis, characterization, crystal structure and theoretical studies of 4-[(E)-(3-chloro-4-hydroxyphenyl) diazenyl]-1, 5-dimethyl-2-phenyl-1, 2-dihydro-3H-pyrazol-3-one. Journal of Molecular Structure, 2017, 1148, 185-195.	1.8	5
5599	Protonationâ€Stateâ€Driven Photophysics in Phenothiazinium Dyes: Intersystem Crossing and Singletâ€Oxygen Production. ChemPhotoChem, 2017, 1, 459-469.	1.5	5
5600	First-principles characterization of native-defect-related optical transitions in ZnO. Journal of Applied Physics, 2017, 122, .	1.1	88
5601	Enhanced Luminescence of Asymmetrical Sevenâ€Coordinate Eu^{III} Complexes Including LMCT Perturbation. European Journal of Inorganic Chemistry, 2017, 2017, 3843-3848.	1.0	53
5602	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	2.3	90
5603	DFT study of IR and Raman spectra of phosphotrihydrazone dendrimer with terminal phenolic groups. Journal of Molecular Structure, 2017, 1144, 466-472.	1.8	2
5604	Synthesis, solvatochromism and crystal structure of trans -[Cu(Et 2 NCH 2 CH 2 NH 2) 2 .H 2 O](NO 3) 2 complex: Experimental withÂDFTÂcombination. Journal of Molecular Structure, 2017, 1148, 328-338.	1.8	22

#	Article	IF	Citations
5605	A critical review of statistical calibration/prediction models handling data inconsistency and model inadequacy. AICHE Journal, 2017, 63, 4642-4665.	1.8	40
5606	Evaluation of SF₆-alternative gas C5-PFK based on arc extinguishing performance and electric strength. Journal Physics D: Applied Physics, 2017, 50, 385202.	1.3	54
5607	Experimental and theoretical studies on oxy-cracking of Quinolin-65 as a model molecule for residual feedstocks. Reaction Chemistry and Engineering, 2017, 2, 703-719.	1.9	16
5608	Synthesis and physicochemical characterization of polyoxymethylene dimethyl ethers. Journal of Fuel Chemistry and Technology, 2017, 45, 837-845.	0.9	29
5609	Z-scan measurements of the third-order optical nonlinearities and vibrational spectral studies by DFT computations on azo dye 1-(2-Methylphenylazo)-2-napthol. Optics and Laser Technology, 2017, 97, 390-399.	2.2	25
5610	Isomeric xylene molecules in the Terahertz-far infrared regime: Computational chemistry and spectral modeling view. Vibrational Spectroscopy, 2017, 92, 220-229.	1.2	2
5611	Analysis and design of resonance Raman reporter molecules by density functional theory. Journal of Raman Spectroscopy, 2017, 48, 1196-1200.	1.2	15
5612	Organic probe molecule adsorption on extended Au(111) surface: a theoretical DFT study. Research on Chemical Intermediates, 2017, 43, 5283-5292.	1.3	0
5613	Multi-properties of a new azo-Schiff base and its binuclear copper(II) chelate: Preparation, spectral characterization, electrochemical, potentiometric and modeling studies. Journal of Molecular Structure, 2017, 1149, 520-529.	1.8	25
5614	Structure and catalytic activity of a newly proposed titanium species in a Ti-YNU-1 zeolite: a density functional theory study. Catalysis Science and Technology, 2017, 7, 4105-4114.	2.1	16
5615	Molecular structure, vibrational analysis (IR and Raman) and quantum chemical investigations of 1-aminoisoquinoline. Journal of Molecular Structure, 2017, 1149, 835-845.	1.8	8
5616	Synthesis, spectroscopic and photophysical studies of xanthene derivatives. Journal of Molecular Structure, 2017, 1149, 862-873.	1.8	13
5617	Waterâ€assisted Dimerization of Hydrogen Cyanide: A Computational Study. Bulletin of the Korean Chemical Society, 2017, 38, 1531-1533.	1.0	8
5618	Theoretical study of the Cl-initiated atmospheric oxidation of methyl isopropenyl ketone. RSC Advances, 2017, 7, 52801-52811.	1.7	6
5619	Copper(I) Chelators for Alzheimerâ€™s Disease. Journal of Physical Chemistry B, 2017, 121, 11304-11310.	1.2	10
5620	Scaling relationships and theory for vibrational frequencies of adsorbates on transition metal surfaces. Nature Communications, 2017, 8, 1842.	5.8	23
5621	Vibrational spectroscopy, electrical characterization, nonlinear optical properties and DFT calculation of (NEt₄)(H₂AsO₄)(H₃AsO₄)₂. Journal of Coordination Chemistry, 2017, 70, 3585-3597.	0.8	10
5622	Experimental and Computational Thermochemical Study of Maleic Anhydride and Vinylene Carbonate. Journal of Physical Chemistry A, 2017, 121, 9474-9484.	1.1	5

#	Article	IF	Citations
5623	Infrared Spectroscopic and Electronic Structure Investigations of Beryllium Halide Molecules, Cations, and Anions in Noble Gas Matrices. Journal of Physical Chemistry A, 2017, 121, 8843-8855.	1.1	8
5624	Computational modelling of the redistribution of copper isotopes by proteins in the liver. Metallomics, 2017, 9, 1809-1819.	1.0	20
5625	Use of Low-Cost Quantum Chemistry Procedures for Geometry Optimization and Vibrational Frequency Calculations: Determination of Frequency Scale Factors and Application to Reactions of Large Systems. Journal of Chemical Theory and Computation, 2017, 13, 6052-6060.	2.3	32
5626	A Decapeptide Hydrated by Two Waters: Conformers Determined by Theory and Validated by Cold Ion Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 9401-9408.	1.1	16
5627	The millimeter and sub-millimeter rotational spectrum of triple ¹³C-substituted ethyl cyanide. Astronomy and Astrophysics, 2017, 601, A2.	2.1	2
5628	Study of molecular structure, anharmonic vibrational dynamic and electronic properties of sulindac using spectroscopic techniques integrated with quantum chemical calculations. Journal of Molecular Structure, 2017, 1147, 603-615.	1.8	11
5629	A combined theoretical and thermal analysis study on the solid state linkage isomerization of Ni(II)-nitrite complexes with ethylenediamine derivatives. Journal of Coordination Chemistry, 2017, 70, 2294-2312.	0.8	3
5630	Ab Initio Investigation of the Micro-species and Raman Spectra in Ca(NO3)2 Solution. Journal of Cluster Science, 2017, 28, 2293-2307.	1.7	2
5631	Chains of benzenes with lithium-atom adsorption: Vibrations and spontaneous symmetry breaking. Chemical Physics Letters, 2017, 684, 86-90.	1.2	1
5632	Spectroscopic and cytotoxic characteristics of (p-cymene)Ru(II) complexes with bidentate coumarins and density functional theory comparison with selected Pd(II) complexes. Inorganica Chimica Acta, 2017, 456, 105-112.	1.2	5
5633	Quantum chemical prediction of vibrational spectra of large molecular systems with radical or metallic electronic structure. Chemical Physics Letters, 2017, 667, 317-321.	1.2	7
5634	Vibrational, structural and electronic study of a pyridinium salt assisted by SXRD studies and DFT calculations. Journal of Molecular Structure, 2017, 1131, 156-162.	1.8	9
5635	Crystal and molecular structures, IR and Raman spectra, vibrational dynamics of aquo 7-methyl-1H-[1,2,3]triazolo[4,5-c]pyridinium nitrate â€“ a new composite material. Journal of Molecular Structure, 2017, 1133, 9-17.	1.8	4
5636	Molecular structure, interatomic interactions and vibrational analysis of 1,4-diazabicyclo[3.2.1]octane parent ring system. Journal of Molecular Structure, 2017, 1130, 395-399.	1.8	3
5637	Calorimetric and computational studies for three nitroimidazole isomers. Journal of Chemical Thermodynamics, 2017, 105, 267-275.	1.0	7
5638	Molecular structure activity on pharmaceutical applications of Phenacetin using spectroscopic investigation. Journal of Molecular Structure, 2017, 1127, 611-625.	1.8	6
5639	Spectral (FT-IR, FT-Raman, UV, and fluorescence), DFT, and solid stateÂinteraction analyses of (E)-4-(3,4-dimethoxybenzylideneamino)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one. Journal of Molecular Structure, 2017, 1128, 174-185.	1.8	19
5640	A DFT study of the mechanism and selectivities of the [3Â+Â2] cycloaddition reaction between 3â€(benzylideneamino)oxindole and transâ€²â€nitrostyrene. Journal of Physical Organic Chemistry, 2017, 30, e3637.	0.9	22

#	Article	IF	Citations
5641	Vibrational properties of fractionally charged molecules and their relevance for molecular electronics and electrochemistry. Chemical Physics, 2017, 482, 311-318.	0.9	6
5642	Computational thermochemistry: Automated generation of scale factors for vibrational frequencies calculated by electronic structure model chemistries. Computer Physics Communications, 2017, 210, 132-138.	3.0	12
5643	Protonated N -alkyl-2-nitroanilines undergo intramolecular oxidation of the alkyl chain upon collisional activation. International Journal of Mass Spectrometry, 2017, 413, 75-80.	0.7	1
5644	Conformational stability, spectral analysis (infrared, Raman and NMR) and DFT calculations of 2-Amino-5-(ethylthio)-1,3,4-thiadiazole. Journal of Molecular Structure, 2017, 1130, 434-441.	1.8	13
5645	Mechanistic study on silver(I)-catalyzed aminofluorination of unactivated alkenes. Journal of Physical Organic Chemistry, 2017, 30, e3655.	0.9	7
5646	Molecular interactions in high conductive gel electrolytes based on low molecular weight gelator. Journal of Colloid and Interface Science, 2017, 490, 279-286.	5.0	11
5647	Experimental and theoretical studies on new 7-(3,6-di-tert-butyl-9H-carbazol-9-yl)-10-alkyl-10H-phenothiazine-3-carbaldehydes. Journal of Molecular Structure, 2017, 1130, 633-643.	1.8	5
5648	Structural, spectroscopic and molecular docking studies on 2-amino-3-chloro-5-trifluoromethyl pyridine: A potential bioactive agent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 175, 51-60.	2.0	48
5649	Vibrational spectra and DFT studies of conjugation in poly(phosphorhydrazone) dendrimers. Vibrational Spectroscopy, 2017, 88, 14-26.	1.2	2
5650	Synthesis, molecular structure and vibrational analysis of D-D-A based carbazole decorated phenothiazine-3-carbaldehyde: Experimental (FT-IR, UV and NMR) and density functional theory (DFT) calculations. Journal of Molecular Structure, 2017, 1128, 674-684.	1.8	10
5651	5. Computational chemistry applied to vibrational spectroscopy: A tool for characterization of nucleic acid bases and some of their 5-substituted derivatives. , 2017, , 117-152.		2
5652	Ab initio based kinetic Monte Carlo analysis to unravel the propagation kinetics in vinyl acetate pulsed laser polymerization. Polymer Chemistry, 2017, 8, 7143-7150.	1.9	35
5653	Simulation and experiment on SF<inf>6</inf> gas decomposition detection based on infrared absorption spectroscopy. , 2017, , .		1
5654	Raman and Infrared Spectra for All-trans-astaxanthin in Dimethyl Sulfoxide Solvent. Chinese Journal of Chemical Physics, 2017, 30, 506-512.	0.6	1
5655	Experimental and Density Functional Theory Calculation Studies on Raman and Infrared Spectra of 1,1â€²-Binaphthyl-2,2â€²-diamine. Chinese Journal of Chemical Physics, 2017, 30, 7-15.	0.6	7
5656	NMR and IR Investigations of Strong Intramolecular Hydrogen Bonds. Molecules, 2017, 22, 552.	1.7	95
5657	Electrochemical and Infrared Absorption Spectroscopy Detection of SF6 Decomposition Products. Sensors, 2017, 17, 2627.	2.1	33
5658	The Antioxidant Activity of Quercetin in Water Solution. Biomimetics, 2017, 2, 9.	1.5	46

#	Article	IF	Citations
5659	Computational chemistry applied to vibrational spectroscopy: A tool for characterization of nucleic acid bases and some of their 5-substituted derivatives. Physical Sciences Reviews, 2017, 2, .	0.8	3
5660	FT-IR, NMR spectroscopic and quantum mechanical investigations of two ferrocene derivatives. Bulletin of the Chemical Society of Ethiopia, 2017, 31, 63.	0.5	4
5661	Photodissociation processes of Bisanthenquinone cation. Proceedings of the International Astronomical Union, 2017, 13, 353-359.	0.0	1
5662	Theoretical Insight into the Structure, Energetic Property and Thermal Stability of C6N6H12 Cages. , 2017, 06, .		0
5663	Synthesis, theoretical, and experimental study of radical scavenging activity of 3-pyridinol containing trans-resveratrol analogs. Medicinal Chemistry Research, 2018, 27, 1298-1308.	1.1	7
5664	Water Dissociative Adsorption on Î±-Al₂O₃(112Ì…0) Is Controlled by Surface Site Undercoordination, Density, and Topology. Journal of Physical Chemistry C, 2018, 122, 6573-6584.	1.5	17
5665	Quantum chemistry as a tool to assess energetic and spectroscopic properties of C1 and C2 hydrocarbons in MOF-74-Mg. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
5666	The Acetylene-Ammonia Co-crystal on Titan. ACS Earth and Space Chemistry, 2018, 2, 366-375.	1.2	30
5667	Catalytic Gasâ€phase Fluorination of Hexachlorobutadiene to 1,2â€Dichlorotetrafluorocyclobutene over Cr/Znâ€based Catalysts. Journal of the Chinese Chemical Society, 2018, 65, 760-770.	0.8	2
5668	Synthesis, molecular structure, Hirshfeld surface, spectral investigations and molecular docking study of 3-(5-bromo-2-thienyl)-1-(4-fluorophenyl)-3-acetyl-2-pyrazoline (2) by DFT method. Journal of Molecular Structure, 2018, 1164, 420-437.	1.8	15
5669	A theoretical study towards thermolysis process of thionesters and thiolesters. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850014.	1.8	3
5670	Comparison of Siliceous Zeolite Potentials from the Perspective of Infrared Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 6093-6102.	1.5	3
5671	Effects of pressure on the structural and electronic properties of linear carbon chains encapsulated in double wall carbon nanotubes. Carbon, 2018, 133, 446-456.	5.4	47
5672	Computational and Spectroscopic Analysis of Î²-Indandione Modified Zinc Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4448-4456.	1.1	6
5673	Raman spectroscopy probing of redox states and mechanism of flavin coenzyme. Journal of Raman Spectroscopy, 2018, 49, 1311-1322.	1.2	9
5674	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45
5675	Dimerization of boryl- and amino-substituted acetylenes by B₂C₂ four-membered ring formation. Chemical Communications, 2018, 54, 5819-5822.	2.2	5
5676	Unassisted formation of hemiaminal ether from 4-aminopyridine and o-vanillin - experimental and theoretical study. Structural Chemistry, 2018, 29, 1189-1200.	1.0	8

#	Article	IF	Citations
5677	Crystal structure, vibrational spectra, optical and DFT studies of poly[bis(L-methionine)-ÎºS:O cadmium (II) di-Î¼-thiocyanato- Îº 2 N:S; Îº 2 S:N]. Journal of Molecular Structure, 2018, 1166, 91-101.	1.8	6
5678	(2 E)-2-[1-(1,3-Benzodioxol-5-yl)-3-(1 H -imidazol-1-yl)propylidene]- N -(4-methoxyphenyl)hydrazinecarboxamide: Synthesis, crystal structure, vibrational analysis, DFT computations, molecular docking and antifungal activity. Journal of Molecular Structure, 2018, 1166, 121-130.	1.8	12
5679	Vibrational investigation on pharmaceutical activity of m-xylene-4-sulphonic acid by quantum computational and experimental support. Journal of Taibah University for Science, 2018, 12, 87-103.	1.1	1
5680	¹³C Kinetic Isotope Effects as a Quantitative Probe To Distinguish between Enol and Enamine Mechanisms in Aminocatalysis. Chemistry - A European Journal, 2018, 24, 8098-8102.	1.7	10
5681	Electronic spectral studies and DFT computational analysis of hydrogen bonded charge transfer complexes between chloranilic acid and 2,5-dihydroxy-p-benzoquinone with 2-amino-4-methylbenzothiazole in methanol. Journal of Molecular Liquids, 2018, 256, 433-444.	2.3	43
5682	DFT application for chlorin derivatives photosensitizer drugs modeling. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 195, 68-74.	2.0	4
5683	Ab initio periodic modelling of the vibrational spectra of molecular crystals: the case of uracil. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	7
5684	Structure and reactivity of oxalate surface complexes on lepidocrocite derived from infrared spectroscopy, DFT-calculations, adsorption, dissolution and photochemical experiments. Geochimica Et Cosmochimica Acta, 2018, 226, 244-262.	1.6	37
5685	Sum-frequency vibrational spectroscopy of limonene chiral liquids due to the nonadiabatic effect. Physical Chemistry Chemical Physics, 2018, 20, 7053-7058.	1.3	5
5686	Probing vibrational activities, electronic properties, molecular docking and Hirshfeld surfaces analysis of 4-chlorophenyl ({[(1E)-3-(1H-imidazol-1-yl)-1-phenylpropylidene]amino}oxy)methanone: A promising anti-Candida agent. Journal of Molecular Structure, 2018, 1159, 83-95.	1.8	21
5687	Charge transfer complex between 2,3-diaminopyridine with chloranilic acid. Synthesis, characterization and DFT, TD-DFT computational studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 196, 247-255.	2.0	39
5688	Strong Hydrogen Bonds at the Interface between Proton-Donating and -Accepting Self-Assembled Monolayers on Au(111). Langmuir, 2018, 34, 2189-2197.	1.6	16
5689	Quantum Chemical Calculations of the Spectroscopic Properties and Nonlinear Optical Activity of 2,6-Dibromo-3-Chloro-4-Fluoroaniline. Journal of Applied Spectroscopy, 2018, 84, 1098-1107.	0.3	0
5690	Density Functional Theory Rate Calculation of Hydrogen Abstraction Reactions of N-Phenyl-Î±-naphthylamine Antioxidants. Industrial & Engineering Chemistry Research, 2018, 57, 876-880.	1.8	11
5691	Molecular structure of hybrid imino-chalcone in the solid state: X-ray diffraction, spectroscopy study and third-order nonlinear optical properties. Journal of Molecular Structure, 2018, 1157, 210-221.	1.8	19
5692	Deducing the Adsorption Geometry of Rhodamine 6G from the Surface-Induced Mode Renormalization in Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 465-473.	1.5	19
5693	Synthesis, spectroscopic and DFT studies of novel 4-(morpholinomethyl)-5-oxo-1-phenylpyrrolidine-3-carboxylic acid. Journal of Molecular Structure, 2018, 1157, 551-559.	1.8	7
5694	Synthesis, characterization and cytotoxicity of areneâ€“ruthenium(ii) complexes with acylpyrazolones functionalized with aromatic groups in the acyl moiety. Dalton Transactions, 2018, 47, 868-878.	1.6	25

#	Article	IF	Citations
5695	Computational study of the structure and properties of bicyclo[3.1.1]heptane derivatives for new high-energy density compounds with low impact sensitivity. Journal of Molecular Modeling, 2018, 24, 17.	0.8	3
5696	Vibrational Properties of Bulk Boric Acid2Aand3TPolymorphs and Their Two-Dimensional Layers: Measurements and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2018, 122, 1312-1325.	1.1	10
5697	Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. Journal of Computational Chemistry, 2018, 39, 889-900.	1.5	10
5698	Theoretical investigations on the kinetics of Cl atom initiated reactions of series of 1-alkenes. Environmental Science and Pollution Research, 2018, 25, 4387-4405.	2.7	4
5699	DFT, spectroscopic studies, NBO, NLO and Fukui functional analysis of 1-(1-(2,4-difluorophenyl)-2-(1H-1,2,4-triazol-1-yl)ethylidene) thiosemicarbazide. Journal of Molecular Structure, 2018, 1158, 1-13.	1.8	62
5700	Searching for a new family of modified CL-20 cage derivatives with high energy and low sensitivity. Structural Chemistry, 2018, 29, 837-845.	1.0	11
5701	Observation of High Capacitance from Molecular Gd@C₈₂ in Aqueous Electrolyte Derived from Energyâ€Level Matching with Proton. Advanced Materials Interfaces, 2018, 5, 1800240.	1.9	5
5702	Theoretical investigation on vibrational frequency fluctuations of SCN-derivatized vibrational probe molecule in water. Chemical Physics, 2018, 512, 82-87.	0.9	6
5703	Clustering of sulfuric acid, bisulfate ion and organonitrate C 10 H 15 O 10 N: Thermodynamics and atmospheric implications. Computational and Theoretical Chemistry, 2018, 1133, 40-46.	1.1	2
5704	Experimental and theoretical investigation of third-order nonlinear optical properties of azo dye 1-(2,) Tj ETQq1 1 0.784314 rgBT /Ove Dyes and Pigments, 2018, 157, 163-178.	2.0	54
5705	Iron versus Ruthenium: Clarifying the Electronic Differences between Prototypical Mixed-Valence Organometallic Butadiyndiyl Bridged Molecular Wires. Organometallics, 2018, 37, 1432-1445.	1.1	44
5706	Molecular Dynamics Simulation of First-Adsorbed Water Layer at Titanium Dioxide Surfaces. Journal of Chemical & Engineering Data, 2018, 63, 2420-2429.	1.0	20
5707	Molecular Modeling, Spectroscopic Investigations, and Computational Studies of DMSO solvated 7â€²-amino-1â€²,3â€²-dimethyl-2,2â€²,4â€²-trioxo-1â€²,2â€²,3â€²,4â€²,4aâ€²,8aâ€²-tetrahydrospiro[indoline-3,5â€²-pyrano[2,3-d]py Journal of Structural Chemistry, 2018, 59, 235-244.	0.8	1
5708	Multicomponentâ€Reactionâ€(MCRâ€) Assisted Synthesis of a Coumarinâ€Based Deep Blue Emitter for OLEDs and Related Applications. ChemistrySelect, 2018, 3, 2951-2957.	0.7	14
5709	Synthesis, spectroscopic characterization, DFT studies and antifungal activity of (E)-4-amino-5-[N'-(2-nitro-benzylidene)-hydrazino]-2,4-dihydro-[1,2,4]triazole-3-thione. Journal of Molecular Structure, 2018, 1164, 386-403.	1.8	43
5710	Theoretical calculation of enthalpy of formation of multiconformational molecules: 1,2-ethanediol, propanediols, and glycerol. Chemical Physics Letters, 2018, 698, 218-222.	1.2	8
5711	Changes of Normal Coordinates and Geometrical Parameters of a Molecule in a Laser Field. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2018, 124, 21-31.	0.2	0
5712	Investigation of the Redox and Acidâ€Base properties of TCNQF and TCNQF₂: Electrochemistry, Vibrational Spectroscopy, and Substituent Effects. ChemElectroChem, 2018, 5, 1173-1185.	1.7	19

#	Article	IF	Citations
5713	Theoretical investigations of transport properties of organic solvents in cation-functionalized graphene oxide membranes: Implications for drug delivery. Nano Research, 2018, 11, 254-263.	5.8	7
5714	FT-IR and FT-Raman spectra of 5-chlorocytosine: Solid state simulation and tautomerism. Effect of the chlorine substitution in the Watson-Crick base pair 5-chlorodeoxycytidine-deoxyguanosine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 418-435.	2.0	6
5715	Spectroscopic investigations using density functional theory on 2-methoxy-4(phenyliminomethyl)phenol: A non linear optical material. Journal of Molecular Structure, 2018, 1155, 249-259.	1.8	5
5716	Synthesis, characterization and computational studies of 3-{(E)-[(2-hydroxyphenyl)imino]methyl}benzene-1,2-diol and molecular structure of its zwitterionic form. Journal of Molecular Structure, 2018, 1152, 21-28.	1.8	5
5717	Structure, spectroscopic analyses (FT-IR and NMR), vibrational study, chemical reactivity and molecular docking study on 3,3'-((4-(trifluoromethyl)phenyl)methylene)bis(2-hydroxynaphthalene-1,4-dione), a promising anticancerous bis-lawsone derivative. Journal of Molecular Structure, 2018, 1154, 596-605.	1.8	7
5718	A combined experimental (IR, Raman and UVâ€“Vis) and quantum chemical study of canadine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 249-258.	2.0	4
5719	Structural investigation of anhydrous nitrofurantion and its monohydrate based on terahertz/Raman vibrational spectroscopy and density functional theory. Journal of Molecular Structure, 2018, 1153, 170-178.	1.8	7
5720	Role of the Diphosphine Chelate in Emissive, Chargeâ€Neutral Iridium(III) Complexes. Chemistry - A European Journal, 2018, 24, 624-635.	1.7	12
5721	Synthesis, spectroscopic investigations, DFT studies, molecular docking and antimicrobial potential of certain new indole-isatin molecular hybrids: Experimental and theoretical approaches. Journal of Molecular Structure, 2018, 1153, 333-345.	1.8	41
5722	Simulated Raman spectra of four tetraphenylbutadiene polymorphs. International Journal of Quantum Chemistry, 2018, 118, e25503.	1.0	2
5723	Infrared multiple photon dissociation spectroscopy of cationized canavanine: Side-chain substitution influences gas-phase zwitterion formation. International Journal of Mass Spectrometry, 2018, 429, 158-173.	0.7	7
5724	Effect of hydrogenâ€bonded interactions on the energetics and spectral properties of the astromolecule aminoacetonitrile. International Journal of Quantum Chemistry, 2018, 118, e25459.	1.0	1
5725	Ring opening of azetidine cycle: First examples of 1-azetidinepropanamine molecules as a template in hybrid organic-inorganic compounds. Journal of Molecular Structure, 2018, 1151, 88-96.	1.8	13
5726	Copper(II) complex with 6-methylpyridine-2-carboxyclic acid: Experimental and computational study on the XRD, FT-IR and UVâ€“Vis spectra, refractive index, band gap and NLO parameters. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 220-230.	2.0	55
5727	Experimental and computational approaches to the analysis of the molecular structure of (E)-3-(3-(4-nitrophenyl)triaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile. Journal of Molecular Structure, 2018, 1155, 239-248.	1.8	5
5728	Raman spectra of thiolated arsenicals with biological importance. Talanta, 2018, 179, 520-530.	2.9	9
5729	Harmonic Force Constants for Molecular Mechanics Force Fields via Hessian Matrix Projection. Journal of Chemical Theory and Computation, 2018, 14, 274-281.	2.3	51
5730	Spectroscopic and theoretical studies of dalbergin and Methyldalbergin. Journal of Molecular Structure, 2018, 1156, 243-254.	1.8	4

#	Article	IF	Citations
5731	Molecular structure and hydrogen bond interactions of a paracetamolâ€“4,4â€²-bipyridine cocrystal studied using a vibrational spectroscopic and quantum chemical approach. CrystEngComm, 2018, 20, 213-222.	1.3	18
5732	Synthesis and characterization of sulfolane-based amino alcohols: A combined experimental and computational study. Journal of Molecular Structure, 2018, 1157, 149-158.	1.8	7
5733	The truth is out there: the metal-Ï€ interactions in crystal of Cr(CO)₃(pcp) as revealed by the study of vibrational smearing of electron density. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 317-336.	0.4	7
5734	ForceGen: atomic covalent bond value derivation for Gromacs. Journal of Molecular Modeling, 2018, 24, 5.	0.8	13
5735	A kinetic study of the gas-phase reactions of 1-methylsilacyclobutane in hot wire chemical vapor deposition. Physical Chemistry Chemical Physics, 2018, 20, 75-85.	1.3	8
5736	Excited state energy fluctuations in the Fennaâ€“Matthewsâ€“Olson complex from molecular dynamics simulations with interpolated chromophore potentials. Physical Chemistry Chemical Physics, 2018, 20, 3310-3319.	1.3	31
5737	Advances in Anharmonic Methods and Their Applications to Vibrational Spectroscopies. , 2018, , 483-512.		9
5738	Optimized molecular geometries, vibrational spectra, and frontier molecular orbital of fluorinated liquid crystals- a comparative quantum chemical calculations. Molecular Crystals and Liquid Crystals, 2018, 669, 12-26.	0.4	6
5739	Structural description, spectral analysis and reactivity descriptors of nematogens containing cyano group- a comparative quantum chemical computational approach. Molecular Crystals and Liquid Crystals, 2018, 669, 61-75.	0.4	8
5740	Crystal structures of racemic and enantiopure synephrine correlated with physicochemical properties from IR spectroscopy and thermal analysis. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1531-1539.	0.2	1
5741	4-(2-Methoxy-4-(prop-1-enyl)phenoxy)phthalonitrile; synthesis, characterization, Hirshfeld surface analysis and chemical activity studies. Molecular Crystals and Liquid Crystals, 2018, 667, 88-111.	0.4	5
5742	In vivo measurement of the dynamics of norepinephrine in an olfactory bulb following ischemia-induced olfactory dysfunction and its responses to dexamethasone treatment. Analyst, The, 2018, 143, 5247-5254.	1.7	2
5743	Effect of the degree of inversion on optical properties of spinel ZnFe₂O₄. Physical Chemistry Chemical Physics, 2018, 20, 28267-28278.	1.3	88
5744	In situ attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy combined with non-negative matrix factorization for investigating the synthesis reaction mechanism of 3-amino-4-amino-oxime furazan. Analytical Methods, 2018, 10, 5817-5822.	1.3	12
5745	The mechanism of pyrolysis of 2-azidoethanol: A theoretical study. Computational and Theoretical Chemistry, 2018, 1146, 10-14.	1.1	2
5746	Temperature Dependent Micro-Structure of KAlF4 from Solid to Molten States. Materials, 2018, 11, 1846.	1.3	4
5747	A systematic benchmarking of computational vibrational spectroscopy with DFTB3: Normal mode analysis and fast Fourier transform dipole autocorrelation function. Journal of Computational Chemistry, 2018, 39, 2067-2078.	1.5	7
5748	Raman Spectroscopic Analysis of Signaling Moleculesâ€“Dopamine Receptors Interactions in Living Cells. ACS Omega, 2018, 3, 14849-14857.	1.6	8

#	Article	IF	Citations
5749	Time-Resolved Spectroscopic Study of N,N-Di(4-bromo)nitrenium Ions in Selected Solutions. Molecules, 2018, 23, 3182.	1.7	6
5750	[((R)-C₈H₁₂N)₄][Bi₂Br₁₀] and [((S)-C₈H₁₂N)₄][Bi₂Br₁₀]: Chiral Hybrid Bismuth Bromides Templated by Chiral Organic Cations. ACS Omega, 2018, 3, 17895-17903.	1.6	54
5751	Effect and Characterization of Stoneâ€“Wales Defects on Graphene Quantum Dot: A First-Principles Study. Condensed Matter, 2018, 3, 50.	0.8	10
5752	Synthesis, spectroscopic investigation, molecular docking and DFT studies of novel (2Z,4Z)-2,4-bis(4-chlorobenzylidene)-5-oxo-1-phenylpyrrolidine-3-carboxylic acid (BCOPCA). Heliyon, 2018, 4, e01009.	1.4	5
5753	Electronic and ligating properties of carbocyclic carbenes: A theoretical investigation. Journal of Computational Chemistry, 2018, 40, 726.	1.5	7
5754	Tuning Hydrogenated Silicon, Germanium, and SiGe Nanocluster Properties Using Theoretical Calculations and a Machine Learning Approach. Journal of Physical Chemistry A, 2018, 122, 9851-9868.	1.1	9
5755	Analytic second derivatives for the efficient electrostatic embedding in the fragment molecular orbital method. Journal of Computational Chemistry, 2018, 39, 2039-2050.	1.5	4
5756	Uncontracted core Pople basis sets in vibrational frequency calculations. International Journal of Quantum Chemistry, 2018, 118, e25761.	1.0	4
5757	Mechanistic Studies on the Base-Promoted Conversion of Alkoxy-Substituted, Ring-Fused gem-Dihalocyclopropanes into Furans: Evidence for a Process Involving Electrocyclic Ring Closure of a Carbonyl Ylide Intermediate. Journal of Organic Chemistry, 2018, 83, 13678-13690.	1.7	7
5758	Spectral Calculations with DFT. , 0, , .		5
5759	Structural, density functional computational studies and antibacterial screening on N,Nâ€²-bis-(4-hydroxy-Î±-methylsalicylidene)ethylenediamine nickel (II) complex. Polyhedron, 2018, 156, 165-173.	1.0	0
5760	Pyrolysis of (thio)carbonates via computation analysis. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850041.	1.8	0
5761	Tuning the optoelectronic and charge transport properties of 2,5-di(pyrimidin-5-yl)thieno[3,2-b]thiophene by oligocene end cores substitution. Results in Physics, 2018, 11, 599-604.	2.0	15
5762	Ligand Design forN,O- orN,N-Pyrazolone-Based Hydrazones Ruthenium(II)-Arene Complexes and Investigation of Their Anticancer Activity. Inorganic Chemistry, 2018, 57, 14123-14133.	1.9	47
5763	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	1.1	25
5764	Three novel Cu(II), Cd(II) and Cr(III) complexes of 6â^'Methylpyridineâ^'2â^'carboxylic acid with thiocyanate: Synthesis, crystal structures, DFT calculations, molecular docking and Î±-Glucosidase inhibition studies. Tetrahedron, 2018, 74, 7198-7208.	1.0	49
5765	Synthesis and Antifungal Activity of Î²-Hydroxysulfides of 1,3-Dioxepane Series. Journal of Chemistry, 2018, 2018, 1-14.	0.9	2
5766	Protonated glycine supramolecular systems: the need for quantum dynamics. Chemical Science, 2018, 9, 7894-7901.	3.7	35

#	Article	IF	Citations
5767	Organic nanoparticles based on Lewis-pair formation: observation of prototropically controlled dual fluorescence. Photochemical and Photobiological Sciences, 2018, 17, 1376-1385.	1.6	3
5768	Role of weak Câ€”H...O and strong Nâ€”H...O intermolecular interactions on the high-symmetry molecular packing of trans-cyclohexane-1,4-dicarboxamide. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 1068-1078.	0.2	3
5769	On avoiding negative electron density in Gram-Charlier refinements of anharmonic motion: the example of glutathione. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 695-706.	0.4	4
5770	Synthesis and characterization of the pyridineâ€”bromine trifluoride (1/1) complex, [pyâ˚™BrF3]. Journal of Fluorine Chemistry, 2018, 215, 17-24.	0.9	5
5771	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye â€“ A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 324-332.	2.0	4
5772	Cluster-model DFT simulations of the infrared spectra of triazine-based molecular crystals. Physical Chemistry Chemical Physics, 2018, 20, 20779-20784.	1.3	14
5773	A combined time-resolved infrared and density functional theory study of the lowest excited states of 9-fluorenone and 2-naphthaldehyde. Chemical Physics, 2018, 512, 44-52.	0.9	9
5774	Substituted 1-(isoxazol-3-yl)methyl-1H-1,2,3-triazoles: Synthesis, palladium(II) complexes, and high-turnover catalysis in aqueous media. Tetrahedron, 2018, 74, 3578-3588.	1.0	10
5775	Practical procedure for a theoretical investigation of thermodynamics and kinetics aspects of different-scale radical reactions from addition and cyclization to cyclocopolymerization involving maleic anhydride and divinyl ether. Polymer, 2018, 146, 429-445.	1.8	2
5776	Investigation into structure and dehydration dynamic of gallic acid monohydrate: A Raman spectroscopic study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 201, 128-133.	2.0	15
5777	Reactions of Laser-Ablated Aluminum Atoms with Cyanogen: Matrix Infrared Spectra and Electronic Structure Calculations for Aluminum Isocyanides Al(NC)_{1,2,3} and Their Novel Dimers. Journal of Physical Chemistry A, 2018, 122, 5342-5353.	1.1	10
5778	Does the Intramolecular Hydrogen Bond Affect the Spectroscopic Properties of Bicyclic Diazole Heterocycles?. Journal of Spectroscopy, 2018, 2018, 1-15.	0.6	5
5779	VUV Absorption Spectra of Gas-Phase Quinoline in the 3.5â€“10.7 eV Photon Energy Range. Journal of Physical Chemistry A, 2018, 122, 5832-5847.	1.1	8
5780	Quantitative Studies on the Structure of Molten Binary Potassium Molybdates by in Situ Raman Spectroscopy and Quantum Chemistry ab Initio Calculations. Analytical Chemistry, 2018, 90, 9085-9092.	3.2	11
5781	Redox Active Quinoidal 1,2,4-Benzotriazines. Journal of Organic Chemistry, 2018, 83, 9391-9402.	1.7	13
5782	Theoretical study of a series of 4,4â€²-azo-1H-1,2,4-triazol-5-one based nitrogen-rich salts as potential energetic compounds. RSC Advances, 2018, 8, 23805-23816.	1.7	7
5783	Isotope Effects Reveal an Alternative Mechanism for â€œIminium-Ionâ€•Catalysis. Journal of the American Chemical Society, 2018, 140, 8396-8400.	6.6	13
5784	Vibrational spectra, structure, theoretical calculations of 3-Fluoro-4-Hydroxybenzaldehyde: With evidence of hydrogen bonding. Journal of Molecular Structure, 2018, 1173, 814-821.	1.8	7

#	Article	IF	Citations
5785	Conjugation in multi-tetrazole derivatives: a new design direction for energetic materials. Journal of Molecular Modeling, 2018, 24, 173.	0.8	4
5786	Synthesis and electronic structure studies of a novel nonlinear optical crystal L-leucinium squarate monohydrate: A spectroscopic view. Journal of Physics and Chemistry of Solids, 2018, 122, 143-153.	1.9	11
5787	From O₂^{â€“}-Initiated SO₂ Oxidation to Sulfate Formation in the Gas Phase. Journal of Physical Chemistry A, 2018, 122, 5781-5788.	1.1	12
5788	Influence of terminal halogen moieties on the phase structure of short-core achiral hockey-stick-shaped mesogens: design, synthesis and structureâ€“property relationship. Molecular Systems Design and Engineering, 2018, 3, 839-852.	1.7	17
5789	Regioselective Functionalization of the [closo-1-CB₉H₁₀]^{â^’} Anion through Iodonium Zwitterions. Inorganic Chemistry, 2018, 57, 10442-10456.	1.9	16
5790	DFT exploration of [3 + 2] cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate. RSC Advances, 2018, 8, 27406-27416.	1.7	7
5791	Fragmentation of chlorpyrifos by thermal electron attachment: a likely relation to its metabolism and toxicity. Physical Chemistry Chemical Physics, 2018, 20, 22272-22283.	1.3	5
5792	Synthesis, crystal structure, and vibrational and DFT simulation studies of benzylammonium dihydrogen phosphite. Journal of Physics and Chemistry of Solids, 2018, 123, 150-156.	1.9	10
5793	Density functional theory calculations, vibration spectral analysis and molecular docking of the antimicrobial agent 6-(1,3-benzodioxol-5-ylmethyl)-5-ethyl-2-{[2-(morpholin-4-yl)ethyl] sulfanyl}pyrimidin-4(3H)-one. Open Chemistry, 2018, 16, 653-666.	1.0	8
5794	An FT-Raman, FT-IR, and Quantum Chemical Investigation of Stanozolol and Oxandrolone. Biosensors, 2018, 8, 2.	2.3	8
5795	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg²⁺. Journal of Physical Chemistry A, 2018, 122, 6147-6155.	1.1	23
5796	A Strongly Luminescent Chromium(III) Complex Acid. Chemistry - A European Journal, 2018, 24, 12555-12563.	1.7	39
5797	Do Mono-oxo Sites Exist in Silica-Supported Cr(VI) Materials? Reassessment of the Resonance Raman Spectra. Journal of Physical Chemistry C, 2018, 122, 17149-17160.	1.5	8
5798	Modulation of Donor-Acceptor Distance in a Series of Carbazole Push-Pull Dyes; A Spectroscopic and Computational Study. Molecules, 2018, 23, 421.	1.7	10
5799	Third-order optical nonlinearities of 1,5-Diaminoanthraquinone for optical limiting application. Optics and Laser Technology, 2018, 108, 218-234.	2.2	56
5800	Oxidopyrylium-Alkene [5 + 2] Cycloaddition Conjugate Addition Cascade (C³) Sequences: Scope, Limitation, and Computational Investigations. Journal of Organic Chemistry, 2018, 83, 9818-9838.	1.7	19
5801	Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. Journal of Chemical Theory and Computation, 2018, 14, 4380-4390.	2.3	26
5802	Excited-State Electronic Asymmetry Prevents Photoswitching in Terthiophene Compounds. Inorganic Chemistry, 2018, 57, 9039-9047.	1.9	1

#	Article	IF	Citations
5803	Mode-Selective Raman Imaging of Dopamineâ€“Human Dopamine Transporter Interaction in Live Cells. ACS Chemical Neuroscience, 2018, 9, 3117-3127.	1.7	8
5804	Experimental and DFT insights into molecular structure and optical properties of new chalcones as promising photosensitizers towards solar cell applications. Applied Surface Science, 2018, 452, 337-351.	3.1	90
5805	First-principles study on vibrationally resolved fluorescence of fused 5,15-(diphenyl)-10,20-(dibromo)porphyrin molecule. Journal of Chemical Physics, 2018, 149, 074312.	1.2	2
5806	A systematic examination of ligand basicity effects on bonding in palladium(0)- and palladium(II)-ethylene complexes. Inorganica Chimica Acta, 2018, 483, 191-202.	1.2	2
5807	Anharmonic vibrational eigenfunctions and infrared spectra from semiclassical molecular dynamics. Journal of Chemical Physics, 2018, 149, 064115.	1.2	28
5808	A Study of the Terahertz Spectra of Crystalline Materials (Polyethylene, Poly(Vinylidene Fluoride)) Tj ETQq1 1 0.784314 rgBT /Overloc 552-559.	0.3	4
5809	A DFT Study on the Selective Oxidation of Ethane Over Pure SBA-15 and SBA-15-supported Vanadium Oxide. Kinetics and Catalysis, 2018, 59, 393-404.	0.3	3
5810	Experimental vibrational spectroscopy (FTIR and FT-Raman) of D-tryptophan and its anharmonic theoretical studies using density functional theory. Journal of Molecular Structure, 2018, 1171, 315-322.	1.8	14
5811	DFT computations on vibrational spectra: Scaling procedures to improve the wavenumbers. ChemistrySelect, 2018, 3, .	0.7	16
5812	Global warming potential estimates for the C₁â€“C₃ hydrochlorofluorocarbons (HCFCs) included in the Kigali Amendment to the Montreal Protocol. Atmospheric Chemistry and Physics, 2018, 18, 6317-6330.	1.9	32
5813	Investigation into tautomeric polymorphism of 2-thiobarbituric acid using experimental vibrational spectroscopy combined with DFT theoretical simulation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 204, 99-104.	2.0	20
5814	Micro-structure studies of the molten binary K₃AlF₆â€“Al₂O₃system byin situhigh temperature Raman spectroscopy and theoretical simulation. Inorganic Chemistry Frontiers, 2018, 5, 1861-1868.	3.0	37
5815	Thermodynamic assessment of carbazole-based organic polycyclic compounds for hydrogen storage applications via a computational approach. International Journal of Hydrogen Energy, 2018, 43, 12158-12167.	3.8	22
5816	Synthesis, molecular structure, quantum chemical analysis, spectroscopic and molecular docking studies of N-(Morpholinomethyl) succinimide using DFT method. Journal of Molecular Structure, 2019, 1175, 609-623.	1.8	10
5817	Structural reactivity analyses of a neoflavonoid 4-methoxydalbergione using vibrational spectroscopy and quantum chemical calculations. Journal of Molecular Structure, 2019, 1175, 28-38.	1.8	7
5818	Synthesis, DFT and biological studies of novel 3,6-dimethyl-1,8-diphenyl-diazocino[3,4-c:7,8-câ€™]bispyrazole. Journal of Molecular Structure, 2019, 1176, 66-72.	1.8	2
5819	Conformational analysis, infrared/Raman spectral assignment, and electronic structural studies of 1,3-dimethyl-2-imidazolidinone using quantum chemical calculations. Journal of Molecular Structure, 2019, 1175, 708-720.	1.8	7
5820	Synthesis, biological evaluation, molecular docking and DFT calculations of novel benzenesulfonamide derivatives. Journal of Molecular Structure, 2019, 1176, 408-421.	1.8	52

#	Article	IF	Citations
5821	A Computational Study of 2-(chloromethyl)oxirane Ring Opening by Bromide and Acetate Anions Considering Electrophilic Activation with Cations of Alkali Metals. Croatica Chemica Acta, 2019, 92, 357-367.	0.1	3
5822	Vibrational spectroscopic characterization, electronic absorption, optical nonlinearity computation and terahertz investigation of (2E) 3-(4-ethoxyphenyl)-1-(3-bromophenyl) prop-2-en-1-one for NLO device fabrication. Journal of Molecular Structure, 2019, 1198, 126909.	1.8	5
5823	Diastereoselective synthesis and cytotoxic evaluation of new isoxazoles and pyrazoles with monoterpenic skeleton. Journal of Molecular Structure, 2019, 1198, 126924.	1.8	37
5824	Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset. Physical Review B, 2019, 100, .	1.1	51
5825	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. Journal of Physical Chemistry A, 2019, 123, 7057-7074.	1.1	19
5826	A novel series of mixed-ligand M(II) complexes containing 2,2â€²-bipyridyl as potent Î±-glucosidase inhibitor: synthesis, crystal structure, DFT calculations, and molecular docking. Journal of Biological Inorganic Chemistry, 2019, 24, 747-764.	1.1	44
5827	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570.	1.3	11
5828	Novel Cu(II), Co(II) and Zn(II) metal complexes with mixed-ligand: Synthesis, crystal structure, Î±-glucosidase inhibition, DFT calculations, and molecular docking. Journal of Molecular Structure, 2019, 1197, 645-655.	1.8	49
5829	Hirshfeld surface analysis and DFT studies on molecular structure, vibrational spectra, NMR chemical shifts and NBO analysis of Bis(2-hydroxyethyl(phenyl)carbamodithioate) nickel (II). Journal of Molecular Structure, 2019, 1197, 308-317.	1.8	14
5830	Theoretical and experimental investigation on the electrochemical properties, structural and spectroscopic parameters of 6,7-dihydroxy-9-thia-1,4a-diaza fluoren-2-one (DTDFO). Journal of Sulfur Chemistry, 2019, 40, 598-613.	1.0	0
5831	Membrane-specific spin trap, 5-dodecylcarbamoyl-5-N-dodecylacetamide-1-pyroline-N-oxide (diC₁₂PO): theoretical, bioorthogonal fluorescence imaging and EPR studies. Organic and Biomolecular Chemistry, 2019, 17, 7694-7705.	1.5	5
5832	Impact of Sodium Cationization on Gas-Phase Conformations of DNA and RNA Cytidine Mononucleotides. Journal of the American Society for Mass Spectrometry, 2019, 30, 1758-1767.	1.2	4
5833	Mechanism and theory of <scp>d</scp>-glucopyranose homogeneous acid catalysis in the aqueous solution phase. Physical Chemistry Chemical Physics, 2019, 21, 17993-18011.	1.3	9
5834	Theoretical investigation of the structure, detonation properties, and stability of bicyclo[3.2.1]octane derivatives. Journal of Molecular Modeling, 2019, 25, 253.	0.8	5
5835	Antioxidant properties of Aloe vera components: a DFT theoretical evaluation. Free Radical Research, 2019, 53, 922-931.	1.5	33
5836	DFT Study of the CNS Ligand Effect on the Geometry, Spin-State, and Absorption Spectrum in Ruthenium, Iron, and Cobalt Quaterpyridine Complexes. ACS Omega, 2019, 4, 10991-11003.	1.6	13
5837	Structural, spectroscopic, Hirshfeld surface and charge distribution analysis of 3-(1H-imidazole-1-yl)-1-phenylpropan-1-ol complemented by molecular docking predictions: An integrated experimental and computational approach. Journal of Molecular Structure, 2019, 1196, 578-591.	1.8	5
5838	Towards a simplified description of thermoelectric materials: accuracy of approximate density functional theory for phonon dispersions. Journal of Physics Condensed Matter, 2019, 31, 395901.	0.7	6

#	Article	IF	Citations
5839	Gear Slippage in Molecular Bevel Gears Bridged with a Group 14 Element. Journal of Organic Chemistry, 2019, 84, 14636-14643.	1.7	8
5840	Structural and Reactivity Analyses of Nitrofurantoinâ€“4-dimethylaminopyridine Salt Using Spectroscopic and Density Functional Theory Calculations. Crystals, 2019, 9, 413.	1.0	7
5841	Pyrazole Compounds : Synthesis, molecular structure, chemical reactivity, experimental and theoretical DFT FTIR spectra. Materials Today: Proceedings, 2019, 13, 956-963.	0.9	7
5842	Benchmarking DFT-D Dispersion Corrections for Anharmonic Vibrational Frequencies and Harmonic Scaling Factors. Journal of Physical Chemistry A, 2019, 123, 9800-9808.	1.1	16
5843	How to Fight Kinetics in Complex Radical Polymerization Processes: Theoretical Case Study of Poly(divinyl etherâ€altâ€maleic anhydride). Macromolecular Chemistry and Physics, 2019, 220, 1900389.	1.1	2
5844	Novel approach to passivation of InAs/GaSb type II superlattice photodetectors. Applied Physics B: Lasers and Optics, 2019, 125, 1.	1.1	4
5845	Molecular-Level Insight into the Hydroxylated Monomeric VO_x/Î¸-Al₂O₃(010) and Its Adsorption of Methanol. Journal of Physical Chemistry C, 2019, 123, 27704-27711.	1.5	6
5846	Infrared Spectra of CH₃CNâ†'M, Mâ^'Î·²-(NC)â€“CH₃, CH₃â€“MNC Prepared by Reactions of Laser-Ablated Fe, Ru, and Pt Atoms with Acetonitrile in Excess Argon. Inorganic Chemistry, 2019, 58, 16194-16204.	1.9	6
5847	Evaluating Computational Chemistry Methods for Isotopic Fractionation between CO2(g) and H2O(g). Journal of Chemical Information and Modeling, 2019, 59, 4663-4677.	2.5	1
5848	IR Spectra of Crystalline Nucleobases: Combination of Periodic Harmonic Calculations with Anharmonic Corrections Based on Finite Models. Journal of Physical Chemistry B, 2019, 123, 10001-10013.	1.2	18
5849	Application of Molecular Electrostatic Potential Surface to Predict Supramolecular Synthons for RDX/Solvent Cocrystals. Crystal Research and Technology, 2019, 54, 1900171.	0.6	6
5850	Development and Implementation of Excited-State Gradients for Local Hybrid Functionals. Journal of Chemical Theory and Computation, 2019, 15, 5508-5522.	2.3	21
5851	Spectroscopic Evidence for Lactam Formation in Terminal Ornithine b₂⁺ and b₃⁺ Fragment Ions. Journal of the American Society for Mass Spectrometry, 2019, 30, 1565-1577.	1.2	2
5852	Detailed kinetic model for hexyl sulfide pyrolysis and its desulfurization by supercritical water. Physical Chemistry Chemical Physics, 2019, 21, 10311-10324.	1.3	12
5853	Raman and FTIR Study of a 2, 3'-difluoro-4''-isothiocyanato-4-propyl-1,1':4',1''-terphenyl compound or C3P(3F)P(3F)P-NCS. Molecular Crystals and Liquid Crystals, 2019, 681, 45-57.	0.4	4
5854	Protoisomerization of Indigo and Isoindigo Dyes Confirmed by Gas-Phase Infrared Ion Spectroscopy. Journal of Physical Chemistry A, 2019, 123, 8226-8233.	1.1	16
5855	FTIR and dispersive gas phase absolute infrared intensities of hydrocarbon fundamental bands. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 1-6.	2.0	7
5856	Theoretical studies on the structures, material properties, and IR spectra of polymorphs of 3,4-bis(1H-5-tetrazolyl)furoxan. Journal of Molecular Modeling, 2019, 25, 51.	0.8	3

#	Article	IF	Citations
5857	Formation of a Toxic Quinoneimine Metabolite from Diclofenac: A Quantum Chemical Study. Drug Metabolism Letters, 2019, 13, 64-76.	0.5	5
5858	Experimental and theoretical study on the kinetics and mechanism of the amine-catalyzed reaction of oxiranes with carboxylic acids. Reaction Kinetics, Mechanisms and Catalysis, 2019, 126, 903-919.	0.8	13
5859	Charge localization in 1D tetramerized organic conductors: the special case of (tTTF)2ClO4. Journal of Physics Condensed Matter, 2019, 31, 155601.	0.7	0
5860	Catalytic dissociation of tris(dimethylamino)silane on hot tungsten and tantalum filament surfaces. Physical Chemistry Chemical Physics, 2019, 21, 14357-14365.	1.3	3
5861	DFT study of the solvation effect on an antiangiogenic deguelin analogue's structure and properties. Chemical Data Collections, 2019, 20, 100185.	1.1	0
5862	Thermochemistry of volatile metal hydroxides and oxyhydroxides at elevated temperatures. Journal of Materials Research, 2019, 34, 394-407.	1.2	12
5863	Synthesis, spectroscopic studies and DFT/TD-DFT/PCM calculations of molecular structure, spectroscopic characterization and NBO of charge transfer complex between 5-amino-1,3-dimethylpyrazole (5-ADMP) with chloranilic acid (CLA) in different solvents. Journal of Molecular Liquids, 2019, 277, 453-470.	2.3	58
5864	Formation of OH radicals from the simplest Criegee intermediate CH2OO and water. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	11
5865	Adsorption mechanism of propyl gallate as a flotation collector on scheelite: A combined experimental and computational study. Minerals Engineering, 2019, 133, 19-26.	1.8	17
5866	Heat evolution and energy analysis of cyanide bioproduction by a cyanogenic microorganism with the potential for bioleaching of precious metals. Journal of Hazardous Materials, 2019, 377, 284-289.	6.5	35
5867	Opening 2,2-diphenyl-2H-chromene to infrared light. Physical Chemistry Chemical Physics, 2019, 21, 11689-11696.	1.3	7
5868	Insight on the Sequential Vapor Infiltration Mechanisms of Trimethylaluminum with Poly(methyl) Tj ETQq1 1 0.784314 rgBT /Overlock 1 123, 16146-16152.	1.5	35
5869	Calculated Oxygen-Isotope Fractionations among Brucite, Portlandite, and Water. ACS Earth and Space Chemistry, 2019, 3, 1584-1593.	1.2	4
5870	Effect of cyclization on bond dissociation enthalpies, acidities and proton affinities of carbamate molecules: A theoretical study. Results in Chemistry, 2019, 1, 100003.	0.9	2
5871	Thermochemistry. Computer Aided Chemical Engineering, 2019, 45, 3-114.	0.3	31
5872	Quantum chemical studies on synthesis, characterization and third order nonlinear optical properties of (E)-2-(benzo[d][1,3]dioxol-5-ylmethylene)hydrazinecarboxamide single crystal. Journal of Materials Science: Materials in Electronics, 2019, 30, 11931-11944.	1.1	10
5873	Chemoselective Reduction of Imines Catalyzed by Ruthenium(II) Halfâ€Sandwich Complexes: A Mechanistic Study. European Journal of Inorganic Chemistry, 2019, 2019, 2947-2955.	1.0	2
5874	Simulations of infrared and Raman spectra in solution using the fragment molecular orbital method. Physical Chemistry Chemical Physics, 2019, 21, 13641-13652.	1.3	11

#	Article	IF	Citations
5875	Quantum molecular dynamic approach to modeling the vibrational spectra of propynenitrile and its 1:1 complexes with water. Computational and Theoretical Chemistry, 2019, 1162, 112499.	1.1	2
5876	First-principles calculation of ideal-gas thermodynamic properties of long-chain molecules by R1SM approachâ€"Application to n-alkanes. Journal of Chemical Physics, 2019, 150, 224101.	1.2	23
5877	Descriptors of transition metal promoters on MoS₂ nanocatalysts for hydrodesulfurization: binding energy of metal sulfides from first principles. Molecular Systems Design and Engineering, 2019, 4, 974-982.	1.7	7
5878	Intramolecular Câ€"H Functionalization Followed by a [2_{Ïƒ} + 2_{Ï€}] Addition via an Intermediate Nickelâ€"Nitridyl Complex. Inorganic Chemistry, 2019, 58, 7131-7135.	1.9	23
5879	Synthesis, molecular structure, spectroscopic properties and biological evaluation of 4-substituted-N-(1H-tetrazol-5-yl)benzenesulfonamides: Combined experimental, DFT and docking study. Journal of Molecular Structure, 2019, 1195, 119-130.	1.8	32
5880	Computational studies of ene reactions between aminoborane (F₃C)₂Bî€N(CH₃)₂ and substituted propenes: additive effects on barriers and reaction energies. Dalton Transactions, 2019, 48, 8161-8174.	1.6	4
5881	Structural, optical, mechanical and dielectric property studies of adduct single crystal 2,4,6-trinitrobenzene-1,3-diol-2-methylimidazole: A spectroscopic and theoretical approach. Physica B: Condensed Matter, 2019, 567, 25-36.	1.3	4
5882	Gauging the Redox Nonâ€Innocence of a Highly Piâ€Acidic Bisâ€Tetrazine Pincer Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2535-2542.	1.0	2
5883	Significant geometry and charge difference between the E₅^{4â^'} bare clusters of group 14 Zintl anions and their coordinated form in [E₅{M(CO)₃}₂]^{4â^'} (E = Si, Ge, Sn, Pb; M = Cr, Mo, W) complexes. New Journal of Chemistry, 2019, 43, 7797-7805.	1.4	9
5884	Cytotoxic Acetogenins from the Roots of Annona purpurea. International Journal of Molecular Sciences, 2019, 20, 1870.	1.8	14
5885	The deconvolution analysis of ATR-FTIR spectra of diacetylene during UV exposure. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 219, 23-32.	2.0	12
5886	3-Substituted Benzo[e][1,2,4]triazines: Synthesis and Electronic Effects of the C(3) Substituent. Journal of Organic Chemistry, 2019, 84, 6377-6394.	1.7	22
5888	A combined experimental and density functional theory study of metformin oxy-cracking for pharmaceutical wastewater treatment. RSC Advances, 2019, 9, 13403-13413.	1.7	24
5889	Impact of fluorination on the photophysics of the flavin chromophore: a quantum chemical perspective. Physical Chemistry Chemical Physics, 2019, 21, 9912-9923.	1.3	16
5890	Collision-induced dissociation of stable nitroxides: A combined tandem mass spectrometry and computational study of TEMPOâ€¢ and SG1â€¢. European Journal of Mass Spectrometry, 2019, 25, 229-238.	0.5	1
5891	A novel series of M(II) complexes of 6â€methylpyridineâ€2â€carboxylic acid with 4(5)methylimidazole: Synthesis, crystal structures, Î±â€glucosidase activity, density functional theory calculations and molecular docking. Applied Organometallic Chemistry, 2019, 33, e4935.	1.7	14
5892	Crystal Structures of Î±- and Î²-Nitrogen Trifluoride. Inorganic Chemistry, 2019, 58, 6422-6430.	1.9	4
5893	Evaluation of Matrix Elements Using Diffusion Monte Carlo Wave Functions. Journal of Physical Chemistry A, 2019, 123, 4370-4378.	1.1	4

#	Article	IF	Citations
5894	Iron(III) complex with N2O2-thiosemicarbazidato and azide ligands. Synthesis mechanism, experimental and theoretical studies. Journal of Molecular Structure, 2019, 1191, 337-344.	1.8	9
5895	Substitution Reactions on Iodine and Bromine: Mechanisms for Facile Halogenations of Heterocycles. Journal of Organic Chemistry, 2019, 84, 5757-5762.	1.7	11
5896	Anharmonicity of Vibrational Modes in Hydrogen Chlorideâ€“Water Mixtures. Journal of Chemical Theory and Computation, 2019, 15, 2535-2547.	2.3	5
5897	Reducing crystallinity on thin film based CMC/PVA hybrid polymer for application as a host in polymer electrolytes. Journal of Non-Crystalline Solids, 2019, 511, 201-211.	1.5	139
5898	Modeling vibrational anharmonicity in infrared spectra of high frequency vibrations of polyatomic molecules. Journal of Chemical Physics, 2019, 150, 090901.	1.2	29
5899	Glucose Can Protect Membranes against Dehydration Damage by Inducing a Glassy Membrane State at Low Hydrations. Membranes, 2019, 9, 15.	1.4	19
5900	Structural Arrangement and Computational Exploration of Guanidinium-Based Ionic Liquids with Benzoic Acid Derivatives as Anions. Crystal Growth and Design, 2019, 19, 2642-2657.	1.4	7
5901	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. Journal of the American Chemical Society, 2019, 141, 6234-6246.	6.6	42
5902	Spectrophotometric and photocatalytic studies of H-bonded charge transfer complex of oxalic acid with imidazole: single crystal XRD, experimental and DFT/TD-DFT studies. New Journal of Chemistry, 2019, 43, 9039-9051.	1.4	36
5903	Triphenylamine-substituted 2-pyridyl-1,2,3-triazole copper(I) complexes: an experimental and computational investigation. Journal of Coordination Chemistry, 2019, 72, 1378-1394.	0.8	8
5904	DFT, molecular docking and experimental FT-IR, FT-Raman, NMR inquisitions on â€œ4-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxy-2-methylpyrimidin-5-amineâ€• Alpha-2-imidazoline receptor agonist antihypertensive agent. Journal of Molecular Structure, 2019, 1186, 468-481.	1.8	83
5905	Firstâ€principles study of vibrational properties of TiSiO₄ clusters. International Journal of Quantum Chemistry, 2019, 119, e25924.	1.0	3
5906	Excited-State Vibrational Frequencies: Restricted Virtual Space Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 2949-2956.	1.1	3
5907	Computational Studies of Relative Stabilities of Low-Spin d⁶ cis- and trans-[M(en)₂X₂]⁺ Complexes (M = Co, Rh, Ir): Steric and Electronic Effects in the Context of the Structural Trans Influence. Journal of Physical Chemistry A, 2019, 123, 2438-2446.	1.1	2
5908	Co-Crystal Formation of Antibiotic Nitrofurantoin Drug and Melamine Co-Former Based on a Vibrational Spectroscopic Study. Pharmaceutics, 2019, 11, 56.	2.0	18
5909	Influence of DFT Functionals and Solvation Models on the Prediction of Far-Infrared Spectra of Pt-Based Anticancer Drugs: Why Do Different Complexes Require Different Levels of Theory?. ACS Omega, 2019, 4, 5254-5269.	1.6	5
5910	Selection rules for estimating the solubility of C4-hydrocarbons in imidazolium ionic liquids determined by machine-learning tools. Journal of Molecular Liquids, 2019, 284, 511-521.	2.3	9
5911	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. Journal of Physical Chemistry A, 2019, 123, 3802-3808.	1.1	26

#	Article	IF	Citations
5912	Two-dimensional copper nanosheets for electrochemical reduction of carbon monoxide to acetate. Nature Catalysis, 2019, 2, 423-430.	16.1	368
5913	Long Carbon-Based Chains of Interstellar Medium Can Have a Triplet Ground State. Why Is This Important for Astrochemistry?. ACS Earth and Space Chemistry, 2019, 3, 863-872.	1.2	18
5914	Experimental and theoretical studies on the thermal decomposition of metformin. Journal of Thermal Analysis and Calorimetry, 2019, 138, 433-441.	2.0	19
5915	Matrix Infrared Spectra and Electronic Structure Calculations of Linear Alkaline Earth Metal Di-isocyanides CNMNC, Ionic (NC)M(NC) Bowties, and Ionic (MNC)₂ Rings. Journal of Physical Chemistry A, 2019, 123, 3743-3760.	1.1	11
5916	Synthesis, spectroscopic and DFT studies of Schiff based (E)-Nâ€²-(Benzo[d][1,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf optical material. Materials Research Express, 2019, 6, 075102.	0.8	8
5917	Probing alkylsilane molecular structure on amorphous silica surfaces by sum frequency generation vibrational spectroscopy: First-principles calculations. Journal of Chemical Physics, 2019, 150, 074703.	1.2	2
5918	Calorimetric and computational study of (1H-Indol-n-yl)methanol and 2-(1H-Indol-n-yl)ethanol (n=2, 3). Thermochimica Acta, 2019, 673, 169-176.	1.2	3
5919	Uncertainty Quantification in First-Principles Predictions of Harmonic Vibrational Frequencies of Molecules and Molecular Complexes. Journal of Physical Chemistry C, 2019, 123, 4072-4084.	1.5	16
5920	A new theoretical calculation of the equilibrium constant and temperature for the carbon isotope exchange reaction between CH4 and CO2. Geothermics, 2019, 79, 140-144.	1.5	6
5921	New Orbital Symmetry-Allowed Route for Cycloreversion of Silacyclobutane and Its Methyl Derivatives. Journal of Physical Chemistry A, 2019, 123, 1749-1757.	1.1	17
5922	Conformational studies of bipyrimidine-based mesogens by combination of DFT calculations and temperature-dependent infrared studies. Liquid Crystals, 2019, 46, 1403-1414.	0.9	2
5923	Thermal and Photophysical Properties of Highly Quadrupolar Liquidâ€Crystalline Derivatives of the [closoâ€B₁₂H₁₂]^{2â^’} Anion. Chemistry - A European Journal, 2019, 25, 2616-2630.	1.7	18
5924	Micro Solid Phase Extraction Surface-Enhanced Raman Spectroscopy (Î¼-SPE/SERS) Screening Test for the Detection of the Synthetic Cannabinoid JWH-018 in Oral Fluid. Analytical Chemistry, 2019, 91, 4780-4789.	3.2	38
5925	A computational study on the electrified Pt(111) surface by the cluster model. Physical Chemistry Chemical Physics, 2019, 21, 6112-6125.	1.3	9
5926	Spectroscopic characterisation of centropolyindanes. Physical Chemistry Chemical Physics, 2019, 21, 4568-4577.	1.3	2
5927	Isoquinoline gas-phase absorption spectrum in the vacuum ultraviolet between 3.7 and 10.7ÂeV. New valence and Rydberg electronic states. RSC Advances, 2019, 9, 5121-5141.	1.7	2
5928	Polymers, Polymerization Reactions, and Computational Quantum Chemistry. , 2019, , 1-16.		3
5929	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. Journal of Physical Chemistry A, 2019, 123, 2142-2152.	1.1	42

#	Article	IF	Citations
5930	A Comparison of Medium-Sized Basis Sets for the Prediction of Geometries, Vibrational Frequencies, Infrared Intensities and Raman Activities for Water. Journal of Physics: Conference Series, 2019, 1290, 012013.	0.3	15
5931	Infrared photodissociation spectroscopy of di-manganese oxide cluster cations. Physical Chemistry Chemical Physics, 2019, 21, 23922-23930.	1.3	8
5932	Structural Effects on the Norrish Type I Î±-Bond Cleavage of Tropospherically Important Carbonyls. Journal of Physical Chemistry A, 2019, 123, 10381-10396.	1.1	11
5933	Simulated NIR spectra as sensitive markers of the structure and interactions in nucleobases. Scientific Reports, 2019, 9, 17398.	1.6	20
5934	Design synthesis and characterization of 2-(4,5-dihydro-2,4,5-triphenylimidazol-1-Yl)-6-methylpyridine:FT-IR, NMR, and computational investigation. AIP Conference Proceedings, 2019, , .	0.3	2
5936	Theoretical Studies on Energetic Nitrogenâ€Rich Heterocyclic Substituted Derivatives of Pyrazino [2, 3â€e] [1, 2, 3, 4] Tetrazineâ€1, 3â€diâ€N â€oxide. ChemistrySelect, 2019, 4, 13646-13655.	0.7	4
5937	Ultrahigh sensitive Raman spectroscopy for subnanoscience: Direct observation of tin oxide clusters. Science Advances, 2019, 5, eaax6455.	4.7	20
5938	Physicochemical studies on proton transfer reaction between methyl[5-(propylthio)-1H-benzoimidazole-2-yl]carbamate (albendazole, ABZ) with 2,4,6- trinitrophenol (picric acid, PA) in chloroform. Journal of Molecular Structure, 2019, 1176, 825-837.	1.8	7
5939	Mechanistic Insights into the Electrochemical Reduction of CO₂ Catalyzed by Iron Cyclopentadienone Complexes. Organometallics, 2019, 38, 1236-1247.	1.1	23
5940	Single-wall carbon nanotube modified with copper-oxamate flat complex probed by synchrotron x-ray photoelectron and x-ray absorption spectroscopies. Journal of Molecular Structure, 2019, 1176, 711-717.	1.8	2
5941	Palladium (II) complex: Synthesis, spectroscopic studies and DFT calculations. Chemical Physics Letters, 2019, 716, 49-60.	1.2	10
5942	Single-Atom Electroplating on Two Dimensional Materials. Chemistry of Materials, 2019, 31, 429-435.	3.2	55
5943	Detecting DNA Methylation Using Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 2019, 123, 698-709.	1.5	11
5944	Structure, Reactivity, Nonlinear Optical Properties and Vibrational Study of 5-Thioxo-1,4-thiazaolidin-3-one and 5-thioxo-1,4,2-thiazasilolidin-3-one (Silicon vs. Carbon). A DFT Study. Silicon, 2019, 11, 2135-2147.	1.8	2
5945	Synthesis, spectroscopic characterization and DFT/TD-DFT computations of a novel charge transfer complex via hydrogen bonding between 3-amino-1,5-dimethylpyrazole with chloranilic acid in different solvents. Journal of Molecular Structure, 2019, 1181, 48-60.	1.8	10
5946	Uncatalyzed gas phase aziridination of alkenes by organic azides. Part 2. Whole azide reaction with alkene. Journal of Chemical Sciences, 2019, 131, 1.	0.7	5
5947	The gas-phase pyrolysis of methyl azidoformate in the absence and presence of water: a theoretical study. Molecular Physics, 2019, 117, 34-41.	0.8	2
5948	Synthesis, biological evaluation and DFT calculation of novel pyrazole and pyrimidine derivatives. Journal of Molecular Structure, 2019, 1179, 304-314.	1.8	58

#	Article	IF	Citations
5949	Screening for potential energetic Câ€“N cages with high energy and good stability: a theoretical comparative study. Molecular Simulation, 2019, 45, 129-136.	0.9	5
5950	A theoretical study on the elimination reaction of acrylonitrile from 2â€²-O-cyanoethylated nucleosides by Bu4NF. Tetrahedron, 2019, 75, 1-9.	1.0	5
5951	A new dinuclear copper (II) complex of 2,5â€“Furandicarboxyclic acid with 4(5)â€Methylimidazole as a high potential Î±â€glucosidase inhibitor: Synthesis, Crystal structure, Cytotoxicity study, and TD/DFT calculations. Applied Organometallic Chemistry, 2019, 33, e4725.	1.7	45
5952	A study of the optical, electrical and structural properties of poly(pyrrole-3,4-dicarboxylic acid). Polymer, 2019, 164, 142-153.	1.8	10
5953	Spectroscopic (FTIR, FT-Raman, 1H NMR and UVâ€“Vis) and DFT/TD-DFT studies on cholesteno [4,6-b,c]-2â€²,5â€²-dihydro-1â€²,5â€²-benzothiazepine. Journal of Molecular Structure, 2019, 1178, 570-582.	1.8	48
5954	Scaling Procedures in Vibrational Spectroscopy. Challenges and Advances in Computational Chemistry and Physics, 2019, , 49-95.	0.6	3
5955	Density functional theory study with and without COSMO of H₂SO₄ reactions in an aqueous environment for metal extraction. Journal of Computational Chemistry, 2019, 40, 591-606.	1.5	2
5956	Improving Vibrational Mode Interpretation Using Bayesian Regression. Journal of Chemical Theory and Computation, 2019, 15, 456-470.	2.3	37
5957	Reverse saturable absorption behavior of Disodium 8-Hydroxy-5,7-Dinitro-2-Naphthalenesulfonate Hydrate for nonlinear optical applications. Journal of Molecular Structure, 2019, 1180, 363-377.	1.8	12
5958	Characterization and absorption properties of newly synthesized mono azo dyes: Experimental and theoretical approach. Journal of Molecular Structure, 2019, 1180, 251-259.	1.8	12
5959	Thermodynamic properties of phase transitions of phenyl derivatives of maleic anhydride and oxazole. Journal of Chemical Thermodynamics, 2019, 131, 489-494.	1.0	3
5960	Theoretical and experimental study by DFT, molecular docking calculations and cytotoxicity assay of 7,7-dimethylaporphine alkaloids type isolated from Guatteria friesiana (Annonaceae). Journal of Molecular Structure, 2019, 1177, 347-362.	1.8	7
5961	Experimental and theoretical studies on the atmospheric degradation of 1, 1, 2, 2, 3, 3, 4-heptafluorocyclopentane. Atmospheric Environment, 2019, 196, 38-43.	1.9	12
5962	Synthesis, spectroscopic investigation and biological activities of copper(II) complex of 2-(2,4-difluorophenyl)pyridine: A combined theoretical and experimental study. Journal of Molecular Structure, 2019, 1177, 242-248.	1.8	6
5963	Spectroscopic exploration in aggregation with in silico molecular modeling and in vitro assay on antioxidant 7-chloro-2-4-fluorophenyl-3-hydroxychromen-4-one. Journal of King Saud University - Science, 2019, 31, 372-383.	1.6	0
5964	Synthesis, structural characterization, and computational study of (E)-Nâ€²-(3,4-dimethoxybenzylidene)furan-2-carbohydrazide. Arabian Journal of Chemistry, 2020, 13, 3571-3584.	2.3	5
5965	X-ray crystal structure, spectroscopic and DFT computational studies of H-bonded charge transfer complexes of tris (hydroxymethyl)aminomethane (THAM) with chloranilic acid (CLA). Journal of Molecular Structure, 2020, 1200, 127066.	1.8	28
5966	Theoretical (DFT) and experimental (Raman and FTIR) spectroscopic study on communic acids, main components of fossil resins. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117405.	2.0	8

#	Article	IF	Citations
5967	On the potential as nonlinear optical material of a new chalcone derivative and its crystal and topological analysis. Journal of Molecular Structure, 2020, 1201, 127131.	1.8	5
5968	The â€œsurfaceâ€•(S) state of the Brâ˜ hydration: An ONIOM-XS MD simulation study. Chemical Physics Letters, 2020, 738, 136853.	1.2	1
5969	DFT, spectroscopic, DSC/TGA, electronic, biological and molecular docking investigation of 2,5-thiophenedicarboxylic acid: A promising anticancer agent. Journal of Molecular Structure, 2020, 1200, 127099.	1.8	14
5970	Influence of the local environment on the intrinsic structures of gas-phase cytidine-5â€²-monophosphates. International Journal of Mass Spectrometry, 2020, 447, 116234.	0.7	0
5971	Effect of solvents on the nonlinear optical behavior and spectral findings of bis [4-(dimethylamino) phenyl] methaniminium chloride. Chemical Physics Letters, 2020, 738, 136833.	1.2	9
5972	Density functional theory, spectroscopic and hydrogen bonding analysis of fenoxycarbâ€“water complexes. Journal of Molecular Structure, 2020, 1201, 127201.	1.8	12
5973	Solvent-free mechanochemical synthesis, hirshfeld surface analysis, crystal structure, spectroscopic characterization and NBO analysis of Bis(ammonium) Bis((4-methoxyphenyl)) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 502 Td (phosphono 1202, 127254.	1.8	21
5974	Synthesis, spectral characterization (FT-IR, NMR, XRD) and computational studies of chloroacetyl chloride incorporated 3t-butyl-2r,6c-diphenyl/di(thiophen-2-yl)piperidin-4-ones. Journal of Molecular Structure, 2020, 1200, 127076.	1.8	5
5975	Density functional calculations on the structural and vibrational properties of 1,4-diaminobutane. Journal of Molecular Structure, 2020, 1199, 126974.	1.8	2
5976	Predominant mechanisms for the removal of nickel metal ion from aqueous solution using cement kiln dust. Journal of Water Process Engineering, 2020, 33, 101033.	2.6	34
5977	PbF[Br 2 F 7], a Fluoridobromate(III) of a pâ€Block Metal. European Journal of Inorganic Chemistry, 2020, 2020, 64-70.	1.0	6
5978	Quantitative analysis on the microstructure of molten binary KFâ€AlF₃ system by in situ Raman spectroscopy assisted with first principles method. Journal of Raman Spectroscopy, 2020, 51, 187-192.	1.2	8
5979	Thermodynamic, kinetic and structural investigation of the catalytic role of some protic solvents on the proton transfer reaction in hydantoin: Density functional theory study. Chemical Physics Letters, 2020, 739, 136931.	1.2	3
5980	Insight into the reaction mechanism for condensation reaction of trioxane and dimethoxymethane over HZSM-5 zeolite. Molecular Catalysis, 2020, 482, 110644.	1.0	2
5981	Synthesis, anti-proliferative activity, computational studies of tetrazole cellulose utilizing different homogenous catalyst. Carbohydrate Polymers, 2020, 229, 115537.	5.1	56
5982	Estimating Systematic Error and Uncertainty in Ab Initio Thermochemistry: II. ATOMIC(hc) Enthalpies of Formation for a Large Set of Hydrocarbons. Journal of Chemical Theory and Computation, 2020, 16, 399-426.	2.3	28
5983	Monoaurated vs. diaurated intermediates: causality or independence?. Chemical Science, 2020, 11, 980-988.	3.7	10
5984	Visualization of vibrational-resolution charge transfer enhanced resonance Raman scattering spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 229, 117945.	2.0	4

#	Article	IF	Citations
5985	Photoelectrochemistry of Ferrites: Theoretical Predictions vs. Experimental Results. Zeitschrift Fur Physikalische Chemie, 2020, 234, 719-776.	1.4	24
5986	Straightforward synthesis, spectroscopic characterizations and comprehensive DFT calculations of novel 1-ester 4-sulfonamide-1,2,3-triazole scaffolds. Journal of Molecular Structure, 2020, 1203, 127405.	1.8	30
5987	Spectral and computational studies on regioselective synthesis of 4-oxo-6-phenyl-2-selenoxo-1,2,3,4-tetrahydropyrimidine-5-carbonitrile. Journal of Molecular Structure, 2020, 1203, 127408.	1.8	2
5988	Statistical molecular fragmentation: which parameters influence the branching ratios?. Physical Chemistry Chemical Physics, 2020, 22, 3160-3172.	1.3	7
5989	Radiative efficiency and global warming potential of the hydrofluoroether HFE-356mec3 (CH3OCF2CHFCF3) from experimental and theoretical infrared absorption cross-sections. Journal of Molecular Spectroscopy, 2020, 367, 111241.	0.4	5
5990	Synthesis, DFT calculations and molecular docking study of mixed ligand metal complexes containing 4,4â€²-dimethyl-2,2â€²-bipyridyl as Î±-glucosidase inhibitors. Journal of Molecular Structure, 2020, 1205, 127655.	1.8	15
5991	Computational study of energetic derivatives of 3,3â€²-bridged ditriazoles. Canadian Journal of Chemistry, 2020, 98, 115-127.	0.6	1
5992	Theoretical Study of the Mechanism of Catalytic Enanteoselective Nâ€“H and Oâ€“H Insertion Reactions. Journal of Physical Chemistry A, 2020, 124, 2-11.	1.1	8
5993	Mechanistic Insight toward Understanding the Role of Charge in Thiourea Organocatalysis. Journal of Organic Chemistry, 2020, 85, 585-593.	1.7	11
5994	The influence of driving force on intramolecular electron transfer: A theoretical study of subphthalocyanineâ€AzaBODIPYâ€C₆₀ supramolecular triad. International Journal of Quantum Chemistry, 2020, 120, e26131.	1.0	4
5995	Static correlation in vibrational frequencies studied using thermally-assisted-occupation density functional theory. Chemical Physics Letters, 2020, 739, 137012.	1.2	13
5996	CO oxidation by linear oxocarbon chains O -C -O (nÂ=Â5â€“10, xÂ=Â1, 2): A theoretical study. Chemical Physics, 2020, 530, 110652.	0.9	3
5997	Relating the thermal properties of a micro pulsating heat pipe to the internal flow characteristics via experiments, image recognition of flow patterns and heat transfer simulations. International Journal of Heat and Mass Transfer, 2020, 163, 120415.	2.5	23
5998	Synthesis and properties of 6,7-dihydroxybenzopyrylium perchlorate halogen derivatives: X-ray, spectroscopic and theoretical studies. Tetrahedron, 2020, 76, 131514.	1.0	10
5999	Steroidal Molecular Rotors with 1,4-Diethynylphenylene Rotators: Experimental and Theoretical Investigations Toward Seeking Efficient Properties. Journal of Physical Chemistry B, 2020, 124, 9625-9635.	1.2	2
6000	Kinetic study of the thermo-oxidative decomposition of metformin by isoconversional and theoretical methods. Thermochimica Acta, 2020, 694, 178797.	1.2	8
6001	Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. Journal of Chemical Theory and Computation, 2020, 16, 7044-7060.	2.3	32
6002	Spectroscopic, quantum chemical and molecular docking studies on 2,4-dimethoxy-1,3,5-triazine: a potent inhibitor of protein kinase CK2 for the development of breast cancer drug. Molecular Simulation, 2020, 46, 1340-1353.	0.9	13

#	Article	IF	Citations
6003	Solvent and catalyst-free synthesis, corrosion protection, thermodynamic, MDS and DFT calculation of two environmentally friendly inhibitors: Bis-phosphonic acids. Journal of Molecular Structure, 2020, 1222, 128813.	1.8	25
6004	Characterization of the simplest sulfenyl thiocyanate: isomers, spectroscopy and implications of astrophysical and biological relevance. Physical Chemistry Chemical Physics, 2020, 22, 17052-17061.	1.3	3
6005	Theoretical study on resonance Raman spectra of meso-tetrakis(3,5-di-tertiarybutylphenyl)-porphyrin due to the second-order Herzberg-Teller mechanism. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 241, 118659.	2.0	1
6006	Isomerization behavior of p-aminoazobenzene directly anchored on MoS2/graphene oxide nanocomposite. Applied Surface Science, 2020, 530, 147216.	3.1	4
6007	Supported Metal Pair-Site Catalysts. ACS Catalysis, 2020, 10, 9065-9085.	5.5	67
6008	Vibrational Spectra of the OH Radical in Water: Ab Initio Molecular Dynamics Simulations and Quantum Chemical Calculations Using Hybrid Functionals. Advanced Theory and Simulations, 2020, 3, 2000174.	1.3	5
6009	Theoretical Investigation on Structure-Property Relationship of Asymmetric Clusters (CH3FBN3)n (nâ€‰=â€‰1â€“â€‰6). Journal of Chemistry, 2020, 2020, 1-11.	0.9	0
6010	Conformers of 1,2,3,4 â€“tetrahydroisoquinoline in S0 and S1: An analysis through potential energy surface, hardness principles and vibrational spectroscopy. Journal of Molecular Structure, 2020, 1207, 127836.	1.8	13
6011	Local Vibrational Mode Analysis of Ï€â€“Hole Interactions between Aryl Donors and Small Molecule Acceptors. Crystals, 2020, 10, 556.	1.0	22
6012	Accessible approaches for vibrational zero point energy calculation of organoboron compounds. Vibrational Spectroscopy, 2020, 110, 103131.	1.2	0
6013	Efficient Computation of Free Energy Contributions for Association Reactions of Large Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6606-6611.	2.1	49
6014	Simple and Accurate Exchange Energy for Density Functional Theory. Molecules, 2020, 25, 3485.	1.7	4
6015	Isoprene polymerizations catalyzed by TiCl4/MgCl2 type Ziegler-Natta catalysts with different titanium contents. Molecular Catalysis, 2020, 494, 111110.	1.0	6
6016	Quantum chemical prediction of the spectroscopic properties and ionic composition of the molten NaF-AlF3 salts. Journal of Molecular Liquids, 2020, 317, 113937.	2.3	12
6017	Sodium Drives Interfacial Equilibria for Semi-Soluble Phosphoric and Phosphonic Acids of Model Sea Spray Aerosol Surfaces. ACS Earth and Space Chemistry, 2020, 4, 1549-1557.	1.2	7
6018	Oxygen isotope fractionation between water and the aqueous hydroxide ion. Geochimica Et Cosmochimica Acta, 2020, 289, 182-195.	1.6	11
6019	Vibrational Zero-Point Energy of Organosilicon Compounds. , 2020, , .		0
6020	Water structure and hydration of polymer network in PMEO2MA hydrogels. Polymer, 2020, 210, 122974.	1.8	19

#	Article	IF	Citations
6021	Diethyl (2-Amino-3-Cyano-4H-Chromen-4-yl)Phosphonate and Its Halogenated Derivatives as Effective Drug: A Theoretical and an Experimental Spectroscopic Study. Polycyclic Aromatic Compounds, 2020, , 1-18.	1.4	0
6022	On the separability of large-amplitude motions in anharmonic frequency calculations. Physical Chemistry Chemical Physics, 2020, 22, 20588-20601.	1.3	1
6023	Analytic first and second derivatives of the energy in the fragment molecular orbital method combined with molecular mechanics. International Journal of Quantum Chemistry, 2020, 120, e26414.	1.0	2
6024	Multiple Reaction Pathways in the Morphinone Reductase-Catalyzed Hydride Transfer Reaction. ACS Omega, 2020, 5, 23468-23480.	1.6	4
6025	Theoretical Investigation of the Atmospheric Cl Oxidation Chemistry of 4-Methyl-3-penten-2-one. ACS Earth and Space Chemistry, 2020, 4, 1957-1965.	1.2	1
6026	Density Functional Theory Calculation and Raman Scattering of the Antihistamine Ebastine. Journal of Applied Spectroscopy, 2020, 87, 608-614.	0.3	4
6027	Semiclassical transition state theory/master equation kinetics of HO + CO: Performance evaluation. International Journal of Chemical Kinetics, 2020, 52, 1022-1045.	1.0	9
6028	Computer-aided design and property prediction of novel insensitive high-energy heterocycle-substituted derivatives of cage NNNAHP. Journal of Molecular Modeling, 2020, 26, 239.	0.8	3
6029	Spectroscopic Study of Solâ€“Gel Entrapped Triruthenium Dodecacarbonyl Catalyst Reveals Hydride Formation. Journal of Physical Chemistry Letters, 2020, 11, 7394-7399.	2.1	4
6030	Ab initio quantum chemical studies of isotopic fractionation during acid digestion reaction of dolomite for clumped isotope application. Rapid Communications in Mass Spectrometry, 2020, 34, e8926.	0.7	0
6031	Theoretical investigation on cis-trans isomerisation of azaphosphatriptycene- based molecular gear. Supramolecular Chemistry, 2020, 32, 569-577.	1.5	1
6032	Theoretical Characterization of the Structure and Spectroscopy of HCNO2 Isomers and Applications. Journal of Physical Chemistry A, 2020, 124, 11061-11071.	1.1	2
6033	FTIR Spectroelectrochemistry of F4TCNQ Reduction Products and Their Protonated Forms. Analytical Chemistry, 2020, 92, 7154-7161.	3.2	18
6034	Probabilistic performance estimators for computational chemistry methods: Systematic improvement probability and ranking probability matrix. II. Applications. Journal of Chemical Physics, 2020, 152, 164109.	1.2	7
6035	Synthesis, spectral characterization, and theoretical investigations of a new azo-stilbene dye for acrylic resins. Journal of Molecular Structure, 2020, 1217, 128380.	1.8	4
6036	The intermolecular anthracene-transfer in a regiospecific antipodal C₆₀difunctionalization. Organic and Biomolecular Chemistry, 2020, 18, 4090-4103.	1.5	1
6037	Optimizing the thermoelectric performances of conjugated polymer backbonesviaincorporating tailored platinum(<scp>ii</scp>) acetylides. Polymer Chemistry, 2020, 11, 3627-3636.	1.9	4
6038	Resonance Raman investigation of dithioniteâ€reduced cobalamin. Journal of Raman Spectroscopy, 2020, 51, 1331-1342.	1.2	6

#	Article	IF	Citations
6039	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. Journal of Chemical Information and Modeling, 2020, 60, 3566-3576.	2.5	13
6040	Tautomers of homophthalic anhydride in the ground and excited electronic states: analysis through energy, hardness and vibrational signatures. Journal of Molecular Modeling, 2020, 26, 173.	0.8	7
6041	Study on the nitrogen migration mechanism during penicillin fermentation residue fast pyrolysis based on the substance transformation and canonical variational theory. Science of the Total Environment, 2020, 737, 139739.	3.9	24
6042	Dissociative electron transfer of copper(<scp>ii</scp>) complexes of glycyl(glycyl/alanyl)tryptophanin vacuo: IRMPD action spectroscopy provides evidence of transition from zwitterionic to non-zwitterionic peptide structures. Physical Chemistry Chemical Physics, 2020, 22, 13084-13091.	1.3	3
6043	Equilibria, kinetics, and boron isotope partitioning in the aqueous boric acidâ€“hydrofluoric acid system. Chemical Geology, 2020, 550, 119693.	1.4	17
6044	Structures, stabilities and electronic properties of the bimetal V2-doped Sin (n = 1â€“10) clusters: a density functional investigation. European Physical Journal D, 2020, 74, 1.	0.6	0
6045	Probing the Structures and Properties of Asymmetric Clusters (CH3ClBN3)n (n = 1â€“6) with Density Functional Theory. Russian Journal of Physical Chemistry A, 2020, 94, 134-142.	0.1	1
6046	Low-dimensional projection approach for efficient sampling of molecular recognition and polymer aggregation. Physical Chemistry Chemical Physics, 2020, 22, 6953-6963.	1.3	1
6047	Boosting Electrocatalytic N₂ Reduction to NH₃ over Two-Dimensional Gallium Selenide by Defect-Size Engineering. Inorganic Chemistry, 2020, 59, 4858-4867.	1.9	44
6048	Conformational Landscapes and Infrared Spectra of Gas-phase Interstellar Molecular Clusters [(C3H3N)(CH3OH)n, n = 1â€“4]. Journal of Physical Chemistry A, 2020, 124, 2398-2407.	1.1	6
6049	Theoretical investigation of neutral decomposition by-products of SF6â€‰+â€‰CO2 mixture in the existence of H2O. Electrical Engineering, 2020, 102, 1451-1467.	1.2	6
6050	Computational insight into polynitromethyl- and polydifluoroaminomethyl-substituted energetic derivatives of 2,3-dihydro pyrazino [2,3-e] [1, 2, 3, 4] tetrazine. Journal of Molecular Modeling, 2020, 26, 78.	0.8	2
6051	A molecular electron density theory study of the [3â€‰+â€‰2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
6052	Quantum Chemical Computations, Molecular Docking, Experimental and DFT Calculation of 4-Amino-3-Phenylbutanoic Acid. Polycyclic Aromatic Compounds, 2022, 42, 1302-1321.	1.4	5
6053	Study of the azoâ€hydrazone tautomerism of Acid Orange 20 by spectroscopic techniques: UVâ€“Visible, Raman, and surfaceâ€enhanced Raman scattering. Journal of Raman Spectroscopy, 2020, 51, 1295-1304.	1.2	11
6054	Polymorphs and pharmacokinetics of an antipsychotic drug candidate. International Journal of Pharmaceutics, 2020, 586, 119600.	2.6	4
6055	Mix and (Mis)match: further studies of the electronic structure and mixed-valence characteristics of 1,4-diethynylbenzene-bridged bimetallic complexes. Dalton Transactions, 2020, 49, 9835-9848.	1.6	8
6056	Spectra, Electronic Structure of 2-Vinyl Naphthalene and Their Oligomeric Scaffold Models: A Quantum Chemical Investigation. Chemistry Africa, 2020, 3, 371-390.	1.2	6

#	Article	IF	Citations
6057	Herzbergâ€“Teller Effect Predominates in Sum-Frequency Vibrational Spectroscopy of Limonene Chiral Liquids. Journal of Physical Chemistry B, 2020, 124, 6642-6650.	1.2	1
6058	Fabrication of hypercrosslinked hydroxyl-rich solid phase extractants for cesium separation from the salt lake brine. Chemical Engineering Journal, 2020, 400, 125991.	6.6	36
6059	Predicting fluorescence quantum yields for molecules in solution: A critical assessment of the harmonic approximation and the choice of the lineshape function. Journal of Chemical Physics, 2020, 152, 054107.	1.2	35
6060	Characterization of coal-based fulvic acid and the construction of a fulvic acid molecular model. RSC Advances, 2020, 10, 5468-5477.	1.7	25
6061	Sterically hindered Re- and Mn-CO2 reduction catalysts for solar energy conversion. Dalton Transactions, 2020, 49, 4230-4243.	1.6	9
6062	A Selenourea-Thiourea BrÃ¸nsted Acid Catalyst Facilitates Asymmetric Conjugate Additions of Amines to Î±,Î²-Unsaturated Esters. Journal of the American Chemical Society, 2020, 142, 5627-5635.	6.6	45
6063	An ab initio study of the effect of hydration on the vibrational spectrum of hydrogen sulfate. Computational and Theoretical Chemistry, 2020, 1176, 112749.	1.1	4
6064	The Methyl Torsion in Unsaturated Compounds. ACS Omega, 2020, 5, 2755-2765.	1.6	11
6065	Raman Optical Activity (ROA) as a New Tool to Elucidate the Helical Structure of Poly(phenylacetylene)s. Angewandte Chemie - International Edition, 2020, 59, 9080-9087.	7.2	22
6066	In Silico Infrared Characterization of Synthetic Cannabinoids by Quantum Chemistry and Chemometrics. Journal of Chemical Information and Modeling, 2020, 60, 2100-2114.	2.5	6
6067	Extensive Quantum Chemistry Study of Neutral and Charged C₄N Chains: An Attempt To Aid Astronomical Observations. ACS Earth and Space Chemistry, 2020, 4, 434-448.	1.2	8
6068	Ab Initio Fragment Molecular Orbital-Based Molecular Dynamics (FMO-MD) Simulations of (NH3)32 Cluster: Effects of Electron Correlation. Bulletin of the Chemical Society of Japan, 2020, 93, 553-560.	2.0	1
6069	Designing and looking for novel low-sensitivity and high-energy cage derivatives based on the skeleton of nonanitro nonaaza pentadecane framework. Structural Chemistry, 2020, 31, 1387-1402.	1.0	7
6070	Removal of Cr (VI) from an aqueous solution using an activated carbon obtained from teakwood sawdust: Kinetics, equilibrium, and density functional theory calculations. Journal of Environmental Chemical Engineering, 2020, 8, 103702.	3.3	51
6071	Formation of Formic Acid Derivatives through Activation and Hydroboration of CO₂ by Low-Valent Group 14 (Si, Ge, Sn, Pb) Catalysts. Journal of Physical Chemistry A, 2020, 124, 1121-1133.	1.1	18
6072	Microsolvation in V⁺(H₂O)_n Clusters Studied with Selected-Ion Infrared Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 1093-1103.	1.1	13
6073	Synthesis, spectral properties,in vitroÎ±â€glucosidase inhibitory activity and quantum chemical calculations of novel mixedâ€ligand M(II) complexes containing 1,10â€phenanthroline. Applied Organometallic Chemistry, 2020, 34, e5412.	1.7	10
6074	Cyanide-free silver immersion deposition involving 3-mercapto-1-propanesulfonic acid for copper finishing. Materials Chemistry and Physics, 2020, 244, 122671.	2.0	9

#	Article	IF	Citations
6075	Theoretical approach to study the formation of C₂H₄O₂ isomers in interstellar medium through reaction between interstellar formaldehyde molecules*. Research in Astronomy and Astrophysics, 2020, 20, 014.	0.7	9
6076	Synthesis, spectroscopic, thermal, structural characterization and DFT/TD-DFT computational studies for charge transfer complexes of 2,4-diamino pyrimidine with some benzoquinone acceptors. Journal of Molecular Liquids, 2020, 309, 113210.	2.3	29
6077	Surface-enhanced Raman scattering for dopamine in Ag colloid: Adsorption mechanism and detection in the presence of interfering species. Applied Surface Science, 2020, 522, 146466.	3.1	44
6078	Raman Optical Activity (ROA) as a New Tool to Elucidate the Helical Structure of Poly(phenylacetylene)s. Angewandte Chemie, 2020, 132, 9165-9172.	1.6	13
6079	Quantum chemical computational and spectroscopic (IR, Raman, NMR, and UV) studies on the 5-(5-methoxy-benzofuran-3-ylmethyl)-3H-[1, 3, 4] oxadiazole-2-thione. Journal of Molecular Structure, 2020, 1210, 128041.	1.8	19
6080	Spectroscopic and in silico study on the conversion of N,Nâ€²-disubstituted hydrazone derivatives of 5-nitrobenzimidazole-2-thione into anion and radical anion products: Implications in hepatotoxicity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 234, 118279.	2.0	3
6081	Anharmonic Frequencies of (MO)₂ and Related Hydrides for M = Mg, Al, Si, P, S, Ca, and Ti and Heuristics for Predicting Anharmonic Corrections of Inorganic Oxides. Journal of Physical Chemistry A, 2020, 124, 3191-3204.	1.1	26
6082	A review on role of tetra-rings in graphene systems and their possible applications. Reports on Progress in Physics, 2020, 83, 056501.	8.1	47
6083	Symmetry breakings in a metal organic framework with a confined guest. Physical Review B, 2020, 101, .	1.1	10
6084	Investigating the conformers of 1, 2, 3, 4-tetrahydroquinoxaline: A combined theoretical and experimental investigation through potential energy surface studies, FT-IR and UVâ€“Vis absorption measurements. Journal of Molecular Structure, 2020, 1211, 128064.	1.8	7
6085	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3307-3315.	2.3	31
6086	Photoexcitation Processes in Oligomethine Cyanine Dyes for Dye-Sensitized Solar Cellsâ€”Synthesis and Computational Study. Nanomaterials, 2020, 10, 662.	1.9	11
6087	Novel metal complexes containing 6-methylpyridine-2-carboxylic acid as potent Î±-glucosidase inhibitor: synthesis, crystal structures, DFT calculations, and molecular docking. Molecular Diversity, 2021, 25, 171-189.	2.1	15
6088	Synthesis, spectra, electronic structure, molecular docking and cytotoxicity investigation on 2-(piperidin-1-ylmethyl)-isoindoline-1,3-dione â€“ A Mannich base system. Journal of Molecular Structure, 2021, 1224, 129151.	1.8	5
6089	Conformer selective monohydrated clusters of 1,2,3,4 â€“tetrahydroisoquinoline in S0: I-Potential energy surface studies, vibrational signatures and NBO analysis. Journal of Molecular Structure, 2021, 1225, 129177.	1.8	8
6090	Pd(II) complexes with ONN pincer ligand: Tailored synthesis, characterization, DFT, and catalytic activity toward the Suzuki-Miyaura reaction. Journal of Molecular Structure, 2021, 1225, 129071.	1.8	13
6091	Highly fluorescent water-soluble PTCA incorporated silver nano-cluster for sensing of dopamine. Materials Chemistry and Physics, 2021, 259, 124086.	2.0	14
6092	A novel quinoxalinedione-bicapped tri-ruthenium carbonyl cluster [Ru3(Î¼-H)2(CO)6(Î¼3-HDCQX)2]: synthesis, characterization, anticancer activity and theoretical investigation of Ruâ€“Ru and Ruâ€“Ligand bonding interactions. Polyhedron, 2021, 193, 114889.	1.0	0

#	Article	IF	Citations
6093	Rapid Evaluation of the Mechanism of Buchwaldâ€“Hartwig Amination and Aldol Reactions Using Intramolecular ¹³C Kinetic Isotope Effects. ACS Catalysis, 2021, 11, 60-67.	5.5	9
6094	Molecular design, property prediction, and intermolecular interactions for highâ€energy cage compounds based on the skeletons of RDX and HMX. Journal of the Chinese Chemical Society, 2021, 68, 557-568.	0.8	2
6095	Cellulose conversion to biofuel precursors using conjugated ionic liquid catalyst: An experimental and DFT studyâ€. Applied Catalysis A: General, 2021, 610, 117951.	2.2	11
6096	Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of infrared spectra of arabidopsis thaliana plant cryptochrome. Physical Chemistry Chemical Physics, 2021, 23, 1666-1674.	1.3	6
6097	Novel Mn(II) and Zn(II) complexes of 6â€bromopicolinic acid as a potential optical material: Synthesis, spectral characterizations, linear, and nonlinear optical properties and density functional theory calculations. Applied Organometallic Chemistry, 2021, 35, e6125.	1.7	10
6098	Spectral behavior peculiarities of the carboxyl functional group in iodine encirclement - the case of 2,6-diiodo-3,4,5-trimethoxybenzoic acid. Journal of Molecular Structure, 2021, 1226, 129303.	1.8	3
6099	Diastereoselective synthesis of new Thiazolyl-Indazole derivatives from R-carvone: A combined experimental and theoretical study. Tetrahedron, 2021, 78, 131830.	1.0	3
6100	Vibrational spectra and molecular structure of sulfanilamide: IR and Low temperature Raman studies and DFT investigation of monomeric and dimeric forms. Vibrational Spectroscopy, 2021, 112, 103199.	1.2	9
6101	Experimental and computational studies of the mechanism of baseâ€catalyzed ring opening of 2â€(chloromethyl)oxirane by benzoic acid. International Journal of Chemical Kinetics, 2021, 53, 356-368.	1.0	3
6102	In silico-driven identification and structural analysis of nitrodihydroquinolinone pesticide candidates with antifungal activity. Journal of Molecular Structure, 2021, 1226, 129326.	1.8	6
6103	Shedding light on ultrafast ring-twisting pathways of halogenated GFP chromophores from the excited to ground state. Physical Chemistry Chemical Physics, 2021, 23, 14636-14648.	1.3	15
6104	Mechanism, kinetics and selectivity of a Williamson ether synthesis: elucidation under different reaction conditions. Reaction Chemistry and Engineering, 2021, 6, 1195-1211.	1.9	10
6105	Computational study of IR, Raman, and NMR spectra of 4-methylmethcathinone drug. Journal of Molecular Modeling, 2021, 27, 3.	0.8	3
6106	Structure, isomerization and dimerization processes of naringenin flavonoids. Physical Chemistry Chemical Physics, 2021, 23, 18068-18077.	1.3	6
6107	The development of an Amber-compatible organosilane force field for drug-like small molecules. Physical Chemistry Chemical Physics, 2021, 23, 12582-12591.	1.3	10
6108	Chemical structure stabilities of a Si_xF_y(xâ‰¤6,yâ‰¤12) series. RSC Advances, 2021, 11, 21832-21839.	1.7	4
6109	Advances, challenges and perspectives of quantum chemical approaches in molecular spectroscopy of the condensed phase. Chemical Society Reviews, 2021, 50, 10917-10954.	18.7	34
6110	Calculation of absolute molecular entropies and heat capacities made simple. Chemical Science, 2021, 12, 6551-6568.	3.7	83

#	Article	IF	Citations
6111	Idarubicinâ€“Gold Complex: From Crystal Growth to Gold Nanoparticles. ACS Omega, 2021, 6, 1235-1245.	1.6	5
6112	An analysis of electrophilic aromatic substitution: a â€œcomplex approachâ€• Physical Chemistry Chemical Physics, 2021, 23, 5051-5068.	1.3	17
6113	Metal-catalyzed aziridination of alkenes by organic azides: a mechanistic DFT investigation. Structural Chemistry, 2021, 32, 1431-1449.	1.0	1
6114	Raman and ROA analyses of twisted anthracenes: connecting vibrational and electronic/photonic structures. Physical Chemistry Chemical Physics, 2021, 23, 13996-14003.	1.3	1
6115	Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 985-995.	2.3	9
6116	Iron Versus Ruthenium: Evidence for the Distinct Differences in the Electronic Structures of Hexa-1,3,5-triyn-1,6-diyl-bridged Complexes [Cp*(dppe)M}{Î¼-(Câ‰¡C)‹sub›3‹/sub›}{M(dppe)Cp*}]‹sup›+‹/sup› (M = Fe, Ru). Organometallics, 2021, 40, 346-357.	2.1	15
6117	Crystal structure, characterization and chemical reactivity of novel piperazine derivative ligand for electrochemical recognition of nitrite anion. Journal of Chemical Sciences, 2021, 133, 1.	0.7	2
6118	Development of a Pantetheine Force Field Library for Molecular Modeling. Journal of Chemical Information and Modeling, 2021, 61, 856-868.	2.5	11
6119	Kinetics of the Reactions of Methyl Radical with Hydrogen, Methyl and Ethyl Peroxides. ChemistrySelect, 2021, 6, 1548-1554.	0.7	0
6120	Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. Journal of Chemical Theory and Computation, 2021, 17, 1701-1714.	2.3	49
6121	Theoretical insight on the solvation properties of Zn2+ in pure liquid ammonia: A quantum mechanical molecular charges field molecular dynamics (QMCF-MD) study. Journal of Molecular Liquids, 2021, 324, 114737.	2.3	1
6122	Density Functional Theory Investigation of Structureâ€“Activity Relationship for Efficient Electrochemical CO‹sub›2‹/sub› Reduction on Defective SnSe‹sub›2‹/sub› Nanosheets. ACS Applied Nano Materials, 2021, 4, 2760-2767.	2.4	6
6123	New evidence on non-covalent interactions in crystalline halo-substituted boron difluoride acetylacetonates from vibrational spectra, model calculations and visualization program tools. Journal of Molecular Structure, 2021, 1227, 129532.	1.8	2
6124	Synthesis, crystal structure, density functional theory calculations, and antimicrobial activity of silver(I) complex derived from 2â€•aminobenzothiazole ligand. Applied Organometallic Chemistry, 2021, 35, e6226.	1.7	3
6125	A comparative DFT study of tetracyanoquinodimethane and its difluoro and tetrafluoro analogs. Journal of the Indian Chemical Society, 2021, 98, 100032.	1.3	6
6126	Selective lithiation of 2,4-lutidine: Role of transition states of lithium dialkylamides. Journal of Organometallic Chemistry, 2021, 936, 121691.	0.8	2
6127	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	1.1	105
6128	Synthesis, and spectroscopic, nanostructure, surface morphology, and density functional theory studies of new charge-transfer complexes of amifampridine with Ï€-acceptors. Journal of Molecular Liquids, 2021, 326, 115199.	2.3	11

#	Article	IF	Citations
6129	Theoretical study of the reactions of hydrogen atom with methyl and ethyl hydroperoxides. Molecular Physics, 0, , e1919324.	0.8	1
6130	DFT Study of Cluster Size-Dependent Structures and Properties of (HClGaN3)n (n = 1â€“6) Clusters. Russian Journal of Physical Chemistry A, 2021, 95, S120-S127.	0.1	0
6131	Infrared spectroscopy of graphene nanoribbons and aromatic compounds with sp3Câ€“H (methyl or) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.7	13
6132	Performance efficiency of MIPOH polymers as organic filler on cellulose pulp waste to form cellulosic paper sheets with biological evaluation and computational studies. Polymer Bulletin, 2022, 79, 4099-4131.	1.7	12
6133	Transient electronic and vibrational signatures during reversible photoswitching of a cyanobacteriochrome photoreceptor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119379.	2.0	7
6134	Atomic charge and atomic dipole modeling of gas-phase infrared intensities of fundamental bands for out-of-plane CH and CF bending vibrations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 251, 119393.	2.0	5
6135	Emergence of fifth-order optical nonlinearity in 2-(2-Quinolyl)-1,3-indandione with strong third-order nonlinear effect under low power CW laser excitation. Chemical Physics Letters, 2021, 769, 138434.	1.2	2
6136	Clues to the non-carcinogenicity of certain N-Nitroso compounds: Role of alkylated DNA bases. Biophysical Chemistry, 2021, 271, 106539.	1.5	4
6137	Effects of edge substitution of subazaphenalenephthalocyanine with electron withdrawing and/or donating groups on electronic and optical properties: A DFT/TDDFT study. Materials Chemistry and Physics, 2021, 263, 124420.	2.0	4
6138	Novel D-Ï€-A phenothiazine and dibenzofuran organic dyes with simple structures for efficient dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 413, 113269.	2.0	21
6139	Cross-conjugated ferrocenyl derivative furan-2-yl-(ferrocenyl)methanone: synthesis, structural analysis, docking and antibacterial evaluation. Spectroscopy Letters, 2021, 54, 326-339.	0.5	0
6140	Vibrational Analysis of Benziodoxoles and Benziodazolotetrazoles. Physchem, 2021, 1, 45-68.	0.5	5
6141	Extraction and Physicochemical Characterization of Dried Powder Mucilage from Opuntia ficus-indica Cladodes and Aloe Vera Leaves: A Comparative Study. Polymers, 2021, 13, 1689.	2.0	26
6142	Surface-enhanced Raman Spectroscopy and Density Functional Theory Study of Glyphosate and Aminomethylphosphonic acid Using Silver Capped Silicon Nanopillars. Universitas Scientiarum, 2021, 26, 51-67.	0.2	5
6143	Sulfide Oxidation by 2,6-Bis[hydroxyl(methyl)amino]-4-morpholino-1,3,5-triazinatodioxomolybdenum(VI): Mechanistic Implications with DFT Calculations for a New Class of Molybdenum(VI) Complex. Inorganic Chemistry, 2021, 60, 7762-7772.	1.9	5
6144	Transfer Learning to CCSD(T): Accurate Anharmonic Frequencies from Machine Learning Models. Journal of Chemical Theory and Computation, 2021, 17, 3687-3699.	2.3	20
6145	Computational Studies on Reactions of Some Organic Azides with Câˆ’H Bonds. ChemistrySelect, 2021, 6, 4368-4381.	0.7	2
6146	Theoretical study of the reactions of nitrogen dioxide with hydrogen and methyl peroxides. Chemical Physics Letters, 2021, 771, 138498.	1.2	4

#	Article	IF	Citations
6147	The electrosorption of 3-bromo-2-nitrothiophene on gold as studied with surface-enhanced Raman spectroscopy. Journal of Chemical Sciences, 2021, 133, 1.	0.7	1
6148	Explicit solvation effects on low-index Fe surfaces and small particles as adsorbents of Arsenic species: a DFT study. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	3
6149	Synthesis of novel Î²-lactams: Antioxidant activity, acetylcholinesterase inhibition and computational studies. Journal of Molecular Structure, 2021, 1233, 130092.	1.8	40
6150	First principles investigation of structural, electronic and optical properties of synthesized radiaannulene oligomers for 6,6,12-graphyne. Journal of Physics and Chemistry of Solids, 2021, 153, 109990.	1.9	13
6151	Computational studies of cisâ€“ and transâ€“isomer preferences of low-spin d6 [M(DABF)2A2]+ and [M(CO)4A2]+ complexes (MÂ=ÂCo, Rh, Ir; AÂ=Âanionic ligand): spectator ligand Ï€-backbonding and DFT exchange. Computational and Theoretical Chemistry, 2021, 1200, 113235.	1.1	1
6152	Shermo: A general code for calculating molecular thermochemistry properties. Computational and Theoretical Chemistry, 2021, 1200, 113249.	1.1	331
6154	Electronic structure theory study of the reactivity and structural molecular properties of halo-substituted (F, Cl, Br) and heteroatom (N, O, S) doped cyclobutane. ChemistrySelect, 2023, 8, 715-739.	0.7	2
6155	Synthesis, spectral, crystallographic, and computational investigation of a novel molecular hybrid 3-(1-((benzoyloxy)imino)ethyl)-2H-chromen-2-ones. European Journal of Chemistry, 2021, 12, 133-146.	0.3	1
6156	Molecular vibrational frequencies from analytic Hessian of constrained nuclearâ€“electronic orbital density functional theory. Journal of Chemical Physics, 2021, 154, 244110.	1.2	8
6157	Firstâ€principles based theoretical investigation of impact of polyolefin structure on photooxidation behavior. Journal of Computational Chemistry, 2021, 42, 1710-1719.	1.5	9
6158	Structures, stabilities and phase diagram assessments of clathrate ices at negative pressures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 401, 127330.	0.9	3
6159	Synthesis, antimicrobial, anti-proliferative activities, molecular docking and DFT studies of novel pyrazolo[5,1-c][1, 2, 4]triazine-3-carboxamide derivatives. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9177-9193.	2.0	26
6160	Fe(II) Redox Chemistry in the Environment. Chemical Reviews, 2021, 121, 8161-8233.	23.0	242
6161	Theoretical design on a series of new cageâ€shaped high energy density compounds. Journal of the Chinese Chemical Society, 2021, 68, 1852.	0.8	0
6162	Effectiveness of smearing and tetrahedron methods: best practices in DFT codes. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 065014.	0.8	9
6163	Giant Spin Splitting in Chiral Perovskites Based on Local Electrical Field Engineering. Journal of Physical Chemistry Letters, 2021, 12, 6492-6498.	2.1	12
6164	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	3.2	4
6165	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). Journal of Chemical Theory and Computation, 2021, 17, 4872-4890.	2.3	22

#	Article	IF	Citations
6166	<scp>2â€Hydroxyâ€5â€nitropyridine and 5â€nitroâ€2â€pyridone: Tautomerism, infrared, Raman, and NMR spectral interpretations, normal coordinate analysis, and DFT calculations</scp>. Journal of the Chinese Chemical Society, 2021, 68, 1863-1879.	0.8	5
6167	SERS and DFT investigations of methyl 4â€‘bromo-1H-pyrrole-2-carboxylate adsorbed on silver and gold substrates: In perspective of biosensor applications. Journal of Molecular Structure, 2021, 1236, 130272.	1.8	14
6168	â€œMoCl3(dme)â€•Revisited: Improved Synthesis, Characterization, and X-ray and Electronic Structures. Inorganic Chemistry, 2021, 60, 12218-12225.	1.9	4
6169	Forcefield evaluation and accelerated molecular dynamics simulation of Zn(II) binding to N-terminus of amyloid-Î². Computational Biology and Chemistry, 2021, 93, 107540.	1.1	6
6170	Density functional theory calculation of the Rennerâ€“Teller effect in NCO : Preliminary assessment of exact exchange energy on the accuracy of the Renner coefficient. International Journal of Quantum Chemistry, 2021, 121, e26804.	1.0	1
6171	Rapid estimation of piperine in black pepper: Exploration of Raman spectroscopy. Phytochemical Analysis, 2022, 33, 204-213.	1.2	5
6172	Tailoring the Gibbs Free Energy of the Nitroxide Exchange Reaction: Substituent and Solvent Effects. Journal of Physical Chemistry A, 2021, 125, 7616-7624.	1.1	2
6173	Structures, Electronic Properties, and Interactions of Cetyl Alcohol with Cetomacrogol and Water: Insights from Quantum Chemical Calculations and Experimental Investigations. ACS Omega, 2021, 6, 20975-20983.	1.6	3
6174	Reliable TDDFT Protocol Based on a Local Hybrid Functional for the Prediction of Vibronic Phosphorescence Spectra Applied to Tris(2,2â€²-bipyridine)-Metal Complexes. Journal of Physical Chemistry A, 2021, 125, 7099-7110.	1.1	13
6175	Variational Energy Decomposition Analysis of Charge-Transfer Interactions between Metals and Ligands in Carbonyl Complexes. Inorganic Chemistry, 2021, 60, 14060-14071.	1.9	5
6176	NONLINEAR OPTICAL AND SPECTRAL PROPERTIES OF HYDROQUINONE & FULLERENE SYSTEMS. EskiÅŸehir Teknik Ãœniversitesi Bilim Ve Teknoloji Dergisi B - Teorik Bilimler, 2021, 9, 47-53.	0.0	0
6177	Structural and vibrational spectral investigation on the identification of Non-Linear Optical properties and wave function analyses (electrostatic potential, electron localisation function,) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.2	2
6178	Theoretical Study of Decomposition Kinetics and Thermochemistry of Bis(dimethylamino)silaneâ€”Formation of Methyleneimine and Silanimine Species. Journal of Physical Chemistry A, 2021, 125, 8175-8186.	1.1	2
6179	Energetic azo compounds based on 2,2â€², 4,4â€², 6,6â€²- hexanitroazobenzene: Structures, detonation performance, and sensitivity. Computational and Theoretical Chemistry, 2021, 1203, 113344.	1.1	1
6180	Kinetics study on the reactions of dimethyl ether with triplet oxygen and hydrogen atoms. Chemical Physics Letters, 2021, 779, 138855.	1.2	4
6181	Theoretical insight into the mechanisms of the gas-phase decomposition of azidoacetone. Chemical Physics Letters, 2021, 778, 138833.	1.2	0
6182	NLO mechanism evaluation by Z-Scan, opto-electronic properties interpretation and chemical potential cavity investigation of 1,8-anthracenedimethanol using quantum computations. Journal of Molecular Structure, 2021, 1240, 130563.	1.8	0
6183	Ab Initio and RRKM/Master Equation Analysis of the Photolysis and Thermal Unimolecular Decomposition of Bromoacetaldehyde. Journal of Physical Chemistry A, 2021, 125, 8282-8293.	1.1	1

#	Article	IF	Citations
6184	Syntheses and Structures of transâ€bis(Alkenylacetylide) Ruthenium Complexes. Chemistry - an Asian Journal, 2021, 16, 3385-3403.	1.7	3
6185	2â€²-Thiophenecarboxaldehyde derived thiosemicarbazone metal complexes of copper(II), palladium(II) and zinc(II) ions: Synthesis, spectroscopic characterization, anticancer activity and DNA binding studies. Inorganica Chimica Acta, 2021, 524, 120440.	1.2	11
6186	Hirshfeld surfaces analysis and DFT study of the structure and IR spectrum of N-ethyl-2-amino-1-(4-chlorophenyl)propan-1-one (4-CEC) hydrochloride. Computational and Theoretical Chemistry, 2021, 1205, 113455.	1.1	8
6187	Enhancement of Molecular imprinted polymer as organic fillers on bagasse cellulose fibers with biological evaluation and computational calculations. Journal of Molecular Structure, 2021, 1241, 130660.	1.8	23
6188	Bifunctional Metalâ€“Organic Layers for Tandem Catalytic Transformations Using Molecular Oxygen and Carbon Dioxide. Journal of the American Chemical Society, 2021, 143, 16718-16724.	6.6	28
6189	Synthesis, crystal structure, Hirshfeld surface analysis and DFT studies of N-(2,6-diisopropylphenyl)-1-(4-methoxyphenyl) methanimine. Journal of Molecular Structure, 2021, 1241, 130620.	1.8	14
6190	Anharmonicity modeling in hydrogen bonded solvent dimers. Journal of Molecular Liquids, 2021, 339, 116735.	2.3	1
6191	Mechanistic and kinetics study on the reaction of methylallyl alcohol with Cl: A theoretical study. Computational and Theoretical Chemistry, 2021, 1204, 113388.	1.1	0
6192	Density functional study of trans,trans,trans-[Pt(N3)2(OH)2(Py)2] on molecular structure and vibrational spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120022.	2.0	3
6193	Analysis of the tautomeric equilibrium of two red monoazo dyes by UVâ€“Visible, Raman and SERS spectroscopies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 261, 120007.	2.0	9
6194	Theoretical investigation of energetic performance and impact sensitivities of nitro and trinitromethyl substituted ozonides of ethylene and cyclopentene. Computational and Theoretical Chemistry, 2021, 1205, 113425.	1.1	2
6195	Synthesis optimization, DFT and physicochemical study of chitosan sulfates. Journal of Molecular Structure, 2021, 1245, 131083.	1.8	54
6196	Spectral estimation from simulations via sketching. Journal of Computational Physics, 2021, 447, 110686.	1.9	0
6197	Arene-ruthenium(II) complexes with pyrazole-based ligands bearing a pyridine moiety: Synthesis, structure, DFT calculations, and cytotoxicity. Inorganica Chimica Acta, 2021, 528, 120610.	1.2	8
6198	A combined experimental and quantum chemical study on molecular structure, spectroscopic properties and biological activity of anti-inflammatory Glucocorticosteroid drug, Dexamethasone. Journal of Molecular Structure, 2021, 1245, 130999.	1.8	25
6199	Ultrasensitive SEIRA detection using gold nanobipyramids: Toward efficient multimodal immunosensor. Journal of Molecular Structure, 2021, 1246, 131160.	1.8	8
6200	Hirshfeld surface analysis, interaction energy calculation and spectroscopical study of 3-chloro-3-methyl-r(2),c(6)-bis(p-tolyl)piperidin-4-one using DFT approaches. Journal of Molecular Structure, 2022, 1248, 131483.	1.8	25
6201	SERS study on the aggregation mechanisms resulting from the orientation of dipyridinic derivatives on gold nanoparticles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 264, 120286.	2.0	4

#	Article	IF	Citations
6202	Development of semiconductive foams based on cellulose- benzenesulfonate/CuFe2O4- nanoparticles and theoretical studies with DFT/ B3PW91/LANDZ2 basis set. Journal of Molecular Structure, 2022, 1247, 131390.	1.8	29
6203	Antioxidant product analysis ofHulu Tea(Tadehagi triquetrum). New Journal of Chemistry, 2021, 45, 20257-20265.	1.4	7
6204	Roles of ethanol and Siâ€“OH in the aldol condensation of ethyl acetate over a Cs/SBA-15 catalyst. Reaction Chemistry and Engineering, 2021, 6, 1002-1015.	1.9	6
6205	Development of the Analytic Second Derivatives for the Fragment Molecular Orbital Method. , 2021, , 425-458.		0
6206	Predicting OH stretching fundamental wavenumbers of alcohols for conformational assignment: different correction patterns for density functional and wave-function-based methods. Physical Chemistry Chemical Physics, 2021, 23, 5629-5643.	1.3	11
6207	Torquoselectivity in the Cationic Cyclopentannelation of (2Z)-Hexa-2,4,5-trienal Acetals. Chemistry - A European Journal, 2000, 6, 4021-4033.	1.7	25
6209	Adaptive Path-Integral Monte Carlo Methods for Accurate Computation of Molecular Thermodynamic Properties. Advances in Chemical Physics, 0, , 117-170.	0.3	11
6210	Catalytic Properties of Single Site Catalysts Prepared via Surface Organometallic Chemistry on Oxides and on Metals. , 0, , 75-135.		2
6211	Reactivity of Copper(III)â€“Oxo Complexes in the Gas Phase. ChemPhysChem, 2017, 18, 2217-2224.	1.0	17
6212	W1 and W2 Theories, and Their Variants: Thermochemistry in the kJ/mol Accuracy Range. , 2001, , 31-65.		25
6213	How Aromaticity Affects the Chemical and Physicochemical Properties of Heterocycles: A Computational Approach. Topics in Heterocyclic Chemistry, 2008, , 155.	0.2	1
6214	Oxirene. , 2008, , 31-52.		2
6215	The Concept of the Potential Energy Surface. , 2016, , 9-49.		10
6216	Semiempirical Calculations. , 2016, , 421-482.		1
6217	Density Functional Calculations. , 2016, , 483-563.		1
6218	First-Principles Quantum Chemical Investigations of Silicon Oxidation. Springer Series in Materials Science, 2001, , 127-141.	0.4	2
6219	Raman Spectroscopic Studies of Polymer Structure. Springer Series in Materials Science, 2000, , 369-445.	0.4	8
6220	Design of Catalysts for Asymmetric Organic Reactions Through Density Functional Calculations. Challenges and Advances in Computational Chemistry and Physics, 2010, , 107-136.	0.6	2

#	Article	IF	Citations
6221	Extracting Thermochemical Information from Ab Initio Data. , 1999, , 353-372.		8
6222	Ab Initio Thermochemistry Beyond Chemical Accuracy for First-and Second-Row Compounds. , 1999, , 373-415.		7
6223	Understanding Alkyl Substituent Effects in R-O Bond Dissociation Reactions in Open- and Closed-Shell Systems. , 2004, , 563-579.		7
6224	On the role of vibrational selective scaling for the calculation of enthalpies of formation using a composite method. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	2
6225	Structural and spectroscopic investigation of glycinium oxalurate. Journal of Molecular Structure, 2017, 1143, 378-387.	1.8	8
6226	Crystal and molecular structures, temperature dependence of the IR and Raman spectra and vibrational dynamics of aquo 4,6-dimethyl-5H-[1,2,3]triazolo[4,5-c]pyridine in a new zwitterionic form. Journal of Molecular Structure, 2017, 1144, 482-495.	1.8	4
6227	Reactions of 2,5-cyclohexadienylidenes investigated by direct spectroscopic methods. Advances in Carbene Chemistry, 2001, , 159-203.	0.1	4
6229	Accurate Assignments of Excited-State Resonance Raman Spectra: A Benchmark Study Combining Experiment and Theory. Journal of Physical Chemistry A, 2017, 121, 7937-7946.	1.1	26
6230	Electroactive Metal Complexes Covalently Attached to Conductive PEDOT Films: A Spectroelectrochemical Study. ACS Applied Materials & Interfaces, 2021, 13, 1301-1313.	4.0	14
6231	Weakened N3 Hydrogen Bonding by 5-Formylcytosine and 5-Carboxylcytosine Reduces Their Base-Pairing Stability. ACS Chemical Biology, 2016, 11, 470-477.	1.6	56
6232	Infrared spectra of CH3â€“MH, CH3â€“M, and CH3â€“MHâ‹¯ prepared via methane activation by laser-ablated Au, Ag, and Cu atoms. Dalton Transactions, 2011, 40, 11115.	1.6	2
6233	Basic Atmospheric Chemistry: A Quantum Chemical Study on Hydration of Mesospheric NaOH. Environmental Chemistry, 2004, 1, 35.	0.7	8
6234	Reactive dynamics and spectroscopy of hydrogen transfer from neural network-based reactive potential energy surfaces. New Journal of Physics, 2020, 22, 055002.	1.2	37
6235	Impact of non-normal error distributions on the benchmarking and ranking of quantum machine learning models. Machine Learning: Science and Technology, 2020, 1, 035011.	2.4	16
6236	Vibrational mode contribution to the dielectric permittivity of disordered small-molecule organic semiconductors. Physical Review Materials, 2020, 4, .	0.9	8
6237	A combined model of electron density and lattice dynamics refined against elastic diffraction data. Thermodynamic properties of crystalline <scp>L</scp>-alanine. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 32-44.	0.0	5
6238	Franck-Condon Dominated Chemistry. Formation and Dissociations of the Dimethylhydroxysulfuranyl Radical. Collection of Czechoslovak Chemical Communications, 2000, 65, 455-476.	1.0	21
6239	Are There Two Different Geometric Isomers of the O=C=N=C=O Cation?. Collection of Czechoslovak Chemical Communications, 2001, 66, 1038-1046.	1.0	2

#	Article	IF	Citations
6240	Atomistic Models and Force Fields. , 2001, , .		16
6241	Theoretical Studies of Molecular Structures, Infrared Spectra, NBO and NLO Properties of Some Novel 5-arylazo-6-hydroxy-4-phenyl-3-cyano-2-pyridone Dyes. Acta Physica Polonica A, 2016, 130, 1273-1287.	0.2	15
6242	Biapenem Inactivation by B2 Metallo Î²-Lactamases: Energy Landscape of the Post-Hydrolysis Reactions. PLoS ONE, 2012, 7, e30079.	1.1	14
6243	Biapenem Inactivation by B2 Metallo Î²-Lactamases: Energy Landscape of the Hydrolysis Reaction. PLoS ONE, 2013, 8, e55136.	1.1	11
6244	VIBRATIONAL SCALING FACTORS FOR Rh(I) CARBONYL COMPOUNDS IN HOMOGENEOUS CATALYSIS. Prilozi: Makedonska Akdemija Na Naukite I Umetnostite Oddelenie Za Prirodno-matematiÄki I BiotehniÄki Nauki, 2017, 38, 43.	0.3	2
6245	AutoGAMESS: A Python package for automation of GAMESS(US) Raman calculations. Journal of Open Source Software, 2019, 4, 1612.	2.0	3
6246	Synthesis, Conformational Analysis, Infrared, Raman and UV-Visible Spectra of Novel Schiff Bases compiled with DFT Calculations. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 568-586.	0.6	3
6247	Lithocholic Acid Derivative as a Model for Artificial Receptors: A Raman Study. Letters in Drug Design and Discovery, 2010, 7, 610-617.	0.4	3
6248	Synthesis, Antitumor Activity, Molecular Docking and DFT Study of Novel Pyrimidiopyrazole Derivatives. Current Computer-Aided Drug Design, 2020, 16, 486-499.	0.8	16
6249	Spectroscopic and quantum chemical elucidation of newly synthesized 1-aryl-3-methyl-3-phenylpyrrolidine-2,5-diones as potentional anticonvulsant agents. Hemijska Industrija, 2019, 73, 125-137.	0.3	1
6250	The quantum-chemical modelling of structure and spectral characteristics for molecular complexes in pentaplast-terlon system. Chemistry and Chemical Technology, 2017, 11, 405-409.	0.2	2
6251	Rationalising the vibrational spectra of biomolecules using atomistic simulations. Frontiers in Bioscience - Landmark, 2009, Volume, 4229.	3.0	11
6252	Ab initio Quantum Chemical Study on Charge Distribution and Molecular Structure of Uranyl (VI) Species with Raman Frequency. , 0, .		8
6253	Association of water and small monocarboxylic acids: Matrix isolation FTIR spectrometry study. Lithuanian Journal of Physics, 2009, 49, 53-62.	0.1	6
6254	Short Synthesis of (+)-Cylindricine C and Formal Total Synthesis of (-)-Lepadiformine. Heterocycles, 2007, 72, 421.	0.4	29
6255	¹³C-¹⁸O Bonds in Precipitated Calcite and Aragonite: An <i>ab Initio</i> Study. Open Journal of Geology, 2014, 04, 436-480.	0.1	3
6256	Reaction Monitoring of Imine Synthesis Using Raman Spectroscopy. Bulletin of the Korean Chemical Society, 2003, 24, 205-208.	1.0	33
6257	Theoretical Studies of the Gas-Phase Identity Nucleophilic Substitution Reactions of Cyclopentadienyl Halides. Bulletin of the Korean Chemical Society, 2003, 24, 583-592.	1.0	2

#	Article	IF	Citations
6258	Structure, Modified Scaled Quantum Mechanical Force Field and A Priori Prediction of Vibrational Spectra and Their Assignment and Exponential Scaling of Frequencies of Triphenylene. Bulletin of the Korean Chemical Society, 2003, 24, 717-722.	1.0	3
6259	Calculation of the Solvation Free Energy of the Proton in Methanol. Bulletin of the Korean Chemical Society, 2005, 26, 589-593.	1.0	49
6260	MP2 Basis Set Limit Binding Energy Estimates of Hydrogen-bonded Complexes from Extrapolation-oriented Basis Sets. Bulletin of the Korean Chemical Society, 2007, 28, 386-390.	1.0	17
6261	Hydrogen-Atom Abstraction Reaction of CF₃CH₂OCF₃by Hydroxyl Radical. Bulletin of the Korean Chemical Society, 2010, 31, 3718-3722.	1.0	12
6262	Zeolite-catalyzed Isomerization of 1-Hexene to trans-2-Hexene: An ONIOM Study. Bulletin of the Korean Chemical Society, 2011, 32, 1851-1858.	1.0	2
6263	Loss of HCN from the Pyrazine Molecular Ion: A Theoretical Study. Bulletin of the Korean Chemical Society, 2011, 32, 2301-2305.	1.0	3
6264	A New Unsymmetrical Zinc Phthalocyanine as Photosensitizers for Dye-sensitized Solar Cells. Bulletin of the Korean Chemical Society, 2012, 33, 1225-1230.	1.0	12
6265	A Theoretical Study on the Alkylation of the Ambident Enolate from a Methyl Glycinate Schiff Base. Bulletin of the Korean Chemical Society, 2012, 33, 2711-2718.	1.0	4
6266	Enhanced Raman Spectrum of Juglone on Ag Surface: Is It a Simile to That of Lawsone?. Bulletin of the Korean Chemical Society, 2013, 34, 68-74.	1.0	6
6267	Does the Gaseous Aniline Cation Isomerize to Methylpyridine Cations Before Dissociation?. Bulletin of the Korean Chemical Society, 2013, 34, 3249-3252.	1.0	6
6268	Decarbonylation of the 2-Hydroxypyridine Radical Cation: A Computational Study. Bulletin of the Korean Chemical Society, 2014, 35, 3021-3024.	1.0	1
6269	Dissociation of the Pyridazine Molecular Ion. Bulletin of the Korean Chemical Society, 2014, 35, 721-724.	1.0	1
6270	Computational Study on OH and Cl Initiated Oxidation of 2,2,2-Trifluoroethyl Trifluoroacetate (CF3C(O)OCH2CF3). Bulletin of the Korean Chemical Society, 2014, 35, 1385-1390.	1.0	5
6271	Synthesis, Antioxidant Activity, Spectroscopic, Electronic, Nonlinear Optical (NLO) and Thermodynamic Properties of 2-Ethoxy-4-[(5-oxo-3-phenyl-1,5-dihydro-1,2,4-triazol-4-ylimino)-methyl]-phenyl-4-methoxybenzoate: A Theoretical and Experimental Study. Journal of the Iranian Chemical Society, 2022, 19, 1015-1038.	1.2	7
6272	Vibrational Properties of Benzoxaboroles and Their Interactions with Candida albicansâ€™ LeuRS. Symmetry, 2021, 13, 1845.	1.1	2
6273	Proving Nanoscale Chiral Interactions of Cyclodextrins and Propranolol Enantiomers by Means of SERS Measurements Performed on a Solid Plasmonic Substrate. Pharmaceutics, 2021, 13, 1594.	2.0	8
6274	Metaâ€anal ysis of uniform scaling factors for harmonic frequency calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1584.	6.2	13
6275	Unusually Large Hydrogen-Bond Cooperativity in Hydrogen Fluoride Clusters, (HF)_n,n= 3 to 8, Revealed by the Molecular Tailoring Approach. Journal of Physical Chemistry A, 2021, 125, 8836-8845.	1.1	16

#	Article	IF	Citations
6276	Determination of the Cohesive Properties and Sublimation Temperatures of Glycine Polymorphs. Crystal Growth and Design, 2021, 21, 6266-6275.	1.4	2
6277	New Charge Transfer Complexes of K+-Channel-Blocker Drug (Amifampridine; AMFP) for Sensitive Detection; Solution Investigations and DFT Studies. Molecules, 2021, 26, 6037.	1.7	3
6278	Ultrasound-Accelerated, Concise, and Highly Efficient Synthesis of 2-Oxazoline Derivatives Using Heterogenous Calcium Ferrite Nanoparticles and Their DFT Studies. Journal of Chemistry, 2021, 2021, 1-12.	0.9	5
6279	A Resonance Raman spectroscopic study on charge transfer enhancement in photosensitizers. Materials Today Advances, 2021, 12, 100180.	2.5	1
6280	Study of a new piperidone as an anti-Alzheimer agent: Molecular docking, electronic and intermolecular interaction investigations by DFT method. Journal of King Saud University - Science, 2021, 33, 101632.	1.6	62
6282	Computer Estimation of Chemical Structures from Infrared Spectra. Journal of Computer Chemistry Japan, 2005, 4, 1-24.	0.0	1
6283	Theoretical Study of NO Adsorption and Decomposition on Si(100) Surfaces. E-Journal of Surface Science and Nanotechnology, 2006, 4, 624-629.	0.1	0
6284	Ab Initio Methods for Simulating and Interpreting hyper-Raman Spectra of Molecules. , 2006, , 317-323.		0
6285	Accurate gas phase acidities of carboxylic acids estimated by scaling of harmonic vibrational frequencies calculated on Hartree-Fock level. , 2006, , 1463-1468.		0
6286	Kinetic Energy Release in the Unimolecular Dissociation of 1-Butanol Cation. Bulletin of the Korean Chemical Society, 2007, 28, 319-321.	1.0	1
6287	Oligomers and Polymers of Carbon Dioxide and CO2/N2. , 2008, , 165-184.		0
6288	Anti-Inflammatory Drugs. , 2008, , 69-96.		1
6289	Tranquilizers and Sedatives. , 2008, , 37-68.		0
6290	A Menagerie of Molecules from Michl and Balaji: Superstrained Molecules. , 2008, , 227-256.		1
6291	10.1007/s11178-008-1003-1. , 2010, 44, 31.		0
6293	Ditopic Binding of Alkali Halide Ions to Trimethylboroxine. Mass Spectrometry Letters, 2010, 1, 9-12.	0.2	0
6294	Spectroscopy of Biological Molecules at Very Low Temperatures. , 2011, , 469-496.		0
6295	Valence XPS, IR, and Solution 13C NMR Spectral Analysis of Representative Polymers by Quantum Chemical Calculations. Progress in Theoretical Chemistry and Physics, 2012, , 393-403.	0.2	0

#	Article	IF	Citations
6296	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Highlights in Theoretical Chemistry, 2014, , 225-239.	0.0	0
6297	Relative Reactivity of Various Al-substituted-dialkylalans in Reduction of Carbonyl Compounds: A Theoretical Study on Substituent Effect. Bulletin of the Korean Chemical Society, 2013, 34, 2335-2339.	1.0	1
6298	MPV-Reduction of C=O bond with Al-substituted-dialkylalan; A Theoretical Study on Relative Reactivity of Various Carbonyl Substrates. Bulletin of the Korean Chemical Society, 2014, 35, 546-550.	1.0	0
6299	ÐšÐ²Ð°Ð½Ñ‚Ð¾Ð²Ð¾-Ñ…Ñ–Ð¼Ñ–Ñ‡Ð½Ñ– Ð¼Ð¾Ð´ÐµÐ»ÑŽÐ²Ð°Ð½Ð½Ñ•ÑÑ€ÑƒÑ‚ÑƒÑ€Ð¸ Ñ‚Ð° ÑžÐ¿Ð¾Ð²Ñ–Ð´Ð°Ð»ÑŒÐ½Ð¾		
6300	Vibrational study of Î±- and Î³-pyridone. , 1999, , 613-614.		0
6301	Uracil molecule: the transferability of the scale factors for the prediction of the infrared spectra. , 1999, , 295-296.		0
6302	Vibrational study of 3-methyluracil. , 1999, , 293-294.		0
6305	Molecular Modeling and Synthesis of Ethyl Benzyl Carbamates as Possible Ixodicide Activity. Computational Chemistry, 2019, 07, 1-26.	0.2	6
6307	1-(4-Chlorophenyl) piperazine: FT-IR, Raman, NMR and Theoretical studies. Anadolu University Journal of Sciences & Technology, 0, , .	0.2	2
6308	Molecular Structural and Vibrational Spectroscopic Assignments of n5-(4-Methoxyphenyl)-3-(1-methylindol-3-yl)-isoxazole using DFT Theory Calculations. Asian Journal of Organic & Medicinal Chemistry, 2019, 4, 147-151.	0.1	0
6309	Design, Synthesis, and Quantum Chemical Calculations of 2,6-Diphenylspiro[cyclohexane-1,3â€™-pyrido[1,2-a]pyrimidine]-2â€™,4,4â€™-trione through DFT approach. Letters in Organic Chemistry, 2019, 16, 983-995.	0.2	1
6310	Vibrational spectroscopic and Hirshfeld surface analysis of N,N'-(azanediylbis(2,1-phenylene))bis(2-chloropropanamide). European Journal of Chemistry, 2019, 10, 386-402.	0.3	1
6311	Hirshfeld surface and theoretical studies of 2,2,2-trichloro-N,N-bis(2-(2,2,2-trichloroacetamido)phenyl)acetamide compound. European Journal of Chemistry, 2019, 10, 323-335.	0.3	0
6312	A QUANTUM CHEMICAL STUDY ON ELUCIDATION OF MOLECULAR STRUCTURE, ELECTRIC MOMENTS AND VIBRATIONAL ANALYSES OF BETA-DAMASCENONE AND ITS ISOMER- A COMPARATIVE STUDY. International Journal of Engineering Technologies and Management Research, 2017, 4, 123-136.	0.1	0
6313	Synthesis, spectral characterization (FT-IR, FT-Raman and NMR) and Quantum computational analysis of (E)-1-(4-Bromophenyl)-3-(5-bromothiophen-2-yl)propâ€2-en-1-one. Chemical Data Collections, 2020, 28, 100415.	1.1	4
6315	Excitedâ€State Dynamics of a metaâ€Dimethylamino Locked GFP Chromophore as a Fluorescence Turnâ€on Water Sensor^{â€}. Photochemistry and Photobiology, 2022, 98, 311-324.	1.3	4
6316	The Vibrational Spectroscopy of the Valence Bonds of Cu-Doped TiO2 Using Electronegativity Principle Quantitative Calculations. Journal of Spectroscopy, 2020, 2020, 1-11.	0.6	6
6317	Study on the reaction mechanism of CH2OÂ+ÂNO2 transformed by PbO/SnO in double-base propellants through theoretical calculation and experiment. Combustion and Flame, 2022, 236, 111768.	2.8	4

#	Article	IF	Citations
6318	Spectroscopic Characterization, Molecular Modeling and DFT/TD-DFT/PCM Calculations of Novel Hydrogen-Bonded Charge Transfer Complex between Chloranilic Acid and 2-Amino-4,6-Dimethylpyridine. Open Journal of Physical Chemistry, 2020, 10, 1-32.	0.1	4
6319	Smart manufacturing of paints and coatings. , 2020, , 179-218.		0
6320	Theoretical Computations on the Pyrolysis of Alkyl (dithio)acetates. Letters in Organic Chemistry, 2020, 17, 224-233.	0.2	1
6321	Study of the conformation and hydrogen bonds of the p-tetrasulfonatothiacalix[4]arene pentasodium salt by vibrational spectroscopy and DFT. Journal of Molecular Modeling, 2021, 27, 326.	0.8	0
6322	Synthesis, single crystal, characterization and computational study of 2-amino-N-cyclopropyl-5-ethyl-thiophene-3-carboxamide. Journal of Molecular Structure, 2022, 1250, 131890.	1.8	27
6323	New Role for Radical SAM Enzymes in the Biosynthesis of Thio(seleno)oxazole RiPP Natural Products. Biochemistry, 2021, 60, 3347-3361.	1.2	11
6325	Valence isomerization of 2-phospha-4-silabicyclo[1.1.0]butane:a high-level ab initio study. , 0, , 531-536.		0
6326	Complex systems in the gas phase. , 2007, , 153-256.		1
6327	Structural and vibrational properties of amines adsorbed on graphene. Nano Structures Nano Objects, 2022, 29, 100816.	1.9	0
6328	Synthesis, Structures, and Properties of Helically Fused Anthraquinones with Unusually Close Carbonylâ€Carbonyl Contacts. Chemistry - A European Journal, 2021, , .	1.7	3
6329	Relativistic Four-Component DFT Calculations of Vibrational Frequencies. Journal of Physical Chemistry A, 2021, 125, 10315-10320.	1.1	2
6330	In Search of the Most Stable Molecular Configuration of Heptakis(2,6-O-dimethyl)-Î²-cyclodextrin and Its Complex with Mianserin: A Comparison of the B3LYP-GD2 and M062X-GD3 Results. Journal of Physical Chemistry B, 2021, 125, 13077-13087.	1.2	4
6331	Mâ†NCCH₃, M-Î·²-(NC)â€“CH₃, and CNâ€“Mâ€“CH₃ Prepared by Reactions of Ce, Sm, Eu, and Lu Atoms with Acetonitrile: Matrix Infrared Spectra and Theoretical Calculations. Inorganic Chemistry, 2021, 60, 17649-17656.	1.9	2
6332	Supramolecular structure and spectroscopic characterization of new 1,3,5-triaza-2-boracyclohex-3-en derivative formed under mild conditions between 2-imino-4-thiobiuret and boric acid. Journal of Molecular Structure, 2021, , 131968.	1.8	1
6333	Filter Feature Selection for Unsupervised Clustering of Designer Drugs Using DFT Simulated IR Spectra Data. ACS Omega, 2021, 6, 32151-32165.	1.6	2
6334	Comparison of Molecular Geometry Optimization Methods Based on Molecular Descriptors. Mathematics, 2021, 9, 2855.	1.1	18
6335	Vital theoretical and inter molecular docking study of (E)-3-[(2,6-dimethylphenyl)diazenyl]-7-methyl-1H-indazole. Journal of the Indian Chemical Society, 2021, 98, 100258.	1.3	0
6336	Exploration of Photophysical and Nonlinear Properties of Salicylaldehyde-Based Functionalized Materials: A Facile Synthetic and DFT Approach. ACS Omega, 2021, 6, 33914-33922.	1.6	8

#	Article	IF	Citations
6337	Spectroscopic studies, quantum chemical investigations, and in silico and in vitro scrutiny of the diuretic drug trichlormethiazide adsorbed on <scp>AuNPs</scp>. Journal of Molecular Recognition, 2022, 35, e2939.	1.1	0
6338	Theoretical Studies of the Reactions of Methyl radical with Dimethyl Ether and 1,2-Ethanediol. Computational and Theoretical Chemistry, 2021, 1207, 113538.	1.1	1
6339	Femtosecond photodecarbonylation of photo-ODIBO studied by stimulated Raman spectroscopy and density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 25637-25648.	1.3	1
6340	Adsorption and orientation characteristics of 1-methylpyrrole-2-carbonyl chloride using SERS and DFT investigations. Journal of Molecular Structure, 2022, 1253, 132201.	1.8	11
6341	Highly-stable cobalt metal organic framework with sheet-like structure for ultra-efficient water oxidation at high current density. Journal of Colloid and Interface Science, 2022, 611, 599-608.	5.0	43
6343	Quasi-Static Two-Dimensional Infrared Spectra of the Carboxyhemoglobin Subsystem under Electric Fields: A Theoretical Study. Journal of Physical Chemistry B, 2020, 124, 9570-9578.	1.2	3
6344	Molecular modelling, spectroscopic characterization and nonlinear optical analysis on N-Acetyl-DL-methionine. Revista Mexicana De FÃsica, 2020, 66, 749-760.	0.2	8
6345	Nuclear Norm Based Spectrum Estimation for Molecular Dynamic Simulations. , 2020, , .		0
6346	Antiureolytic activity of new water-soluble thiadiazole derivatives: Spectroscopic, DFT, and molecular docking studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 272, 120971.	2.0	8
6347	Comparison of Proton Acceptor and Proton Donor Properties of H2O and H2O2 in Organic Crystals of Drug-like Compounds: Peroxosolvates vs. Crystallohydrates. Molecules, 2022, 27, 717.	1.7	11
6348	Atmospheric chemistry of CF3CN: kinetics and products of reaction with OH radicals, Cl atoms and O3. Physical Chemistry Chemical Physics, 2022, 24, 2638-2645.	1.3	1
6349	Conformational analysis, molecular structure, spectroscopic, NBO, reactivity descriptors, wavefunction and molecular docking investigations of 5,6-dimethoxy-1-indanone: A potential anti Alzheimer's agent. Heliyon, 2022, 8, e08821.	1.4	7
6350	Performance of Vibrational Self-Consistent Field Theory for Accurate Potential Energy Surfaces: Fundamentals, Excited States, and Intensities. Journal of Physical Chemistry A, 2022, 126, 608-622.	1.1	6
6351	State-of-the-art of computational green chemistry in leading universities in Russia. , 2022, , 55-77.		0
6352	Synthesis, photophysical, electrochemical, and DFT examinations of two new organic dye molecules based on phenothiazine and dibenzofuran. Journal of Molecular Modeling, 2022, 28, 34.	0.8	16
6353	New 1,2,3-Triazoles from (R)-Carvone: Synthesis, DFT Mechanistic Study and In Vitro Cytotoxic Evaluation. Molecules, 2022, 27, 769.	1.7	14
6354	Interfacial Dynamics in Inverted-Headgroup Lipid Membranes. Journal of Chemical Physics, 2022, 156, 075102.	1.2	3
6355	Electrostatic Perturbations in the Substrateâ€Binding Pocket of Taurine/Îąâ€Ketoglutarate Dioxygenase Determine its Selectivity. Chemistry - A European Journal, 2022, 28, .	1.7	32

#	Article	IF	Citations
6356	Synthesis, crystal structure, Hirshfeld surface analysis and molecular docking analysis of new cadmium(II) iodide complex with the pyridine, 4-(1,1-dimethylethyl). Journal of Coordination Chemistry, 0, , 1-23.	0.8	2
6357	Theoretical structural and thermochemical characterization of partially fluorinated alcohols. Computational and Theoretical Chemistry, 2022, 1209, 113600.	1.1	0
6358	Synthesis, spectroscopic characterizations, biological activity, DNA-binding investigation combined with DFT studies of new proton-transfer complexes of 2,4-diaminopyrimidine with 2,6-dichloro-4-nitrophenol and 3,5-dinitrosalicylic acid. Journal of Molecular Liquids, 2022, 350, 118508.	2.3	4
6359	Influence of fluorosubstitution on physical properties of the smectogenic chiral ester. Materials Research Bulletin, 2022, 150, 111756.	2.7	10
6360	Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation. Journal of Physical Chemistry Letters, 2022, 13, 1382-1388.	2.1	12
6361	Metalâ€“organic frameworks properties from hybrid density functional approximations. Journal of Chemical Physics, 2022, 156, 094706.	1.2	10
6362	Plasmonically Generated Tryptophan Radical Anion on Gold Nanoparticles Investigated by Combined Surface-Enhanced Raman Scattering and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 27596-27606.	1.5	4
6363	Nickel Adsorption by Biogenic Selenium Nanoparticles (Senps): Characterization and Simulation of Non-Symmetric Breakthrough Curves in Continuous-Flow Packed-Bed Columns. SSRN Electronic Journal, 0, , .	0.4	0
6364	Oxalate promoted iron dissolution of hematite via proton coupled electron transfer. Environmental Science: Nano, 2022, 9, 1770-1779.	2.2	7
6365	Total synthesis of monoterpenoid indole alkaloid (â€“)-arbophyllidine. Organic Chemistry Frontiers, 0, , .	2.3	0
6366	Deamidation reaction network mapping of pharmacologic and related proteins: impact of solvation dielectric on the degradation energetics of asparagine dipeptides. Reaction Chemistry and Engineering, 2022, 7, 1525-1543.	1.9	6
6367	Critical Computational Evidence Regarding the Long-Standing Controversy over the Main Electrophilic Species in Hypochlorous Acid Solution. Molecules, 2022, 27, 1843.	1.7	2
6368	Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CLâ€20) Lattice: Part I, Infrared Spectra. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.0	2
6369	The long road to calibrated prediction uncertainty in computational chemistry. Journal of Chemical Physics, 2022, 156, 114109.	1.2	12
6370	Isopropyl-naphthylamide-hydrazine as a novel fluorescent reagent for ultrasensitive determination of carbonyl species on UPLC. Microchemical Journal, 2022, 177, 107308.	2.3	0
6371	Theoretical study of nimetazepam, a real-life chiral molecule without an asymmetric carbon atom. Journal of Molecular Structure, 2022, 1259, 132720.	1.8	0
6372	Crystal structure, spectroscopic studies, DFT calculations, and biological activity of 5-bromosalicylaldehydeâ€“based Schiff bases. Journal of Molecular Structure, 2022, 1262, 132976.	1.8	5
6373	An Efficient Method for Determining Matrix Elements of the Dipole Moment Operator and Corrections to the Energy of a Polyatomic Molecule Using the Perturbation Theory within the Polynomials of Quantum Numbers Formalism. Optics and Spectroscopy (English Translation of Optika I) Tj ETQq1 1 0.784314 rgBT /Ov	0.2	0

#	Article	IF	Citations
6374	Methane and Acetylene Detection in Transformer Oil Based on Raman Spectroscopy. , 2021, , .		0
6375	NH Stretching Frequencies of Intramolecularly Hydrogen-Bonded Systems: An Experimental and Theoretical Study. Molecules, 2021, 26, 7651.	1.7	12
6376	Synthesis, spectroscopic, DFT, and molecular docking studies on 1,4-dihydropyridine derivative compounds: a combined experimental and theoretical study. Journal of Molecular Modeling, 2022, 28, 5.	0.8	6
6377	Synthesis, structural, spectroscopic and docking studies on (E)-1-Ferrocenyl-3-phenylÂpropen-1-one by the density functional theory. Molecular Simulation, 2022, 48, 387-402.	0.9	0
6378	Reduction Mechanism of Alcohols Contents Caused by Acids During Oil-Paper Insulation Aging. IEEE Transactions on Dielectrics and Electrical Insulation, 2021, 28, 1867-1874.	1.8	7
6379	Probing computational methodologies in predicting mid-infrared spectra for large polycyclic aromatic hydrocarbons. Monthly Notices of the Royal Astronomical Society, 2022, 513, 3663-3681.	1.6	9
6380	Heuristics and Uncertainty Quantification in Rational and Inverse Compound and Catalyst Design. , 2024, , 485-495.		0
6381	Characterizing Raman modes and gas sensing features of functionalized tetragonal graphyne quantum dots: A first principles study. Journal of Physics and Chemistry of Solids, 2022, 167, 110737.	1.9	3
6382	Poly (O-Aminophenol) Produced by Plasma Polymerization Has IR Spectrum Consistent with a Mixture of Quinoid & Keto Structures. Plasma, 2022, 5, 196-205.	0.7	0
6383	Gallium and scandium doping effect on the sensing performance of aluminum phosphide nanotubes toward toxic ethylene oxide gas. Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 441, 128145.	0.9	2
6384	Cp₂TiCl₂: Synthesis, Characterization, Modeling and Catalysis. Journal of Chemical Education, 2022, 99, 2121-2128.	1.1	5
6385	Vibrational Spectra and Surface-Enhanced Vibrational Spectra of Azamacrocycles. , 0, , 725-800.		0
6388	Competitive Hydrogen Migration in Silicon Nitride Nanoclusters: Reaction Kinetics Generalized from Supervised Machine Learning. Journal of Physical Chemistry A, 2022, 126, 2677-2689.	1.1	4
6389	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	1.3	15
6390	Design, Synthesis, Spectroscopic Characterization, Molecular Docking and Biological Evaluation of 9H-Carbazole Linked 4-Nitrophenol: A DFT Approach. Journal of Computational Biophysics and Chemistry, 2022, 21, 909-926.	1.0	1
6391	Testing the limitations of harmonic approximation in the determination of Raman intensities. Molecular Physics, 2022, 120, .	0.8	1
6392	Pyrolysis process and mechanism for calcium elimination of used lubricating oil. Journal of Analytical and Applied Pyrolysis, 2022, 165, 105540.	2.6	1
6393	Theoretical and experimental study of the infrared and Raman spectra of L-lysine acetylation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 278, 121371.	2.0	4

#	Article	IF	Citations
6394	Solvent effects on the vibrational modes of (R)-3-methylcyclohexanone conformers. Journal of Molecular Liquids, 2022, 359, 119317.	2.3	2
6395	Density functional studies and spectroscopic analysis (FT-IR, FT-Raman, UVâ€“visible, and NMR) with molecular docking approach on an anticancer and antifungal drug 4â€hydroxy-3-methoxybenzaldehyde. Journal of Molecular Structure, 2022, 1264, 133134.	1.8	2
6396	Synthesis, structural, photo-physical properties and DFT studies of some diarylheptanoids. Journal of Molecular Structure, 2022, 1264, 133254.	1.8	5
6397	Vibrational Probes of Anharmonic Interactions in the Molecular Ferroelectric 2-Methylbenzimidazole. Vibrational Spectroscopy, 2022, , 103384.	1.2	0
6398	Geometrical benchmarking and analysis of redox potentials of copper(I/<scp>II</scp>) <scp>guanidineâ€quinoline</scp> complexes: Comparison of semiâ€empirical tightâ€binding and <scp>DFT</scp> methods and the challenge of describing the entatic state (part <scp>III</scp>). Journal of Computational Chemistry, 2023, 44, 319-328.	1.5	1
6399	Quantum computational, spectroscopic (FT-IR, NMR and UVâ€“Vis) profiling, Hirshfeld surface, molecular docking and dynamics simulation studies on pyridine-2,6-dicarbonyl dichloride. Journal of Molecular Structure, 2022, 1265, 133374.	1.8	26
6400	Does an Enol Pathway Preclude High Stereoselectivity in Iron-Catalyzed Indole Câ€“H Functionalization via Carbene Insertion?. Journal of Organic Chemistry, 2022, 87, 7919-7933.	1.7	10
6401	Theoretical assessment of the solvent effect on the functionalization of Au32 and C60 nanocages with fluorouracil drug. Diamond and Related Materials, 2022, 126, 109142.	1.8	40
6404	Khalifa University of Science and Technology. SSRN Electronic Journal, 0, , .	0.4	0
6405	Infrared Spectrum Analysis and Quantitative Detection of SF₆ Characteristic Decomposition Components SO₂F₂ and SOF₂. IEEE Transactions on Dielectrics and Electrical Insulation, 2022, 29, 1316-1323.	1.8	6
6406	VIBFREQ1295: A New Database for Vibrational Frequency Calculations. Journal of Physical Chemistry A, 2022, 126, 4100-4122.	1.1	11
6407	Fast Predictions of Reaction Barrier Heights: Toward Coupled-Cluster Accuracy. Journal of Physical Chemistry A, 2022, 126, 3976-3986.	1.1	26
6408	Comprehensive quantum chemical calculations and molecular docking analysis of uracil mustard by first principle. Journal of the Indian Chemical Society, 2022, , 100580.	1.3	0
6409	DPPC phospholipid interaction with cholesterol and melatonin: Raman spectroscopy and density functional theory study. Journal of Raman Spectroscopy, 0, , .	1.2	1
6410	Synthesis, Spectroscopic, Crystal Structure, DFT, Hirshfeld Surface and Molecular Docking Analysis of Hexahydroquinoline Derivative (HQ). Polycyclic Aromatic Compounds, 2023, 43, 4242-4270.	1.4	12
6411	Estimating ignition delay times of nitroglycerin: A chemical kinetic modeling study. Combustion Science and Technology, 2024, 196, 406-420.	1.2	3
6412	Stabilities, electronic and piezoelectric properties of blue-phosphorene-phase MXs (MÂ=ÂGe, Sn; XÂ=ÂS, Se,) Tj ETQq0 0 0 rgBT /Overlo	3.1	2
6413	Correlation between Câ•O Stretching Vibrational Frequency and pK_a Shift of Carboxylic Acids. Journal of Physical Chemistry B, 2022, 126, 4999-5006.	1.2	10

#	Article	IF	Citations
6414	Spectroscopic, computational, electronic state and non-linear optical analysis on 1, 8-dihydroxyanthraquinone by density functional theory. Materials Today: Proceedings, 2022, 67, 462-470.	0.9	1
6415	Synthesis, single crystal X-ray, DFT, Hirshfeld surface and molecular docking studies of 9-(2,4-dichlorophenyl)-4a-hydroxy-tetramethyl-octahydro-1H-xanthene-1,8(2H)-dione. Journal of Molecular Structure, 2022, 1268, 133613.	1.8	15
6416	Portable Models for Entropy Effects on Kinetic Selectivity. Journal of the American Chemical Society, 2022, 144, 13996-14004.	6.6	9
6417	Olive oil authentication based on quantitative Î²-carotene Raman spectra detection. Food Chemistry, 2022, 397, 133763.	4.2	8
6418	Theoretical estimates of sulfoxyanion triple-oxygen equilibrium isotope effects and their implications. Geochimica Et Cosmochimica Acta, 2022, 336, 353-371.	1.6	2
6419	Strontium Nitridoborate Hydride Sr₂BN₂H Verified by Single-Crystal X-ray and Neutron Powder Diffraction. Inorganic Chemistry, 2022, 61, 12685-12691.	1.9	5
6420	Investigation of the Geometric and Spectroscopic Properties of Four Twisted Triphenylpyridinium Donorâ€“Acceptor Dyes. Journal of Physical Chemistry A, 0, , .	1.1	1
6421	Zinc(II) Complex with Pyrazolone-Based Hydrazones is Strongly Effective against Trypanosoma brucei Which Causes African Sleeping Sickness. Inorganic Chemistry, 2022, 61, 13561-13575.	1.9	5
6422	Temperature, pressure, and adsorptionâ€dependent redox potentials: I. Processes of CO₂ reduction to valueâ€added compounds. Energy Science and Engineering, 2022, 10, 4520-4543.	1.9	3
6423	Direct and Water-Mediated Adsorption of Stabilizers on SERS-Active Colloidal Bimetallic Plasmonic Nanomaterials: Insight into Citrateâ€“AuAg Interactions from DFT Calculations. Journal of Physical Chemistry A, 2022, 126, 5236-5251.	1.1	3
6424	Structural, vibrational characterization and DFT calculations of urea: DL-malic acid (1:1) â€“ co-crystal. Journal of Molecular Structure, 2022, 1270, 133930.	1.8	6
6425	Growth and characterization of nitrophenol complexes with piperazine and pyridine derivatives. Journal of Molecular Structure, 2022, 1270, 133884.	1.8	3
6426	Nickel removal by biogenic selenium nanoparticles (SeNPs): Characterization and simulation of non-symmetric breakthrough curves in continuous-flow packed-bed columns. Environmental Nanotechnology, Monitoring and Management, 2022, 18, 100729.	1.7	1
6427	IR, UV-Visible, NMR Spectra and Aromaticity of the Covalent Organic Tetraoxa[8]Circulene Frameworks. SSRN Electronic Journal, 0, , .	0.4	0
6428	Design, Synthesis, Theoretical, Spectroscopic and Molecular Docking Studies of Ruthenium and Zinc Complexes and their Antimycobacterial Study. Asian Journal of Chemistry, 2022, 34, 2611-2622.	0.1	0
6429	Catalytic formation of oxalic acid on the partially oxidised greigite Fe₃S₄(001) surface. Physical Chemistry Chemical Physics, 2022, 24, 20104-20124.	1.3	2
6430	Molecules of life: studying the interaction between water and phosphine in argon matrices. Physical Chemistry Chemical Physics, 2022, 24, 22426-22430.	1.3	1
6431	Experimental, NBO, NLO and docking analysis of a novel ligand derived from vanillin and N(4)-methyl-N(4)-phenylthiosemicarbazide and its transition metal complexes. Results in Chemistry, 2022, 4, 100453.	0.9	0

#	Article	IF	Citations
6432	Experimental, insilico, DFT studies of novel compound 2-{2-[(3,4-dimethoxyphenyl)methylidene]hydrazinecarbonothioyl}-N-methyl-N-phenylhydrazine-1-carbothioamide. Results in Chemistry, 2022, 4, 100534.	0.9	1
6433	Role of hydrazone substituents in determining the nuclearity and antibacterial activity of Zn(<scp>ii</scp>) complexes with pyrazolone-based hydrazones. Dalton Transactions, 2022, 51, 14165-14181.	1.6	7
6434	Exploring the evolution patterns of melem from thermal synthesis of melamine to graphitic carbon nitride. RSC Advances, 2022, 12, 24311-24318.	1.7	3
6435	Simple and high-precision DFT-QSPR prediction of enthalpy of combustion for sesquiterpenoid high-energyâ€“density fuels. Fuel, 2023, 332, 126157.	3.4	3
6436	Comparative Analysis of Interaction Mode between MABA and Silver Nanoparticles in the Silver Colloidal Solution. Russian Journal of Physical Chemistry B, 2022, 16, 590-595.	0.2	0
6437	A wave function correction-based approach to the identification of resonances for vibrational perturbation theory. Journal of Chemical Physics, 2022, 157, .	1.2	8
6438	Iridium Complexes with a Naphthyridine-Based Si,N-Ligand: Synthesis and Catalytic Activity toward Olefin Hydrogenation. Organometallics, 2022, 41, 2612-2621.	1.1	3
6439	Static Electron Correlation in Anharmonic Molecular Vibrations: A Hybrid TAO-DFT Study. Journal of Physical Chemistry A, 2022, 126, 7273-7282.	1.1	5
6440	IR, UV-visible, NMR spectra and aromaticity of the covalent organic tetraoxa[8]circulene frameworks. Computational and Theoretical Chemistry, 2022, 1217, 113900.	1.1	0
6441	Synthesis, X-Ray Diffraction, DFT and Hirshfeld Surface Studies of		

#	Article	IF	Citations
6450	Hidden Intermediate Activation: A Concept to Elucidate the Reaction Mechanism of the Schmittel Cyclization of Enyne-Allenes. Physical Chemistry Chemical Physics, 0, , .	1.3	4
6451	Synthesis, Spectroscopic (FTIR, FT-Raman and UV-Vis), Structural Investigation, Hirshfeld, AIM, NBO, Chemical Reactivity, In-Vitro and In-Silico Analysis of N-(2-Hydroxyphenyl)-4-Toluenesulfonamide. Polycyclic Aromatic Compounds, 2023, 43, 8005-8036.	1.4	2
6452	Towards pharmaceutical protein stabilization: DFT and statistical learning studies on non-enzymatic peptide hydrolysis degradation mechanisms. Computational and Theoretical Chemistry, 2022, 1218, 113938.	1.1	1
6453	How Cu(II) binding affects structure and dynamics of Î±-synuclein revealed by molecular dynamics simulations. Journal of Inorganic Biochemistry, 2023, 239, 112068.	1.5	6
6454	Synthesis, characterization, and quantum chemical study of cobalt(II) chelates with N-phenethyl-iminodiacetate(2-)-like ligands. Influence of p-(R)-phenethyl group on crystal pattern. Journal of Coordination Chemistry, 2022, 75, 2814-2828.	0.8	1
6455	Bis(Vinylenedithio)â€Tetrathiafulvaleneâ€Based Coordination Networks. Chemistry - A European Journal, 2023, 29, .	1.7	4
6456	Design of a Zr-based metalâ€“organic framework as an efficient fosfomycin carrier: a combined experimental and DFT study. New Journal of Chemistry, 2023, 47, 1278-1290.	1.4	1
6457	Quantum chemistry of cocaine and its isomers II: Spectroscopy. Computational and Theoretical Chemistry, 2023, 1219, 113952.	1.1	0
6458	Nanoporous cyanuric acid nanosheets for semiconductors: Insights from chemical bonding. Chemical Physics Letters, 2023, 811, 140236.	1.2	0
6459	Theoretical study on the vibrational structures in the conductance spectra of a weakly coupled polycyclic aromatic hydrocarbon molecule. Chemical Physics Letters, 2023, 812, 140272.	1.2	0
6460	A combined experimental and computational thermodynamic study of fluoronitrophenol isomers. Journal of Chemical Thermodynamics, 2023, 178, 106954.	1.0	0
6461	Density Functional Theory Investigation on the Molecular Structure and Vibrational Spectra of Triclosan. Spectroscopy (Santa Monica), 2022, , 23-32.	0.3	0
6462	Local mode analysis of characteristic vibrational coupling in nucleobases and Watsonâ€“Crick base pairs of DNA. Electronic Structure, 2022, 4, 044005.	1.0	9
6463	Weak Interactions between Poly(ether imide) and Carbon Dioxide: A Multiscale Investigation Combining Experiments, Theory, and Simulations. Macromolecules, 2022, 55, 10773-10787.	2.2	7
6464	Molecular Dynamics Simulation of Poly(Ether Ether Ketone) (PEEK) Polymer to Analyze Intermolecular Ordering by Low Wavenumber Raman Spectroscopy and X-ray Diffraction. Polymers, 2022, 14, 5406.	2.0	2
6465	Soft x-ray spectroscopy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">coronene</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mo>(</mml:mo><mml:mtext>coronene</mml:mtext></mml:mrow></mml:msup></mml:math>	1.0	2
6466	Computing the Differences between Asn-X and Gln-X Deamidation and Their Impact on Pharmaceutical and Physiological Proteins: A Theoretical Investigation Using Model Dipeptides. Journal of Physical Chemistry A, 2023, 127, 57-70.	1.1	0
6467	Synthesis, Crystal Structure, DFT Studies on Tetramethyl-(p-Tolyl)-Hexahydro-1H-Xanthene-1,8(2H)-Dione. Polycyclic Aromatic Compounds, 0, , 1-23.	1.4	1

#	Article	IF	Citations
6468	Comprehensive studies of spiropyrrolidines towards spectroscopic characterization, X-ray diffraction, Hirshfeld surface and DFT computations. Journal of Molecular Structure, 2023, 1278, 134872.	1.8	0
6469	Synthesis, Quantum Computational Analysis and Molecular Docking of 3-(2-Hydroxyphenyl)-1-Phenyl Propanone: A Combined Experimental and Theoretical Analysis. Polycyclic Aromatic Compounds, 2023, 43, 8903-8932.	1.4	1
6470	Thermo-oxidative conversion of PDC as a molecular model of residual feedstocks to oxygen-rich chemicals. Reaction Chemistry and Engineering, 2023, 8, 1083-1096.	1.9	2
6471	Understanding the mechanism and regioâ€•and stereo selectivity of [3â€‰+â€‰2] cycloaddition reactions between substituted azomethine ylide and 3,3,3â€•<scp>trifluoro</scp> â€1â€•nitropropâ€1â€•ene, within the molecular electron density theory. Journal of Computational Chemistry, 0, , .	1.5	1
6472	Sum-frequency vibrational spectroscopy of centrosymmetric molecule at interfaces. Journal of Chemical Physics, 0, , .	1.2	3
6474	Organic Base-Catalyzed Cascade Reaction of Electron-Deficient Cyclopentadienone with Prop-2-yn-1-ols: Formation of 3-Methylenetetrahydrofuran Ring Condensed with Cyclopentenone. Heterocycles, 2023, 106, .	0.4	0
6475	Dissecting amide-I vibrations in histidine dipeptide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 292, 122424.	2.0	0
6476	Dechlorination of CDCl3 on Fe(111): Implications for disinfection by-product degradation. Surface Science, 2023, 732, 122271.	0.8	0
6477	Quantum Chemical Analysis and Effect of Super Alkali/Super Halogen Doping on the Opto-Electronic Properties of L-Lysine p-Nitrophenolatemonohydrate (LLPNP) Using First Principle. Polycyclic Aromatic Compounds, 2023, 43, 8667-8689.	1.4	0
6478	Physical Chemistry in Context: Using Quantum Mechanics to Understand the Greenhouse Effect. Journal of Chemical Education, 2023, 100, 1333-1342.	1.1	0
6479	Dinuclear Phenoxo-Bridged Nickel(II) and Copper(II) Complexes of Phenolate-Based Tripodal Ligand: Theoretical and Experimental Insights. Polycyclic Aromatic Compounds, 2024, 44, 313-332.	1.4	1
6480	Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. Journal of Physical Chemistry A, 2023, 127, 1715-1735.	1.1	19
6481	Multi-componential metal intercalated graphite hybrids synthesized by co-intercalation polymerization towards high-efficient microwave absorptions. Nano Research, 2023, 16, 6369-6379.	5.8	8
6482	Hirshfeld and AIM Analysis of the Methylone Hydrochloride Crystal Structure and Its Impact on the IR Spectrum Combined with DFT Study. Crystals, 2023, 13, 383.	1.0	2
6483	Nonlinear optical response and characteristic Raman spectra of phagraphene quantum dots. Physica Scripta, 2023, 98, 045109.	1.2	2
6484	Free-Radical Propagation Rate Coefficients of Diethyl Itaconate and Di-n-Propyl Itaconate Obtained via PLPâ€“SEC. Polymers, 2023, 15, 1345.	2.0	1
6485	Determination of the molecular structure and spectroscopic properties of capsaicin. Radiation Physics and Chemistry, 2023, 208, 110879.	1.4	4
6486	Surface-Enhanced Raman Spectroscopic Analysis of Flavoenzyme Cofactors: Guidance for Flavin-Related Bio- and Chemo- Sensors. Chemosensors, 2023, 11, 190.	1.8	0

#	Article	IF	Citations
6487	Combining Experimental and Theoretical Tools to Probe Radio-Oxidation Products in Polyethylene. Polymers, 2023, 15, 1537.	2.0	1
6488	Probing radical versus proton migration in the aniline cation with IRMPD spectroscopy. Molecular Physics, 2024, 122, .	0.8	0
6489	Oxidized Bridged Carbenoids as Viable Intermediates in a Fe(III) Catalyzed Câˆ'H Insertion Reaction. Chemistry - A European Journal, 2023, 29, .	1.7	2
6490	Application of Low-Frequency Raman Spectroscopy to Probe Dynamics of Lipid Mesophase Transformations upon Hydration. Journal of Physical Chemistry B, 2023, 127, 3223-3230.	1.2	2
6519	Benchmark Accuracy in Thermochemistry, Kinetics, and Noncovalent Interactions. , 2024, , 47-68.		0
6556	Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry with Re-Engineered 2, a 5-Dihydroxypheny Acid Derivative. , 2024, , 313-337.		0