

Reaction path following in mass-weighted internal coord

The Journal of Physical Chemistry

94, 5523-5527

DOI: 10.1021/j100377a021

Citation Report

#	ARTICLE	IF	CITATIONS
36	A reduction of the reaction path formalism to the space of internal variables. <i>Chemical Physics Letters</i> , 1991, 178, 49-54.	1.2	14
37	Extended transition-state theory and constant-energy chemical-reaction molecular-dynamics method for liquid-phase chemical reactions. <i>Journal of Chemical Physics</i> , 1992, 97, 8143-8155.	1.2	17
38	Chapter 3. Theoretical organic chemistry. <i>Annual Reports on the Progress of Chemistry Section B</i> , 1992, 89, 35.	0.8	1
39	On coordinate transformations in steepest descent path and stationary point locations. <i>International Journal of Quantum Chemistry</i> , 1992, 43, 855-871.	1.0	40
40	Algorithmic tools in the study of semiempirical potential surfaces. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 723-741.	1.0	83

41 Following gradient extremal paths. *Theoretica Chimica Acta*, 1992, 83, 15-20. 0.9 45

42

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54	Dynamically defined reaction path (DDRP) method. Journal of Molecular Structure, 1994, 311, 29-35.	1.8	2
55	Reaction path as a gradient line on a potential energy surface. International Journal of Quantum Chemistry, 1994, 49, 105-127.	1.0	35
56	Ab initio calculations to the reactions of HF and HCl with Si(OH) <sub>4</sub> and (HO) <sub>3</sub> SiSi(OH) <sub>3</sub> : Modeling of SiO <sub>2</sub> etching reactions. International Journal of Quantum Chemistry, 1994, 52, 117-125.	1.0	4
57	The determination of intrinsic reaction coordinates by density functional theory. International Journal of Quantum Chemistry, 1994, 52, 731-765.	1.0	126
58	Gradient line reaction path of HF addition to ethylene. Chemical Physics Letters, 1994, 218, 413-421.	1.2	35
59	An ab initio molecular orbital study of SiH <sub>2</sub> + F <sub>2</sub> †SiH <sub>2</sub> F <sub>2</sub> . Chemical Physics Letters, 1994, 225, 410-415.	1.2	2
60	Dynamically defined reaction path (DDRP) method. Computational and Theoretical Chemistry, 1994, 311, 29-35.	1.5	9
61	A direct ab initio dynamics approach for calculating thermal rate constants using variational transition state theory and multidimensional semiclassical tunneling methods. An application to the CH <sub>4</sub> +H†CH <sub>3</sub> +H <sub>2</sub> reaction. Journal of Chemical Physics, 1994, 100, 8014-8025.	1.2	95
62	A new direct ab initio dynamics method for calculating thermal rate constants from density functional theory. Journal of Chemical Physics, 1994, 101, 7408-7414.	1.2	86
63	Transition structures of the Friedel-Crafts reaction in solution. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1757-1761.	1.7	17
64	Ab initio quantum chemistry study of the gas-phase reaction of ClO with HO <sub>2</sub> . Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1811.	1.7	23
65	Enzyme catalysis and transition structures in vacuo. Transition structures for the enolization, carboxylation and oxygenation reactions in ribulose-1,5-bisphosphate carboxylase/oxygenase enzyme (Rubisco). Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2365-2374.	1.7	43
66	Some thoughts on reaction-path following. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1569.	1.7	73
67	Ab initio molecular orbital calculations of the mechanism of oxidation of boron and aluminum monohalides. Chemical Physics Letters, 1995, 241, 516-521.	1.2	1
68	Geometry optimisation on a hypersphere. Application to finding reaction paths from a conical intersection. Chemical Physics Letters, 1995, 243, 1-8.	1.2	112
69	Is there a hydride transfer between N <sub>2</sub> OH <sup>+</sup> and saturated hydrocarbons?. Chemical Physics, 1995, 192, 99-110.	0.9	3
70	Theoretical investigation of isotopic scrambling mechanisms in 2-chloroethyl methyl sulfide. Structural Chemistry, 1995, 6, 243-254.	1.0	1
71	Theoretical implications involved in the DDRP method. Journal of Mathematical Chemistry, 1995, 17, 377-393.	0.7	3

#	ARTICLE	IF	CITATIONS
72	Searching for transition states: Theline-then-plane(LTP) approach. International Journal of Quantum Chemistry, 1995, 55, 429-439.	1.0	18
73	Proton transfer in H5O2+ and H3O2? with an external restraining force. International Journal of Quantum Chemistry, 1995, 56, 567-575.	1.0	5
74	Gas-phase stability of cluster ions SF <sub>m</sub> + (SF <sub>6</sub> ) <sub>n</sub> with m = 0-5 and n = 1-3. Journal of the American Society for Mass Spectrometry, 1995, 6, 1137-1142.	1.2	7
75	Charge analysis along the intrinsic reaction coordinate for the insertion reactions CFX + HY (X = H, F; Y = O, S). Journal of Physical Chemistry, 1995, 357, 75-86.	1.5	5
76	An ab initio investigation on transition states and reactivity of chloroethane with OH radical. Journal of Chemical Physics, 1995, 102, 7504-7518.	1.2	42
77	Direct ab initio dynamics studies of vibrational state selected reaction rate of the OH+H <sub>2</sub> →H+H <sub>2</sub> O reaction. Journal of Chemical Physics, 1995, 102, 5335-5341.	1.2	33
78	Thermal and vibrational state selected rates of the CH <sub>4</sub> +Cl→HCl+CH <sub>3</sub> reaction. Journal of Chemical Physics, 1995, 103, 9642-9652.	1.2	154
79	Ab initio calculations to the reactions of CF <sub>m</sub> (m = 4-1) and NF <sub>n</sub> (n = 3-1) species with models of SiO <sub>2</sub> surface structures. Surface Science, 1995, 331-333, 1503-1507.	0.8	8
80	Theoretical study of the cyclization of $\alpha$ -iminothioaldehydes into dihydrothiazoles. Journal of the Chemical Society Perkin Transactions II, 1995, , 1077-1086.	0.9	4
81	Reaction path potential and vibrational frequencies in terms of curvilinear internal coordinates. Journal of Chemical Physics, 1995, 102, 3188-3201.	1.2	202
82	Prototype Si-H insertion reaction of silylene with silane. Absolute rate constants, temperature dependence, RRKM modelling and the potential-energy surface. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2723-2732.	1.7	87
83	A density functional study on olefin insertion and hydrogen transfer in the reaction between Cl <sub>2</sub> Ti-ethyl and ethylene. Possible implications for the stereochemistry and chain termination in olefin polymerization. Canadian Journal of Chemistry, 1995, 73, 989-998.	0.6	33
84	Current Status of Transition-State Theory. The Journal of Physical Chemistry, 1996, 100, 12771-12800.	2.9	1,795
85	Spontaneous DNA Mutations Induced by Proton Transfer in the Guanine-Cytosine Base Pairs: An Energetic Perspective. Journal of the American Chemical Society, 1996, 118, 3010-3017.	6.6	273
86	Is It [4 + 2] or [2 + 4]? A New Look at Lewis Acid Catalyzed Diels-Alder Reactions. Journal of the American Chemical Society, 1996, 118, 11680-11681.	6.6	24
87	Isomers on the Si <sub>2</sub> CH <sub>4</sub> <sup>+</sup> Potential Energy Surface. Organometallics, 1996, 15, 5391-5398.	1.1	5
88	The C <sub>7</sub> H <sub>6</sub> Potential Energy Surface Revisited: Relative Energies and IR Assignment. Journal of the American Chemical Society, 1996, 118, 1535-1542.	6.6	155
89	Transition Structures for the Aromatic Claisen Rearrangements by the Molecular Orbital Method. Journal of Organic Chemistry, 1996, 61, 6218-6226.	1.7	50

#	ARTICLE	IF	CITATIONS
90	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral $\hat{I}\pm$ -Alkoxy Carbonyl Compounds. <i>Journal of Organic Chemistry</i> , 1996, 61, 3467-3475.	1.7	25
91	Bond-Stretch Isomerism in Tetrasilabicyclo[1.1.0]butane Derivatives. <i>Organometallics</i> , 1996, 15, 2118-2124.	1.1	37
92	Gas-Phase Identity $S_N2$ Reactions of Halide Anions and Methyl Halides with Retention of Configuration. <i>Journal of the American Chemical Society</i> , 1996, 118, 11258-11264.	6.6	108
93	Are Anion Radicals Nucleophiles and/or Outersphere Electron Donors? An Ab Initio Study of the Reaction of Ethylene and Formaldehyde Anion Radicals with Methyl Fluoride and Chloride. <i>Journal of the American Chemical Society</i> , 1996, 118, 5737-5744.	6.6	26
94	Experimental and Theoretical Study of the $C_2H_3^{\hat{+}}$ , $H + C_2H_2$ Reaction. Tunneling and the Shape of Falloff Curves. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16899-16911.	2.9	101
95	Electronic Factors Influencing the Decarboxylation of $\hat{I}^2$ -Keto Acids. A Model Enzyme Study. <i>Journal of Organic Chemistry</i> , 1996, 61, 6346-6353.	1.7	51
96	Theoretical Characterization of the Mechanism of $Hg\hat{\sim}C$ Bond Cleavage by Halogenic Acids. <i>Organometallics</i> , 1996, 15, 1465-1469.	1.1	23
97	Structured Electron Transfer Transition State. Valence Bond Configuration Mixing Analysis and ab Initio Calculations of the Reactions of Formaldehyde Radical Anion with Methyl Chloride. <i>The Journal of Physical Chemistry</i> , 1996, 100, 12241-12252.	2.9	48
98	Reaction Paths for Aqueous Decomposition of $CCl_2$ . <i>The Journal of Physical Chemistry</i> , 1996, 100, 12410-12413.	2.9	46
99	Combined ab initio and density functional study of ring chain tautomerism in benzofurazan-1-oxide. <i>Journal of Computational Chemistry</i> , 1996, 17, 1848-1856.	1.5	15
100	Equilibrium and non-equilibrium solvent effects in electrophilic halogenation of ethylenic compounds. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 107-116.	1.5	17
101	Searching critical points of fitted potential energy surfaces. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 85-90.	1.5	7
103	Ab initio study of the formation of $C_3H_3^+$ from the reaction of $CH_3^+$ with acetylene. <i>Journal of Computational Chemistry</i> , 1996, 17, 905-909.	1.5	11
104	Use of multivariate methods in the analysis of calculated reaction pathways. <i>Journal of Computational Chemistry</i> , 1996, 17, 1197-1216.	1.5	4
105	Computational investigations of carbonyl reactions: Comparison between nucleophilic addition versus enolate formation in the reaction of acetaldehyde with hydroxide ion. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 711-716.	0.9	7
106	A Gaussian-2 molecular orbital study of the sigmatropic 1,3-hydrogen shift in 1-silapropene. <i>Chemical Physics Letters</i> , 1996, 254, 302-306.	1.2	2
107	Density functional theory and ab initio study of $CH_3NC$ and $HNC$ isomerization. <i>Chemical Physics Letters</i> , 1996, 256, 213-219.	1.2	41
108	Ab initio and density functional theory study of the diazene isomerization. <i>Chemical Physics Letters</i> , 1996, 261, 13-17.	1.2	40

#	ARTICLE	IF	CITATIONS
109	What Do Ab Initio Calculations Predict for the Structure of Lithiated Azaenolates of Peptides?. Chemistry - A European Journal, 1996, 2, 9-18.	1.7	9
110	Towards the Definition of the Maximum Allowable Tightness of an Electron Transfer Transition State in the Reactions of Radical Anions and Alkyl Halides. Angewandte Chemie International Edition in English, 1996, 35, 1098-1100.	4.4	35
111	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. Tetrahedron, 1996, 52, 10693-10704.	1.0	33
112	A theoretical study of a model of N-tert-butyl- $\beta$ -phenylnitrone (PBN) as active oxygen species scavenger. Chemical Physics, 1996, 204, 313-326.	0.9	3
113	Reaction dynamics of the four-centered elimination $\text{CH}_2\text{OH}+\text{CHO}+\text{H}_2$ : Measurement of kinetic energy release distribution and classical trajectory calculation. Journal of Chemical Physics, 1996, 104, 4517-4529.	1.2	30
114	The effective fragment model for solvation: Internal rotation in formamide. Journal of Chemical Physics, 1996, 105, 11081-11090.	1.2	122
115	An interpolated unrestricted Hartree-Fock potential energy surface for the $\text{OH}+\text{H}_2\rightarrow\text{H}_2\text{O}+\text{H}$ reaction. Journal of Chemical Physics, 1996, 104, 4600-4610.	1.2	69
116	Reaction path dynamics in curvilinear internal coordinates including torsions. Journal of Chemical Physics, 1996, 104, 6491-6496.	1.2	74
117	Proton Abstraction from Carbon Acids. Ab Initio Molecular Orbital Study on the Proton Abstraction from Acetaldehyde by $\text{NH}_2^-$ , $\text{OH}^-$ , $\text{F}^-$ , $\text{SiH}_3^-$ , $\text{PH}_2^-$ , and $\text{SH}^-$ . The Journal of Physical Chemistry, 1996, 100, 3441-3447.	2.9	9
118	Kinetics of the $\text{C}_2\text{H}_3+\text{H}_2$ , $\text{H}+\text{C}_2\text{H}_4$ and $\text{CH}_3+\text{H}_2$ , $\text{H}+\text{CH}_4$ Reactions. The Journal of Physical Chemistry, 1996, 100, 11346-11354.	2.9	116
119	Synthesis of $\beta$ -Lactams from Fluoroketenes and Imines: Ab Initio Potential Energy Surfaces in Gas Phase and in Solution. The Journal of Physical Chemistry, 1996, 100, 10600-10608.	2.9	24
120	Ring Opening of Cyclopropylidene and Internal Rotation of Allene. The Journal of Physical Chemistry, 1996, 100, 16147-16154.	2.9	77
121	Hydrogen Transfer in 7-Azaindole. The Journal of Physical Chemistry, 1996, 100, 3974-3979.	2.9	77
122	A combined method for determining reaction paths, minima, and transition state geometries. Journal of Chemical Physics, 1997, 107, 375-384.	1.2	284
123	Potential energy surfaces for polyatomic reactions by interpolation with reaction path weight: $\text{CH}_2\text{OH}+\text{CHO}+\text{H}_2$ reaction. Journal of Chemical Physics, 1997, 106, 1003-1012.	1.2	43
124	Thermochemistry of the reactions of $\text{F}+(3\text{P})$ and $\text{F}+(1\text{D})$ with hydrogen sulphide a molecular orbital study. Molecular Physics, 1997, 91, 503-512.	0.8	2
125	Nonenzymatic and enzymatic hydrolysis of alkyl halides: A theoretical study of the $\text{S}_{\text{N}}2$ reactions of acetate and hydroxide ions with alkyl chlorides. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 6591-6595.	3.3	31
126	Transition Structures of [2,3]-Wittig Rearrangement of 2-Oxa-5-methylhexene-1-carboxylic Acid. Chemistry Letters, 1997, 26, 81-82.	0.7	5

#	ARTICLE	IF	CITATIONS
127	Open Dimer Participation in Chelation Controlled Addition of Methyllithium Dimer to $\alpha$ - and $\beta$ -Alkoxy Aldehydes. <i>Chemistry Letters</i> , 1997, 26, 1079-1080.	0.7	12
128	Molecular decompositions of acetaldehyde and formamide: theoretical studies using Hartree-Fock, Moller-Plesset and density functional theories. <i>Molecular Physics</i> , 1997, 92, 497-502.	0.8	10
129	Density Functional Study of the [2+2]- and [2+3]-Cycloaddition Mechanisms for the Osmium-Catalyzed Dihydroxylation of Olefins. <i>Organometallics</i> , 1997, 16, 13-19.	1.1	122
130	Theoretical Study of the Atmospheric Reaction between Dimethyl Sulfide and Chlorine Atoms. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9738-9744.	1.1	27
131	Reaction-Path Dynamics and Theoretical Rate Constants for the $\text{CH}_3\text{F} + \text{Cl} \rightarrow \text{HCl} + \text{CH}_2\text{F}$ Reaction by Direct Dynamics Method. <i>Journal of the American Chemical Society</i> , 1997, 119, 9033-9038.	6.6	35
132	An ab Initio Study of Nucleophilic Attack of Trimethyl Phosphate: Factors Influencing Site Reactivity. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8706-8713.	1.1	32
133	Reaction-Path Dynamics of Hydroxyl Radical Reactions with Ethane and Haloethanes. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4245-4253.	1.1	43
134	Theoretical Investigation of the Reaction between Aluminum and Propene. Comparison between Calculated and Experimental ESR Results. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4814-4820.	1.1	5
135	Ab Initio Study of Hydrogen Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4416-4431.	1.1	105
136	Hydrogen-Bond Networks for Hydrolyses of Anhydrides. <i>Journal of Organic Chemistry</i> , 1997, 62, 7049-7053.	1.7	16
137	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. <i>Journal of the American Chemical Society</i> , 1997, 119, 6415-6422.	6.6	51
138	G2 Molecular Orbital Study of the Reactions of Water with $\text{Cl}^+(3\text{P})$ and $\text{Cl}^+(1\text{D})$ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 1722-1730.	1.1	10
139	Theoretical Study of the Oxidation of Alcohol to Aldehyde by d <sup>0</sup> Transition-Metal <sup>n</sup> Oxo Complexes: A Combined Approach Based on Density Functional Theory and the Intrinsic Reaction Coordinate Method. <i>Organometallics</i> , 1997, 16, 716-724.	1.1	45
140	Quantum Chemical Reaction Path and Transition State for a Model Cope (and Reverse Cope) Elimination. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3554-3560.	1.1	32
141	Combining Quantum Mechanical Reaction Pathways with Force Field Lattice Interactions To Model a Solid-State Phototransformation. <i>Journal of the American Chemical Society</i> , 1997, 119, 1474-1475.	6.6	20
142	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1859-1865.	1.1	44
143	Novel Aspects of the [1,3] Sigmatropic Silyl Shift in Allylsilane. <i>Journal of the American Chemical Society</i> , 1997, 119, 807-815.	6.6	28
144	Primary and Solvent Kinetic Isotope Effects in the Water-Assisted Tautomerization of Formamidine: An ab Initio Direct Dynamics Study. <i>Journal of Physical Chemistry A</i> , 1997, 101, 7802-7808.	1.1	27

#	ARTICLE	IF	CITATIONS
145	A DFT Study of the Simmons-Smith Cyclopropanation Reaction. <i>Journal of the American Chemical Society</i> , 1997, 119, 12300-12305.	6.6	59
146	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of $\beta$ -Lactam Antibiotics. A Theoretical Study Including Solvent Effects. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3581-3588.	1.2	56
147	Relaxation Paths from a Conical Intersection: The Mechanism of Product Formation in the Cyclohexadiene/Hexatriene Photochemical Interconversion. <i>Journal of Physical Chemistry A</i> , 1997, 101, 2023-2032.	1.1	149
148	Theoretical Studies on the Addition of Polymetallic Lithium Organocuprate Clusters to Acetylene. Cooperative Effects of Metals in a Trap-and-Bite Reaction Pathway. <i>Journal of the American Chemical Society</i> , 1997, 119, 4887-4899.	6.6	73
149	An ab Initio QCISD Study of the Potential Energy Surface for the Reaction $\text{HNO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{OH}$ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 9430-9438.	1.1	25
150	Potential Energy Surfaces for Dissociation Reactions of High-Energy Isomers of $\text{N}_2\text{O}_2$ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 4283-4289.	1.1	21
151	A Theoretical Study of the Favorskii Rearrangement. Calculation of Gas-Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the $\beta$ -Chlorocyclobutanone. <i>Journal of the American Chemical Society</i> , 1997, 119, 1941-1947.	6.6	24
152	Mechanism of Acid-Catalyzed Epoxidation of Alkenes with Peroxy Acids. <i>Journal of Organic Chemistry</i> , 1997, 62, 5191-5197.	1.7	79
153	A general methodology for quantum modeling of free-energy profile of reactions in solution: An application to the Menshutkin $\text{NH}_3 + \text{CH}_3\text{Cl}$ reaction in water. <i>Journal of Chemical Physics</i> , 1997, 107, 1881-1889.	1.2	79
154	Theory versus Experiment in Jet Spectroscopy: Glycolic Acid. <i>Journal of the American Chemical Society</i> , 1997, 119, 2232-2239.	6.6	72
155	Direct evidence for anchimeric assistance in alcohol elimination from gas-phase $\text{MH}^+$ ions of 1,4-dialkoxycyclohexanes under chemical ionisation. Experiment and theory. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 1221-1234.	0.9	11
156	Understanding the activation energy trends for the $\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{C}_2\text{H}_4\text{OH}$ reaction by using canonical variational transition state theory. <i>Journal of Chemical Physics</i> , 1997, 107, 7266-7274.	1.2	50
157	Rearrangements of $\text{C}_7\text{H}_6$ Isomers: Computational Studies of the Interconversions of Bicyclo[3.2.0]hepta-1,3,6-triene, Bicyclo[3.2.0]hepta-3,6-diene-2-ylidene, Bicyclo[3.2.0]hepta-2,3,6-triene, and Cyclohepta-1,2,4,6-tetraene. <i>Journal of Organic Chemistry</i> , 1997, 62, 4398-4405.	1.7	38
158	Theoretical Study of the Zwitterionic Cleavage of 4-Azido-2-pyrrolinones: The Role of Solvent and Substituents. <i>Journal of the American Chemical Society</i> , 1997, 119, 10291-10301.	6.6	15
159	A Gaussian-2 molecular orbital study of the unimolecular reactions of acetyl cyanide. <i>Chemical Physics Letters</i> , 1997, 270, 363-368.	1.2	11
160	Theoretical study on $\text{CH}_2\text{CNH}/\text{CH}_3\text{CN}$ : isomerization reaction in small clusters containing $\text{H}_2\text{O}$ molecules. <i>Computational and Theoretical Chemistry</i> , 1997, 389, 27-35.	1.5	1
161	Mechanisms, energetics and dynamics of a key reaction sequence during the decomposition of nitromethane: $\text{HNO} + \text{HNO} \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$ . <i>Computational and Theoretical Chemistry</i> , 1997, 393, 59-71.	1.5	17
162	Parallelization strategies and experiences with the dynamically defined reaction path (DDRP) method. <i>Computational and Theoretical Chemistry</i> , 1997, 398-399, 111-119.	1.5	4



#	ARTICLE	IF	CITATIONS
163	Microcalorimetric, FTIR, and DFT studies of the adsorption of isobutene on silica. <i>Catalysis Letters</i> , 1997, 47, 119-128.	1.4	8
164	On the cleavage of the peroxide O—O bond in methyl hydroperoxide and dimethyl peroxide upon protonation. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1997, 163, 101-119.	1.9	20
165	Bromine Complexes of Ethylene and Cyclopropene: Matrix-IR Spectroscopic Identification, Photochemical Reactions, Ab Initio Studies. <i>Liebigs Annalen</i> , 1997, 1997, 317-326.	0.8	12
166	On the Oxenoid Character of Alkylperoxy Anions and Their Lithium Compounds: A Combined Mass Spectrometric and Theoretical Investigation. <i>Chemische Berichte</i> , 1997, 130, 1085-1097.	0.2	21
167	Ab Initio Models for the Nitroaldol (Henry) Reaction. <i>Chemistry - A European Journal</i> , 1997, 3, 20-28.	1.7	34
168	Dimethyl Peroxide Radical Cation: A New Theoretical and Experimental Approach to the $C_2H_6O^+$ Potential Energy Surface. <i>Chemistry - A European Journal</i> , 1997, 3, 626-638.	1.7	17
169	Diabatic ordering of vibrational normal modes in reaction valley studies. <i>Journal of Computational Chemistry</i> , 1997, 18, 1282-1294.	1.5	26
170	The ene reaction: Comparison of results of Hartree-Fock, Møller-Plesset, CASSCF, and DFT calculations. <i>International Journal of Quantum Chemistry</i> , 1997, 62, 509-514.	1.0	18
171	Understanding the mechanism of the addition of organomagnesium reagents to 2-hydroxypropanal: An ab initio molecular orbital analysis. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 719-728.	1.0	3
172	A semiempirical study on the ring-opening process for the cyclopropanone, 2,2-dimethylcyclopropanone, trans-2,3-di-tert-butylcyclopropanone, and spiro(bicyclo[2.2.1]heptane-2,1'-cyclopropan)-2-one systems in solution. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 729-738.	1.0	4
173	A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere. <i>Chemical Physics Letters</i> , 1997, 269, 469-474.	1.2	1
174	Ab initio molecular orbital study on the H <sub>2</sub> loss reaction from ethane cation, C <sub>2</sub> H <sub>6</sub> <sup>+</sup> . <i>Chemical Physics Letters</i> , 1997, 277, 291-298.	1.2	10
175	Transition structures of carbon dioxide fixation, hydration and C <sub>2</sub> inversion for a model of Rubisco catalyzed reaction. <i>Chemical Physics Letters</i> , 1997, 278, 291-296.	1.2	17
176	Kinetic isotope effect in hydrogen abstraction from 2-propanol by hydrogen and deuterium radicals. A pulse radiolysis Fourier transform electron spin resonance study. <i>Chemical Physics Letters</i> , 1997, 280, 353-358.	1.2	12
177	A density functional theory and ab initio study of the hydrolysis of dinitrogen pentoxide. <i>Chemical Physics Letters</i> , 1998, 285, 459-466.	1.2	40
178	A theoretical study on the decomposition mechanism of $\hat{1}^2$ -propiolactone and $\hat{1}^2$ -butyrolactone. <i>Chemical Physics Letters</i> , 1998, 288, 261-269.	1.2	9
179	A direct isomerization path for the H <sub>6</sub> <sup>+</sup> cluster.. <i>Chemical Physics Letters</i> , 1998, 293, 59-64.	1.2	19
180	Combined AM1/MM3 computations on organic systems: the Diels-Alder reaction as a test case. <i>Chemical Physics Letters</i> , 1998, 296, 239-244.	1.2	7

#	ARTICLE	IF	CITATIONS
181	Microcalorimetric, FTIR, and DFT Studies of the Adsorption of Methanol, Ethanol, and 2,2,2-Trifluoroethanol on Silica. <i>Journal of Catalysis</i> , 1998, 175, 252-268.	3.1	111
182	A theoretical study of the addition of CH <sub>3</sub> MgCl to chiral $\hat{\text{I}}\pm$ -alkoxy carbonyl compounds. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 263-275.	1.5	3
183	A PM3 semiempirical study of the molecular mechanism for the Favorskii rearrangement of the $\hat{\text{I}}\pm$ -chlorocyclobutanone. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 299-306.	1.5	5
184	A theoretical analysis of the $\hat{\text{I}}\epsilon$ attack of CH <sub>2</sub> F <sup>+</sup> on acetylene. <i>Computational and Theoretical Chemistry</i> , 1998, 429, 275-279.	1.5	1
185	Reaction pathways for proton exchange between protonated formamide and water. <i>Computational and Theoretical Chemistry</i> , 1998, 429, 61-69.	1.5	7
186	PM3 study of the [2 + 3] cycloaddition of 1-nitropropene to methylazide. <i>Computational and Theoretical Chemistry</i> , 1998, 432, 229-234.	1.5	9
187	Theoretical study of the thermal interconversion mechanism between the norbornadiene and quadricyclane radical cations. <i>Computational and Theoretical Chemistry</i> , 1998, 434, 59-66.	1.5	20
188	Exploring the possibility of a bimolecular reaction channel for the F <sub>2</sub> SS/FSSF rearrangement process. <i>Computational and Theoretical Chemistry</i> , 1998, 455, 123-129.	1.5	5
189	An electronic structure investigation of the BNO-BON-NBO system. <i>Computational and Theoretical Chemistry</i> , 1998, 430, 137-148.	1.5	12
190	Enthalpy and Entropy in Ring Closure Reactions. <i>Bioorganic Chemistry</i> , 1998, 26, 193-199.	2.0	31
191	A Combined Neutralization-Reionization Mass Spectrometric and Theoretical Study of Oxyallyl and Other Elusive [C <sub>3</sub> , H <sub>4</sub> , O] Neutrals. <i>European Journal of Organic Chemistry</i> , 1998, 1998, 987-1009.	1.2	34
192	Theoretical investigation of the abnormal Reimer-Tiemann reaction. <i>Journal of Physical Organic Chemistry</i> , 1998, 11, 670-677.	0.9	3
194	Theoretical investigations of NMR chemical shifts and reactivities of oxovanadium(v) compounds. <i>Journal of Computational Chemistry</i> , 1998, 19, 113-122.	1.5	51
195	Theoretical investigation of unimolecular decomposition channels of furan <sup>4</sup> . <i>Journal of Computational Chemistry</i> , 1998, 19, 240-249.	1.5	42
196	TheRate: Program for ab initio direct dynamics calculations of thermal and vibrational-state-selected rate constants. <i>Journal of Computational Chemistry</i> , 1998, 19, 1039-1052.	1.5	263
197	Theoretical study of ester enolate-imine condensation route to $\gamma$ -lactams. <i>Journal of Computational Chemistry</i> , 1998, 19, 1826-1833.	1.5	9
198	Conformers of gaseous protonated glycine. <i>Journal of Computational Chemistry</i> , 1998, 19, 1862-1876.	1.5	40
199	Ab initio MO study on the direct and migratory reaction mechanism for the formation of HF in H + CIF system. <i>Science in China Series B: Chemistry</i> , 1998, 41, 97-102.	0.8	3

#	ARTICLE	IF	CITATIONS
200	Application of reaction path concept in intramolecular proton transfer. <i>Computers &amp; Chemistry</i> , 1998, 22, 13-20.	1.2	1
201	Isomerization of $\text{CH}_3\text{O}^+=\text{CHCH}_3$ to $\text{CH}_2=\text{O}+\text{CH}_2\text{CH}_3$ . <i>Journal of the American Society for Mass Spectrometry</i> , 1998, 9, 130-137.	1.2	13
202	Phosphate Ester Hydrolysis in Aqueous Solution: $\hat{\text{A}}\%$ Associative versus Dissociative Mechanisms. <i>Journal of Physical Chemistry B</i> , 1998, 102, 719-734.	1.2	234
203	Benzene Oxidation in the Troposphere. Theoretical Investigation on the Possible Competition of Three Postulated Reaction Channels. <i>Journal of the American Chemical Society</i> , 1998, 120, 6753-6757.	6.6	51
204	Reactivity and Regioselectivity of Hydroxyl Radical Addition to Halogenated Ethenes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1583-1594.	1.1	81
205	Elimination of Ethylene from Metastable Isomeric Silylenium Ions in the Gas Phase: $\hat{\text{A}}\%$ Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6942-6949.	1.1	14
206	Predictions of rate constants and estimates for tunneling splittings of concerted proton transfer in small cyclic water clusters. <i>Journal of Chemical Physics</i> , 1998, 109, 2672-2679.	1.2	57
207	Ab initio molecular orbital and density functional characterization of the potential energy surface of the $\text{N}_2\text{O}+\text{Br}$ reaction. <i>Journal of Chemical Physics</i> , 1998, 109, 9410-9416.	1.2	11
208	Modern Valence-Bond Description of Chemical Reaction Mechanisms: $\hat{\text{A}}$ Diels $\hat{\text{A}}$ Alder Reaction. <i>Journal of the American Chemical Society</i> , 1998, 120, 3975-3981.	6.6	45
209	A Theoretical Study of Homogeneous Ziegler $\hat{\text{A}}$ Natta Catalysis. <i>Organometallics</i> , 1998, 17, 16-24.	1.1	78
210	Density Functional Study of Bergman Cyclization of Enediyne. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2584-2593.	1.1	43
211	Ab Initio Molecular Orbital Study of the Thermochemistry and Reactions of the Chlorinated Disilenes and Their Isomers ( $\text{Si}_2\text{H}_n\text{Cl}_{4-n}$ ). <i>Journal of Physical Chemistry A</i> , 1998, 102, 785-792.	1.1	33
212	Potential Energy Surfaces for the Bis-Silylation of Ethylene. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4666-4668.	1.1	3
213	Neutral and Alkaline Hydrolyses of Model $\hat{\text{I}}^2$ -Lactam Antibiotics. An ab Initio Study of Water Catalysis. <i>Journal of the American Chemical Society</i> , 1998, 120, 2146-2155.	6.6	71
214	Density Functional Theory Study of a Lewis Acid Catalyzed Diels $\hat{\text{A}}$ Alder Reaction. The Butadiene + Acrolein Paradigm. <i>Journal of the American Chemical Society</i> , 1998, 120, 2415-2420.	6.6	123
215	Rearrangements on the $\text{C}_6\text{H}_6$ Potential Energy Surface and the Topomerization of Benzene. <i>Journal of the American Chemical Society</i> , 1998, 120, 5741-5750.	6.6	58
216	Mechanism of Dioxirane Oxidation of CH Bonds: $\hat{\text{A}}$ Application to Homo- and Heterosubstituted Alkanes as a Model of the Oxidation of Peptides. <i>Journal of Organic Chemistry</i> , 1998, 63, 5413-5422.	1.7	59
217	Study of Small Water Clusters Using the Effective Fragment Potential Model. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2650-2657.	1.1	73

#	ARTICLE	IF	CITATIONS
218	Molecular Modeling of Methane Diffusion in Glassy Atactic Polypropylene via Multidimensional Transition State Theory. <i>Macromolecules</i> , 1998, 31, 7068-7090.	2.2	86
219	Theoretical Study of the Reaction $1[:CH_2] + CHO + CH_3 + CO$ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 9918-9924.	1.1	6
220	Reaction-Path and Dual-Level Dynamics Calculations of the $CH_3F + OH$ Reaction. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10715-10722.	1.1	23
221	Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for $C_2H_4 + H$ and $C_2H_5$ : Variable Scaling of External Correlation Energy for Association Reactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 5559-5567.	6.6	30
222	A Theoretical Study of the Interaction of Ammonia with Silicon Trimer. <i>Journal of Physical Chemistry A</i> , 1998, 102, 9531-9536.	1.1	3
223	Mechanistic Crossover Induced by Steric Hindrance: A Theoretical Study of Electron Transfer and Substitution Mechanisms of Cyanoformaldehyde Anion Radical and Alkyl Halides. <i>Journal of the American Chemical Society</i> , 1998, 120, 2131-2145.	6.6	32
224	A Density Functional Study of [2+3] versus [2+2] Addition of Ethylene to Chromium-Oxygen Bonds in Chromyl Chloride. <i>Inorganic Chemistry</i> , 1998, 37, 1307-1314.	1.9	42
225	On the Origin of Substrate Directing Effects in the Epoxidation of Allyl Alcohols with Peroxyformic Acid. <i>Journal of the American Chemical Society</i> , 1998, 120, 680-685.	6.6	50
226	Theoretical Evidence for a Concerted Mechanism of the Oxirane Cleavage and A-Ring Formation in Oxidosqualene Cyclization. <i>Journal of the American Chemical Society</i> , 1998, 120, 4045-4046.	6.6	48
227	Ab Initio Tests of the Marcus Equation for the Prediction of the Position of the Transition State for the Reaction $H + C_2H_5R \rightarrow CH_3 + CH_2R$ with $R = H, CH_3, NH_2, CN, CF_3$ , and $C_6H_5$ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 2332-2341.	1.1	14
228	Hybridization as a Metric for the Reaction Coordinate of Chemical Reactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 10494-10496.	6.6	42
229	Theoretical Study of the Insertion Reactions of Aluminum with $H_2O, NH_3, HCl$ , and $Cl_2$ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 1005-1017.	1.1	37
230	High Level and Dual Level Direct Dynamics in the Intramolecular Proton Transfer of Hydrogenoxalate Anion. Influence of Tunneling and Isotopic Effect. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2954-2961.	1.1	16
231	The Mechanism of the Gas-Phase Ion-Molecule Reaction between $Al^+$ and Ethanol. <i>Journal of Physical Chemistry A</i> , 1998, 102, 10493-10500.	1.1	12
232	Direct Dynamics Study of the Dissociation and Elimination Channels in the Thermal Decomposition of Methyl Nitrite. <i>Journal of the American Chemical Society</i> , 1998, 120, 7594-7601.	6.6	14
233	Theoretical Study of the Mechanism of Zeolite-Catalyzed Isomerization Reactions of Linear Butenes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 982-989.	1.1	105
234	Modeling of Peptide Hydrolysis by Thermolysin. A Semiempirical and QM/MM Study. <i>Journal of the American Chemical Society</i> , 1998, 120, 8825-8833.	6.6	76
235	A Computational Study on the Reaction Mechanism of the Boulton-Katritzky Rearrangement. <i>Journal of the American Chemical Society</i> , 1998, 120, 13478-13484.	6.6	48

#	ARTICLE	IF	CITATIONS
236	Theoretical Study on the Reaction Path and Variational Rate Constant of the Reaction $\text{HNCO} + \text{NH} \hat{\rightarrow} \text{NCO} + \text{NH}_2$ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 1194-1199.	1.1	15
237	8-Endo Cyclization of (Alkoxy carbonyl)methyl Radicals: A Radical Way for Preparation of Eight-Membered-Ring Lactones. <i>Journal of the American Chemical Society</i> , 1998, 120, 7469-7478.	6.6	52
238	Ab initio study on the reaction mechanism of ozone with the chlorine atom. <i>Journal of Chemical Physics</i> , 1998, 109, 10847-10852.	1.2	33
239	Initial H <sub>2</sub> O-induced oxidation of C(001)-(2 $\times$ 1): A study with hybrid density-functional theory. <i>Physical Review B</i> , 1998, 58, 6760-6763.	1.1	24
240	Theoretical study of an isotope effect on rate constants for the $\text{CH}_3 + \text{H}_2 \hat{\rightarrow} \text{CH}_4 + \text{H}$ and $\text{CD}_3 + \text{H}_2 \hat{\rightarrow} \text{CD}_3\text{H} + \text{H}$ reactions using variational transition state theory and the multidimensional semiclassical tunneling method. <i>Journal of Chemical Physics</i> , 1999, 110, 10830-10842.	1.2	20
241	Acetylacetonate (acac) anion in the gas phase: predicted structures, vibrational spectra, and photodetachment energies. <i>International Journal of Mass Spectrometry</i> , 1999, 185-187, 577-587.	0.7	6
242	Ab initio study of the addition of atomic carbon with water. <i>Chemical Physics</i> , 1999, 244, 143-149.	0.9	18
243	Unimolecular decomposition of the isomers of $[\text{HNO}_2]^+$ and $[\text{HNO}_2]^{\hat{\rightarrow}}$ systems: a DFT study. <i>Chemical Physics</i> , 1999, 248, 147-159.	0.9	10
244	A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase. <i>Chemical Physics</i> , 1999, 246, 1-12.	0.9	25
245	A density functional study on the formation of stereoerrors in the stereoselective propene polymerization with zirconocene catalysts. <i>Journal of Organometallic Chemistry</i> , 1999, 592, 11-21.	0.8	23
246	A theoretical study on an isotope effect in the $\text{CH}_3 + \text{H}_2 \hat{\rightarrow} \text{CH}_4 + \text{H}$ reaction. <i>Chemical Physics Letters</i> , 1999, 299, 57-63.	1.2	14
247	A Gaussian-2 molecular orbital study of the reaction of $\text{CF}_3$ with $\text{NO}_2$ . <i>Chemical Physics Letters</i> , 1999, 313, 307-312.	1.2	4
248	Ab initio and density functional theory study of the mechanism of synthesis of the $\text{N}_5^+$ cation. <i>Chemical Physics Letters</i> , 1999, 314, 300-306.	1.2	31
249	DFT Study of the Isomerization of Hexyl Species Involved in the Acid-Catalyzed Conversion of 2-Methyl-Pentene-2. <i>Journal of Catalysis</i> , 1999, 181, 124-144.	3.1	48
250	Theoretical study of dynamical properties on reaction path in molecular internal coordinates. <i>Science in China Series B: Chemistry</i> , 1999, 42, 605-611.	0.8	1
251	Ab initio study on reaction path and rate constant of the hydrogen atom abstraction reaction $\text{HNCO} + \text{N} \hat{\rightarrow} \text{NCO} + \text{NH}$ . <i>Computational and Theoretical Chemistry</i> , 1999, 459, 37-46.	1.5	12
252	Theoretical study for the $\text{HNSi} \hat{\leftrightarrow} \text{HSiN}$ isomerization: ab initio and DFT calculations. <i>Computational and Theoretical Chemistry</i> , 1999, 460, 213-220.	1.5	9
253	Finding, optimization, and verification of transition state structures with semi-empirical and ab-initio computational methods. <i>Computational and Theoretical Chemistry</i> , 1999, 465, 173-182.	1.5	8

#	ARTICLE	IF	CITATIONS
254	A quantum mechanical study of the transfer of biological sulfate. Computational and Theoretical Chemistry, 1999, 461-462, 105-111.	1.5	11
255	A theoretical study on reaction mechanism of oxidative coupling reaction of p-phenylenediamine with phenol: a proposal of the route via a [5,5]-sigmatropic rearrangement. Computational and Theoretical Chemistry, 1999, 461-462, 429-438.	1.5	5
256	A Gaussian-2 ab initio study of [C <sub>2</sub> H <sub>5</sub> S] <sup>+</sup> ions: III. H <sub>2</sub> and CH <sub>4</sub> eliminations from CH <sub>3</sub> CHSH <sup>+</sup> and CH <sub>3</sub> SCH <sub>2</sub> <sup>+</sup> . Computational and Theoretical Chemistry, 1999, 490, 109-124.	1.5	9
257	Generation, Microwave Spectrum, and Ab Initio MO Calculation of trans-1-Nitrosopropene, CH <sub>3</sub> CH=CHNO (synform). Journal of Molecular Spectroscopy, 1999, 194, 79-86.	0.4	12
258	Interconversions of Z-1,3,5-hexatriene conformers: A theoretical study. International Journal of Quantum Chemistry, 1999, 72, 295-305.	1.0	10
259	On the kinetic stability of the SH <sub>3</sub> X species with X=F, Cl. International Journal of Quantum Chemistry, 1999, 73, 37-43.	1.0	1
260	Serine peptidase catalytic machinery: Cooperative one-step mechanism. International Journal of Quantum Chemistry, 1999, 73, 161-174.	1.0	21
261	Theoretical study of reactions between AlH(?) and HF molecule. International Journal of Quantum Chemistry, 1999, 73, 417-424.	1.0	2
262	A spin-coupled investigation of the electrophilic addition of hydrochloric acid to ethylene. International Journal of Quantum Chemistry, 1999, 74, 231-239.	1.0	5
263	Thermolysis mechanism of N-acetylpropanamide. International Journal of Quantum Chemistry, 1999, 74, 337-342.	1.0	1
264	Theoretical studies of heterogeneous reaction mechanisms relevant for stratospheric ozone depletion. International Journal of Quantum Chemistry, 1999, 75, 683-692.	1.0	20
265	Theoretical study of a vanadate peptide complex. Journal of Computational Chemistry, 1999, 20, 1254-1261.	1.5	19
266	Ab initio study of the reaction of CHO <sup>+</sup> with H <sub>2</sub> O and NH <sub>3</sub> . Journal of Computational Chemistry, 1999, 20, 1432-1443.	1.5	2
267	Hydrogen as a migrating group in some pinacol rearrangements: a DFT study. Journal of Physical Organic Chemistry, 1999, 12, 741-746.	0.9	12
268	Ground State and Transition State Contributions to the Rates of Intramolecular and Enzymatic Reactions. Accounts of Chemical Research, 1999, 32, 127-136.	7.6	274
269	Cycloaddition Reactions of 1,3-Cyclohexadiene on the Silicon(001) Surface. Journal of the American Chemical Society, 1999, 121, 11311-11317.	6.6	118
270	Theoretical Studies on the Reaction Path Dynamics and Variational Transition-State Theory Rate Constants of the Hydrogen-Abstraction Reactions of the NH(X) Radical with Methane and Ethane. Journal of Physical Chemistry A, 1999, 103, 4910-4917.	1.1	13
271	Mechanism of the Gas-Phase HO + H <sub>2</sub> O → H <sub>2</sub> O + OH Reaction and Several Associated Isotope Exchange Reactions: A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053.	1.1	34

#	ARTICLE	IF	CITATIONS
272	A theoretical ab initio and Monte Carlo simulation study of the pyridine+CCl <sub>2</sub> reaction kinetics in the gas phase and in carbon tetrachloride solution using canonical flexible transition state theory. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1031-1036.	1.3	7
273	Flowing afterglow study of the gas phase nucleophilic reactions of some formyl, acetyl and cyclic esters. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 2397-2407.	0.9	16
274	A reaction class approach for modeling gas phase reaction rates. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1061-1065.	1.3	79
275	Theoretical investigations of reactions between AlH(1 $\hat{1}$ ) and X $\hat{1}$ / <sub>2</sub> H (X=Cl, OH). <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 657-664.	1.3	5
276	Ab initio quantum mechanical calculations of p K <sub>a</sub> s of isolated molecules and molecules undergoing chemical reactions: p K <sub>a</sub> of acetic acid during $\hat{1}$ -proton abstraction. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 5643-5647.	1.3	25
277	Pathways for HCl formation in HO+ClO reaction. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 5429-5432.	1.3	6
278	Solvation of the Menshutkin Reaction: A Rigorous Test of the Effective Fragment Method. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1265-1273.	1.1	78
279	Facile formation of azines from reactions of singlet methylene and dimethylcarbene with precursor diazirines: theoretical explorations. <i>Canadian Journal of Chemistry</i> , 1999, 77, 540-549.	0.6	14
280	2-Alkoxy carbonylpyridinium N-Aminides: A 1,3-Dipoles or 1,4-Nucleophile Electrophile Synthons? Experimental and Theoretical Evidence for the Mechanism of Pyrido[1,2-b]pyridazinium Inner Salt Formation. <i>Journal of Organic Chemistry</i> , 1999, 64, 9001-9010.	1.7	17
282	A New Mechanism for the Reaction of Carbenes with OH Groups. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3904-3909.	1.1	40
283	Intrinsic reaction coordinate analysis of the conversion of methane to methanol by an iron oxo species: A study of crossing seams of potential energy surfaces. <i>Journal of Chemical Physics</i> , 1999, 111, 538-545.	1.2	191
284	Mechanism of Chorismate Mutase: Contribution of Conformational Restriction to Catalysis in the Claisen Rearrangement. <i>Journal of the American Chemical Society</i> , 1999, 121, 11831-11846.	6.6	77
285	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3935-3943.	1.1	33
286	Theoretical Study of Addition Reactions of SiX <sub>2</sub> to Acetylene (X = H, CH <sub>3</sub> , t-Bu, Cl, F). <i>Organometallics</i> , 1999, 18, 4881-4883.	1.1	10
287	The Ionization Energy of CF <sub>3</sub> : When Does Entropy Matter in Gas-Phase Reactions?. <i>Journal of the American Chemical Society</i> , 1999, 121, 7689-7695.	6.6	30
288	Donor Acceptor-Assisted Diels Alder Reaction of Anthracene and Tetracyanoethylene. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8279-8287.	1.1	39
289	Structures, Energetics, and Transition States of the Silicon Phosphorus Compounds Si <sub>2</sub> PH <sub>n</sub> (n = 7, 5). <i>Journal of Physical Chemistry A</i> , 1999, 103, 11394-11405.	1.1	4
290	Dual-Level Direct Dynamics of the Hydroxyl Radical Reaction with Ethane and Haloethanes: Toward a General Reaction Parameter Method. <i>Journal of Physical Chemistry A</i> , 1999, 103, 11394-11405.	1.1	33

#	ARTICLE	IF	CITATIONS
291	Excited-State Energy and Geometry Changes during the [1,7]H-Shift Reaction of Cycloheptatriene. <i>Organic Letters</i> , 1999, 1, 1889-1891.	2.4	9
292	Mechanism of Formamide Hydroxylation Catalyzed by a Molybdenum <sup>VI</sup> Dithiolene Complex: A Model for Xanthine Oxidase Reactivity. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5406-5412.	1.2	58
293	A QM/MM Monte Carlo Simulation Study of Solvent Effects on the Decarboxylation Reaction of N-Carboxy-2-imidazolidinone Anion in Aqueous Solution. <i>Journal of Organic Chemistry</i> , 1999, 64, 1151-1159.	1.7	7
294	Ab Initio Study of the Reaction Mechanism of CH <sub>3</sub> <sup>+</sup> and CH <sub>3</sub> <sup>-</sup> with CH <sub>2</sub> CNa(OH). <i>Journal of Physical Chemistry A</i> , 1999, 103, 3472-3480.	1.1	0
295	Theoretical Study of the Ion <sup>+</sup> Molecule Reaction of the Vinyl Cation with Ethane. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5996-6002.	1.1	10
296	A Quantum-Chemical Study of the C <sub>2</sub> H <sub>3</sub> F <sub>2</sub> <sup>+</sup> and C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> <sup>+</sup> Isomers and Their Interconversion. CBS-QB3 Proton Affinities of Difluoroethenes and Dichloroethenes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7872-7882.	1.1	3
297	The Mechanism of Methoxy Radical Oxidation by O <sub>2</sub> in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent O <sup>+</sup> ...O Bonding Interaction. <i>Journal of the American Chemical Society</i> , 1999, 121, 1337-1347.	6.6	77
298	Ab Initio Study of the Reactions between a Series of Substituted Singlet Nitrenium Ions and Water. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6191-6199.	1.1	19
299	Direct ab Initio Dynamics Studies of the Hydrogen Abstraction Reactions of Hydrogen Atom with Fluoromethanes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2152-2159.	1.1	49
300	Theoretical Study on the Mechanism of Formation of Cyanate Resins. <i>Journal of Organic Chemistry</i> , 1999, 64, 4742-4748.	1.7	3
301	Mechanism of Hydroxyl Radical Addition to Imidazole and Subsequent Water Elimination. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5598-5607.	1.2	33
302	Insertion of Difluorovinylidene into Hydrogen and Methane. <i>Journal of the American Chemical Society</i> , 1999, 121, 8891-8897.	6.6	52
303	NH <sub>3</sub> -Assisted Ammonolysis of $\beta$ -Lactams: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1999, 64, 3281-3289.	1.7	16
304	Monte Carlo Investigations of Solvent Effects on the Decarboxylation Reaction of Neutral N-Carboxy-2-imidazolidinone in Aqueous Solution. <i>Journal of Organic Chemistry</i> , 1999, 64, 4492-4501.	1.7	6
305	Competitive Mechanisms and Origins of Stereocontrol in the [2 + 2] Thermal Cycloaddition between Imines and Ketiminium Cations. A Complementary Entry to 2-Azetidinones ( $\beta$ -Lactams) and Related Compounds. <i>Journal of Organic Chemistry</i> , 1999, 64, 1831-1842.	1.7	33
306	Intersystem Crossings in Model Energetic Materials. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9349-9354.	1.1	43
307	Equilibrium Structure and Stability of AlC <sub>n</sub> (n = 2, 3) and AlC <sub>n</sub> N (n = 1, 2) Species. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9275-9279.	1.1	25
308	Mechanism of Alkaline Hydrolysis of Cyclic and Acyclic Sulfates: An ab Initio Study with Solvation Correction. <i>Journal of the American Chemical Society</i> , 1999, 121, 5548-5558.	6.6	19



#	ARTICLE	IF	CITATIONS
309	Ab Initio Molecular Orbital Study of the N(2D) + H2O Reaction. Journal of Physical Chemistry A, 1999, 103, 436-442.	1.1	19
310	Experimental and Computational Study of Hydration Reactions of Aluminum Oxide Anion Clusters. Journal of Physical Chemistry A, 2000, 104, 7079-7090.	1.1	44
312	A theoretical study of the reaction of HCO+ with C2H2. Journal of Computational Chemistry, 2000, 21, 35-42.	1.5	4
313	Improving description of hydrogen bonds at the semiempirical level: water-water interactions as test case. Journal of Computational Chemistry, 2000, 21, 572-581.	1.5	70
314	Carbonyl insertion reaction into the Pt-C bond in heterobimetallic Pt(SnCl3)(PH3)2(CO)(CH3) compound: Theoretical study. Journal of Computational Chemistry, 2000, 21, 668-674.	1.5	17
315	Quantum mechanical study of regioselectivity of radical additions to substituted olefins. Journal of Computational Chemistry, 2000, 21, 675-691.	1.5	10
316	Insertion reaction of propene into Rh-H bond in HRh(CO)(PH3)2(C3H6) compound: A density functional study. International Journal of Quantum Chemistry, 2000, 78, 42-51.	1.0	32
317	The protonated betaine/ammonia complex: how stable is the gas-phase zwitterion structure?. Chemical Physics Letters, 2000, 320, 513-517.	1.2	17
318	Theoretical study on the reversible storage of H2 by BeO. Chemical Physics Letters, 2000, 321, 95-100.	1.2	13
319	Theoretical study on reforming of CO2 catalyzed with Be. Chemical Physics Letters, 2000, 325, 639-644.	1.2	11
320	The role of bridged structures in the mechanism of the reaction between chlorine atom and ethylene. Chemical Physics Letters, 2000, 325, 693-697.	1.2	9
321	Chiral diamines. 1. Relative energies of (â <sup>+</sup> )-sparteine conformers, interconversion barriers, and allyllithium complexes. Journal of Molecular Structure, 2000, 556, 239-244.	1.8	28
322	An ab initio study on the structure and reactivity of 1,4-disilabenzene. Journal of Organometallic Chemistry, 2000, 611, 280-287.	0.8	9
323	Spin-forbidden F+ transfer between 2NF+ and CO: a computational study on the detailed mechanistic aspects. International Journal of Mass Spectrometry, 2000, 201, 151-160.	0.7	3
324	A density functional theory study of methyl shifts and methylcyclopropanol ion formation in C4H8O+ ions. International Journal of Mass Spectrometry, 2000, 199, 41-57.	0.7	5
325	The fragmentation pathways of protonated glycine: A computational study. Journal of the American Society for Mass Spectrometry, 2000, 11, 687-696.	1.2	62
326	Ab initio study of the reaction mechanism of singlet and triplet N2O and their intersystem crossing. Chemical Physics, 2000, 259, 89-97.	0.9	23
327	The attractive quartet potential energy surface for the CH3C(+)+CO reaction. Chemical Physics, 2000, 252, 17-23.	0.9	2

#	ARTICLE	IF	CITATIONS
328	Ab initio/Rice-Kramersperger-Kassel-Marcus approach to carbon nitride formation: CH <sub>3</sub> NH <sub>2</sub> decomposition. <i>Chemical Physics Letters</i> , 2000, 321, 101-105.	1.2	9
329	Ab initio method study on the isomerization of 3-amino-2-pyridone. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 321-325.	1.5	1
330	Stability of N <sub>8</sub> isomers and isomerization reaction of N <sub>8</sub> (C <sub>2v</sub> ) to N <sub>8</sub> (C <sub>s</sub> ). <i>Computational and Theoretical Chemistry</i> , 2000, 531, 135-141.	1.5	17
331	Ab initio molecular orbital study of the reaction. <i>Computational and Theoretical Chemistry</i> , 2000, 503, 231-240.	1.5	12
332	Ab initio molecular orbital study of potential energy surface for the H <sub>2</sub> NO(2B <sub>1</sub> ) + NO(2 $\Sigma$ ) + H <sub>2</sub> reaction. <i>Computational and Theoretical Chemistry</i> , 2000, 507, 119-126.	1.5	7
333	Unimolecular Decomposition of the 2-Oxepinoxy Radical: A Key Seven-Membered Ring Intermediate in the Thermal Oxidation of Benzene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8121-8130.	1.1	40
334	Origins of the Loss of Concertedness in Pericyclic Reactions: Theoretical Prediction and Direct Observation of Stepwise Mechanisms in [3 + 2] Thermal Cycloadditions. <i>Journal of the American Chemical Society</i> , 2000, 122, 6078-6092.	6.6	107
335	An ab initio quantum-chemical study of proton addition to F-, CH <sub>3</sub> -, and CF <sub>3</sub> -substituted ethylene derivatives. <i>Russian Chemical Bulletin</i> , 2000, 49, 1327-1331.	0.4	0
336	Toward elimination of discrepancies between theory and experiment: The rate constant of the atmospheric conversion of SO <sub>3</sub> to H <sub>2</sub> SO <sub>4</sub> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000, 97, 8874-8878.	3.3	91
337	A reaction-path Hamiltonian described with quasirectilinear vibrational coordinates constructed from a nonlinear combination of curvilinear internal coordinates: Application to examination of the reaction CH <sub>4</sub> + F + CH <sub>3</sub> + HF. <i>Journal of Chemical Physics</i> , 2000, 113, 3136-3140.	1.2	15
338	A combined reaction class approach with integrated molecular orbital+molecular orbital (IMOMO) methodology: A practical tool for kinetic modeling. <i>Journal of Chemical Physics</i> , 2000, 112, 24-30.	1.2	24
339	Direct ab initio dynamics studies of N + H <sub>2</sub> + NH + H reaction. <i>Journal of Chemical Physics</i> , 2000, 113, 6149-6153.	1.2	31
340	A General Reaction Path Dual-Level Direct Dynamics Calculation of the Reaction of Hydroxyl Radical with Dimethyl Sulfide. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8779-8786.	1.1	18
341	Heats of Formation for Cyclic C <sub>4</sub> F <sub>n</sub> , n = 4-8, and Their Cations. <i>Journal of Physical Chemistry A</i> , 2000, 104, 9026-9028.	1.1	10
342	Theoretical Studies on Reactions of Transition-Metal Complexes. <i>Chemical Reviews</i> , 2000, 100, 353-406.	23.0	811
343	Ultrafast Radiationless Deactivation of Organic Dyes: Evidence for a Two-State Two-Mode Pathway in Polymethine Cyanines. <i>Journal of the American Chemical Society</i> , 2000, 122, 2911-2924.	6.6	185
344	Hydrolysis of sulfur trioxide to form sulfuric acid in small water clusters. <i>Journal of Chemical Physics</i> , 2000, 112, 8830-8838.	1.2	114
345	Rearrangement Pathways of Arylperoxy Radicals. 2. Five-Membered Heterocycles. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6324-6331.	1.1	13

#	ARTICLE	IF	CITATIONS
346	Is SH <sub>4</sub> , the simplest 10-S-4 sulfurane, observable?. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2239-2244.	1.3	7
347	Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2000, 122, 324-330.	6.6	65
348	A theoretical study on proton transfer in the mutarotation of sugars. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2707-2713.	1.3	22
349	Ab initio and RRKM studies of the unimolecular reactions of CH <sub>2</sub> XCHFO (X=H, F) radicals. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 61-66.	1.3	11
350	Mechanism of the OH+CH <sub>2</sub> CO reaction. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2329-2334.	1.3	23
351	A quantum-chemical study of the geometries and electronic structures of ArO and [Ar,O,H] <sup>+</sup> : proton affinities of singlet and triplet ArO. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2271-2274.	1.3	12
352	Theoretical Study of the Triplet N <sub>4</sub> Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11999-12005.	1.1	45
353	Selective C <sup>α</sup> -C vs C <sup>β</sup> -H Bond Activation by Rhodium(I) PCP Pincer Complexes. A Computational Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 7095-7104.	6.6	85
354	An ab Initio Study of the Kinetics of the Reactions of Halomethanes with the Hydroxyl Radical. 1. CH <sub>2</sub> Br <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2000, 104, 2931-2938.	1.1	25
355	Theoretical Study of the Reversible Storage of H <sub>2</sub> by BeS. <i>Journal of the American Chemical Society</i> , 2000, 122, 11406-11410.	6.6	12
356	Mechanism of Addition of Allylmetal to Vinylmetal. Dichotomy between Metallo <sup>α</sup> -Ene Reaction and Metallo <sup>β</sup> -Claisen Rearrangement. <i>Journal of the American Chemical Society</i> , 2000, 122, 11791-11798.	6.6	41
357	Theoretical Study of the Gas-Phase Reaction of Diborane(3) Anion B <sub>2</sub> H <sub>3</sub> <sup>-</sup> with CO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2000, 104, 11952-11960.	1.1	5
358	Computational Study of the Unimolecular Decomposition Pathways of Phenylperoxy Radical. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3004-3011.	1.1	62
359	An ab Initio Study of the Photochemical Decomposition of 3,3-Dimethyldiazirine. <i>Journal of Organic Chemistry</i> , 2000, 65, 7847-7857.	1.7	28
360	Production and IR Absorption of Cyclic CS <sub>2</sub> in Solid Ar. <i>Journal of the American Chemical Society</i> , 2000, 122, 661-667.	6.6	31
361	Theoretical Studies of Fundamental Pathways for Alkaline Hydrolysis of Carboxylic Acid Esters in Gas Phase. <i>Journal of the American Chemical Society</i> , 2000, 122, 1522-1530.	6.6	58
362	Ab Initio Mechanism and Multichannel RRKM <sup>α</sup> -TST Rate Constant for the Reaction of Cl(2P) with CH <sub>2</sub> CO (Ketene). <i>Journal of Physical Chemistry A</i> , 2000, 104, 320-328.	1.1	46
363	Ab initio molecular dynamics studies of the photodissociation of formaldehyde, H <sub>2</sub> CO <sup>α</sup> →H <sub>2</sub> +CO: Direct classical trajectory calculations by MP2 and density functional theory. <i>Journal of Chemical Physics</i> , 2000, 113, 10062-10067.	1.2	127

#	ARTICLE	IF	CITATIONS
364	Ab Initio Calculations on the 5-exo versus 6-endo Cyclization of 1,3-Hexadiene-5-yn-1-yl Radical: Formation of the First Aromatic Ring in Hydrocarbon Combustion. <i>Journal of the American Chemical Society</i> , 2000, 122, 11416-11422.	6.6	20
365	A Density Functional Study of Ethene Hydrogenation Reactions Catalyzed by Titanocene Complexes. <i>Journal of the American Chemical Society</i> , 2000, 122, 6476-6487.	6.6	6
366	Mechanism of Peroxynitrite Oxidation of Aliphatic CH Bonds in Saturated and Unsaturated Hydrocarbons. A Theoretical Model for the CH Oxidation of Lipids. <i>Journal of the American Chemical Society</i> , 2000, 122, 1191-1199.	6.6	26
367	Reaction Pathways and Energy Barriers for Alkaline Hydrolysis of Carboxylic Acid Esters in Water Studied by a Hybrid Supermolecule-Polarizable Continuum Approach. <i>Journal of the American Chemical Society</i> , 2000, 122, 2621-2627.	6.6	107
368	Mechanism and Quantum Mechanical Tunneling Effects on Inner Hydrogen Atom Transfer in Free Base Porphyrin: A Direct ab Initio Dynamics Study. <i>Journal of the American Chemical Society</i> , 2000, 122, 897-906.	6.6	60
369	Chemically and Thermally Activated Decomposition of Secondary Butyl Radical. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10747-10765.	1.1	57
370	Hydride Transfer Reduction of Carbonyls by a Rhodium(I) Complex: A Theoretical Study. 1. The Two-Step Mechanism. <i>Organometallics</i> , 2000, 19, 1589-1598.	1.1	30
371	Reactivity and Secondary Kinetic Isotope Effects in the SN2 Reaction Mechanism: A Dioxxygen Radical Anion and Related Nucleophiles. <i>Journal of the American Chemical Society</i> , 2000, 122, 1740-1748.	6.6	44
372	Competition between SN2 and Single Electron Transfer Reactions as a Function of Steric Hindrance Illustrated by the Model System AlkylCl + NO-. <i>Journal of the American Chemical Society</i> , 2000, 122, 2329-2338.	6.6	21
373	Cheletropic Decomposition of Cyclic Nitrosoamines Revisited: The Nature of the Transition States and a Critical Role of the Ring Strain. <i>Journal of Organic Chemistry</i> , 2000, 65, 3612-3619.	1.7	4
374	Adsorption of Multiple H2 Molecules on Pd3 and Pd4 Clusters. A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11606-11614.	1.1	48
375	Theoretical Study of the Mechanisms of Palladation of Methylene cyclopropane and [3 + 2] Cycloadditions. <i>Inorganic Chemistry</i> , 2000, 39, 1113-1119.	1.9	40
376	An Ab Initio Study of Potential Energy Surfaces for N8 Isomers. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5647-5650.	1.1	189
377	A Three-Center Orbital Interaction in the Diels-Alder Reactions Catalyzed by Lewis Acids. <i>Journal of Organic Chemistry</i> , 2000, 65, 1830-1841.	1.7	40
378	New Insights on the Origins of the Stereocontrol of the Staudinger Reaction: A [2 + 2] Cycloaddition between Ketenes and N-Silylimines. <i>Journal of Organic Chemistry</i> , 2000, 65, 8458-8464.	1.7	37
379	Activation of Small Alkanes in Ga-Exchanged Zeolites: A Quantum Chemical Study of Ethane Dehydrogenation. <i>Journal of Physical Chemistry A</i> , 2000, 104, 2468-2475.	1.1	82
380	Density Functional Study of the Reppe Carbonylation of Acetylene. <i>Organometallics</i> , 2000, 19, 4104-4116.	1.1	23
381	A Theoretical Study of the Molecular Mechanism of the Reaction between N,N-Dimethylmethyleammonium Cation and Cyclopentadiene. <i>Journal of Organic Chemistry</i> , 2001, 66, 3211-3214.	1.7	51

#	ARTICLE	IF	CITATIONS
382	Nature of the 2-Bicyclo[3.2.1]octanyl and 2-Bicyclo[3.2.2]nonanyl Cations. <i>Journal of Organic Chemistry</i> , 2001, 66, 376-380.	1.7	9
383	Energetics of Aluminum Combustion. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7473-7480.	1.1	56
384	Corannulene as a Lewis Base: An Computational Modeling of Protonation and Lithium Cation Binding. <i>Journal of the American Chemical Society</i> , 2001, 123, 6687-6695.	6.6	67
385	A Combined Experimental and Theoretical Study of the Homogeneous, Unimolecular Decomposition Kinetics of 3-Chloropivalic Acid in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1869-1875.	1.1	4
386	Adsorption of Water on the Si(100) Surface: An Ab Initio and QM/MM Cluster Study. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4039-4044.	1.2	39
387	Effective Monkey Saddle Points and Berry and Lever Mechanisms in the Topomerization of SF <sub>4</sub> and Related Tetracoordinated AX <sub>4</sub> Species. <i>Inorganic Chemistry</i> , 2001, 40, 1756-1769.	1.9	24
388	Revisiting Markovnikov Addition to Alkenes via Molecular Electrostatic Potential. <i>Journal of Organic Chemistry</i> , 2001, 66, 6883-6890.	1.7	66
389	Branching Ratio and Pressure Dependent Rate Constants of Multichannel Unimolecular Decomposition of Gas-Phase $\dot{I} \pm HMX$ : An Ab Initio Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2427-2434.	1.1	55
390	On the Reaction Path Hamiltonian for Polyatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5022-5029.	1.1	18
391	Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3887-3893.	1.1	70
392	Hydrogen bond cooperativity and electron delocalization in hydrogen fluoride clusters. <i>Journal of Chemical Physics</i> , 2001, 114, 5552-5561.	1.2	90
393	Glyoxal photodissociation. An ab initio direct classical trajectory study of C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> + H <sub>2</sub> + 2 h $\nu$ $\rightarrow$ CO. <i>Journal of Chemical Physics</i> , 2001, 114, 8897-8904.	1.2	34
394	A Mechanistic Study of the Reactions of H, O (3P), and OH with Monocyclic Aromatic Hydrocarbons by Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 140-152.	1.1	66
395	A Study of the Mechanism of the Reaction between Ozone and the Chlorine Atom Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4065-4070.	1.1	18
396	Interactions and Reactions of Sulfur Trioxide, Water, and Ammonia: An ab Initio and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4344-4350.	1.1	35
397	Theoretical studies of reaction pathways and energy barriers for alkaline hydrolysis of phosphotriesterase substrates paraoxon and related toxic phosphofluoridate nerve agents. <i>Perkin Transactions II RSC</i> , 2001, , 2355-2363.	1.1	6
398	Ab initio study of oxygen atom transfer from hydrogen peroxide to trimethylamine. <i>Chemical Communications</i> , 2001, , 1748-1749.	2.2	4
399	Theoretical studies of nonenzymatic reaction pathways for the three reaction stages of the carboxylation of ribulose-1,5-bisphosphate. <i>Perkin Transactions II RSC</i> , 2001, , 23-29.	1.1	21

#	ARTICLE	IF	CITATIONS
400	RAIL: Reaction-path and variational rate constants using the integrated molecular orbital with harmonic cap method. <i>Journal of Chemical Physics</i> , 2001, 115, 3021-3030.	1.2	6
401	Quantum Mechanical Study of the Competitive Hydration between Protonated Quinazoline and Li+, Na+, and Ca2+ Ions. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9717-9724.	1.1	8
402	Hydrolysis of 1,8- and 2,3-naphthalic anhydrides and the mechanism of cyclization of 1,8-naphthalic acid in aqueous solutions. The IUPAC name for naphthalic acid is naphthalenedicarboxylic acid. Electronic supplementary information (ESI) available: tables containing the values of the rate constants. See <a href="http://www.rsc.org/suppdata/p2/b1/b104148g/">http://www.rsc.org/suppdata/p2/b1/b104148g/</a> . <i>Perkin Transactions II RSC</i> , 2001, , 2342-2350.	1.1	22
403	Mechanistic Aspects of the Abstraction of an Allylic Hydrogen in the Chlorine Atom Reaction with 2-Methyl-1,3-Butadiene (Isoprene). <i>Journal of the American Chemical Society</i> , 2001, 123, 10348-10353.	6.6	24
404	A Theoretical Study of the Gas-Phase Pyrolysis of 2-Azidoacetic Acid. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3140-3147.	1.1	18
405	Hindered Inversion of Chiral Ion-Dipole Pairs. <i>Journal of the American Chemical Society</i> , 2001, 123, 2251-2254.	6.6	12
406	Positional Isomerization of Dialkyl-naphthalenes: A Comprehensive Interpretation of the Selective Formation of 2,6-DIPN over HM Zeolite. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6513-6518.	1.1	27
407	The Reaction of N(4S) with CH2F: A Comparative ab Initio and DFT Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9917-9925.	1.1	11
408	CS2 Fixation by Carbonic Anhydrase Model Systems: A New Substrate in the Catalytic Cycle. <i>Inorganic Chemistry</i> , 2001, 40, 1006-1013.	1.9	23
409	Direct Observation of a Hydrogen Atom Adduct to C-5 in Uracil. A Neutralization-Reionization Mass Spectrometric and ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8339-8351.	1.1	26
410	Theoretical Study on the Potential Energy Surface of the 1CH2+N2O Reaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5885-5895.	1.1	7
411	A Theoretical Study of the 2NCO + 2OH Reaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 229-237.	1.1	15
412	A Gaussian-2 ab Initio Study of the [C2H5S]- Potential Energy Surface: I. Structures and Energetics of [C2H5S]- Anions and Fragmentation Pathways of the Thioethoxide Anion. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7651-7664.	1.1	4
413	Formation of (SiN2SiC) Five-Membered Rings by Intramolecular Insertion into the Si-N Bond: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3875-3880.	1.1	5
414	Theoretical Studies on the Potential Energy Surfaces of N8 Clusters. <i>Journal of Physical Chemistry A</i> , 2001, 105, 1979-1982.	1.1	18
415	Ab Initio Molecular Orbital Study of the Reaction of GeH2 with H2O and Decomposition Reactions of H3GeOH. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4988-4991.	1.1	5
416	Origin of the Enantioselectivity in the Hydrogen Transfer Reduction of Carbonyls by a Rhodium(I) Complex: A Theoretical Study. <i>Organometallics</i> , 2001, 20, 2207-2214.	1.1	25
417	Silyl Group Insertion into the N-N Bond: Experimental and Quantum Chemical Results. <i>Journal of the American Chemical Society</i> , 2001, 123, 378-382.	6.6	15

#	ARTICLE	IF	CITATIONS
418	Kinetics of Reactions of H Atoms With Methane and Chlorinated Methanes. Journal of Physical Chemistry A, 2001, 105, 3107-3122.	1.1	72
419	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
420	Mechanism of Olefin Cyclopropanation by Diazomethane Catalyzed by Palladium Dicarboxylates. A Density Functional Study. Journal of the American Chemical Society, 2001, 123, 6157-6163.	6.6	53
421	Reaction of Carbon Atoms, C (2p2,3P), with Hydrogen Sulfide, H <sub>2</sub> S (X1A1): Overall Rate Constant and Product Channels. Journal of Physical Chemistry A, 2001, 105, 9893-9900.	1.1	24
422	Theoretical Studies of Competing Reaction Pathways and Energy Barriers for Alkaline Ester Hydrolysis of Cocaine. Journal of Physical Chemistry A, 2001, 105, 1296-1301.	1.1	45
423	Kinetics of Reactions of H Atoms With Ethane and Chlorinated Ethanes. Journal of Physical Chemistry A, 2001, 105, 6900-6909.	1.1	40
424	Modeling the 1,3-Dipolar Cycloaddition of Nitrones to Vinylboranes in Competition with Boration, Cyclization, and Oxidation Reactions. Journal of Organic Chemistry, 2001, 66, 2449-2458.	1.7	25
425	Charge-Separation Process of the C <sub>2</sub> H <sub>4</sub> + Cl <sub>2</sub> Reaction in Water: ab Initio Molecular Orbital Study Using a Cluster Model. Journal of Physical Chemistry A, 2001, 105, 11080-11087.	1.1	3
426	Methane to Methanethiol Conversion by FeS+. A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 2005-2014.	1.1	26
427	First-Principle Molecular Dynamic Simulations along the Intrinsic Reaction Paths. Journal of Physical Chemistry A, 2001, 105, 4333-4343.	1.1	45
428	Use of Quantum Methods with Transition State Theory: Application to H-Atom Metathesis Reactions. Journal of Physical Chemistry A, 2001, 105, 1669-1675.	1.1	30
429	DFT/ECP Study of C-H Activation by (PCP)Ir and (PCP)Ir(H) <sub>2</sub> (PCP = 1,3-C <sub>6</sub> H <sub>3</sub> (CH <sub>2</sub> PR <sub>2</sub> ) <sub>2</sub> ). Enthalpies and Free Energies of Associative and Dissociative Pathways. Journal of Chemical Information and Computer Sciences, 2001, 41, 56-63.	2.8	52
430	A theoretical study on reactivity of singlet phosphinidene by its reacting with polar water molecule. Chemical Physics, 2001, 264, 1-8.	0.9	9
431	A study on the effect of Lewis acid catalysis on the molecular mechanism of the cycloaddition between (E)-methyl cinnamate and cyclopentadiene. Tetrahedron, 2001, 57, 6877-6883.	1.0	9
433	Merging of 4+2 and 2+4 cycloaddition paths in the regiospecific dimerization of methacrolein. A case of concerted crypto-diradical cycloaddition. Tetrahedron Letters, 2001, 42, 5077-5080.	0.7	30
434	Catalyzed keto-enol tautomerism of ionized acetone: a Fourier transform ion cyclotron resonance mass spectrometry study of proton transport isomerization. International Journal of Mass Spectrometry, 2001, 210-211, 429-446.	0.7	35
435	Using theozymes for designing transition-state analogs for the intramolecular aldol reaction of $\beta$ -diketones. International Journal of Quantum Chemistry, 2001, 83, 338-347.	1.0	6
436	Theoretical study of reactions between MH (M=B, Al) and the H <sub>2</sub> S molecule. International Journal of Quantum Chemistry, 2001, 85, 127-135.	1.0	8

#	ARTICLE	IF	CITATIONS
437	Nitrenes as intermediates in the thermal decomposition of aliphatic azides. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 241-248.	1.0	27
438	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. <i>Journal of Computational Chemistry</i> , 2001, 22, 387-406.	1.5	52
439	Chemistry with ADF. <i>Journal of Computational Chemistry</i> , 2001, 22, 931-967.	1.5	8,854
440	Theoretical studies on a possible synthesis reaction pathway on N <sub>8</sub> (CS) clusters. <i>Journal of Computational Chemistry</i> , 2001, 22, 1334-1339.	1.5	17
441	Gas-phase detection of the HBCC (X1?) molecule: a combined crossed beam and computational study of the B(2P)+C <sub>2</sub> H <sub>2</sub> (1?g+) reaction. <i>Journal of Computational Chemistry</i> , 2001, 22, 1359-1365.	1.5	24
442	Monomer~Dimer Equilibria of Oxo/Imido Complexes of Heptavalent Rhenium: Theoretical and Spectroscopic Investigations. <i>European Journal of Inorganic Chemistry</i> , 2001, 2001, 981-991.	1.0	11
443	Theoretical Study of Amine-Assisted Aminolysis of Penicillins ~ The Kinetic Role of the Carboxylate Group. <i>European Journal of Organic Chemistry</i> , 2001, 2001, 793-801.	1.2	4
444	An Experimental and Theoretical Study of the Basicity of Tetra-tert-butyltetrahedrane. <i>Chemistry - A European Journal</i> , 2001, 7, 342-346.	1.7	27
445	Computational Study of a New Heck Reaction Mechanism Catalyzed by Palladium(II/IV) Species. <i>Chemistry - A European Journal</i> , 2001, 7, 1703-1711.	1.7	160
446	Solvated CH <sub>5</sub> <sup>+</sup> in Liquid Superacid. <i>Chemistry - A European Journal</i> , 2001, 7, 1936-1943.	1.7	31
447	Ab Initio Calculations on the Mechanism of the Oxidation of the Hydroxymethyl Radical by Molecular Oxygen in the Gas Phase: A Significant Reaction for Environmental Science. <i>Chemistry - A European Journal</i> , 2001, 7, 3377-3386.	1.7	35
448	Thermal Rearrangements of 2-Vinylcyclopropylidene to Cyclopentadiene and Vinylallene: A Theoretical Investigation. <i>Chemistry - A European Journal</i> , 2001, 7, 3951-3960.	1.7	8
449	Modeling quantitative structure~property relationships in calculated reaction pathways using a new 3D quantum topological representation. <i>Analytica Chimica Acta</i> , 2001, 446, 3-13.	2.6	15
450	Theoretical study on the reaction mechanism of BH <sub>2</sub> <sup>+</sup> and ethylene in gas-phase. <i>Chemical Physics Letters</i> , 2001, 339, 140-146.	1.2	2
451	A density-functional study of the reaction of neutral scandium with water. <i>Chemical Physics Letters</i> , 2001, 342, 169-176.	1.2	9
452	Theoretical study of the reaction of beryllium oxide with methane. <i>Chemical Physics Letters</i> , 2001, 348, 303-310.	1.2	25
453	Theoretical study on gas-phase proton transfer reactions between ~proton-donor and ~acceptor systems. <i>Chemical Physics Letters</i> , 2001, 348, 95-101.	1.2	5
454	3 Theoretical description of reaction mechanisms: reaction pathways and electronic structure rearrangements. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2001, 97, 61-90.	4.4	2



#	ARTICLE	IF	CITATIONS
455	An ab initio study of the enolboration of 3-pentanone mediated by boron monochlorides L2BCl. <i>Tetrahedron</i> , 2001, 57, 6239-6247.	1.0	8
456	An ab initio study of the reaction of CH <sub>2</sub> F <sup>+</sup> with acetylene. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 193-198.	1.5	1
457	A density functional theory investigation of the polytopal rearrangement of square-based pyramidal clusters: C <sub>5</sub> H <sub>5</sub> <sup>+</sup> , P <sub>5</sub> <sup>+</sup> and Sb <sub>5</sub> <sup>+</sup> . <i>Computational and Theoretical Chemistry</i> , 2001, 571, 1-6.	1.5	7
458	On the isomerization of $\hat{I}^2$ -pinene: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2001, 544, 213-220.	1.5	16
459	Mechanism of trans $\hat{a}^{\prime\prime}$ cis isomerization reaction in 3-substituted thietane-1-oxide. <i>Computational and Theoretical Chemistry</i> , 2001, 572, 235-242.	1.5	5
460	The Elusive 7-Silanorbornadien-7-ylum: $\hat{A}$ Synthesis and Characterization of Nitrilium and Oxonium Ions Deriving from 2,3-Benzo-7-silanorbornadien-7-ylum. <i>Organometallics</i> , 2001, 20, 4584-4592.	1.1	38
461	The reactions CH <sub>n</sub> D <sub>4-n</sub> <sup>+</sup> +OH <sup>+</sup> and CH <sub>4</sub> +OD <sup>+</sup> as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I. <i>Journal of Chemical Physics</i> , 2001, 114, 2154-2165.	1.2	44
462	Topological analysis of the electron localization function applied to the study of the [1,3] sigmatropic shift of fluorine in 3-fluoropropene. <i>Journal of Chemical Physics</i> , 2001, 114, 23.	1.2	23
463	Glyoxal photodissociation. II. An ab initio direct classical trajectory study of C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> <sup>+</sup> CO+H <sub>2</sub> CO. <i>Journal of Chemical Physics</i> , 2001, 115, 6907-6912.	1.2	19
464	The potential energy surface of excited states by time-dependent density functional theory: The reaction of sulfur atom and nitrogen dioxide. <i>Journal of Chemical Physics</i> , 2001, 115, 7495-7502.	1.2	11
465	Lifetime and decomposition pathways of a chemically bound helium compound. <i>Journal of Chemical Physics</i> , 2001, 115, 7341-7343.	1.2	41
466	A theoretical study of Si <sub>4</sub> H <sub>2</sub> cluster with ab initio and density functional theory methods. <i>Journal of Chemical Physics</i> , 2001, 114, 1278-1285.	1.2	9
467	Inversion vs Retention of Configuration in Gas-Phase Ammonium Ion/Alcohol Reactions. <i>Journal of Organic Chemistry</i> , 2002, 67, 1221-1226.	1.7	8
468	Controlled Alcohol $\rightleftharpoons$ Ketone Interconversion by Dihydrogen Transfer: $\hat{A}$ An ab Initio Study of the Methanol $\rightleftharpoons$ Formaldehyde Complex. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9512-9519.	1.1	11
469	Theoretical Study of Intramolecular Proton Transfer Reactions in Some Thiooxalic Acid Derivatives. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3891-3898.	1.1	18
470	The Bonding Nature of Some Simple Sigmatropic Transition States from the Topological Analysis of the Electron Localization Function. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11533-11539.	1.1	22
471	Chlorination Chemistry. 3. Ab Initio Study of the Reaction of Chlorine Atom with Allene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1739-1745.	1.1	9
472	A Computational Study on the Substituent Effect of Diallylamine Monomers in Their Cyclopolymerization Reactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8184-8190.	1.1	14

#	ARTICLE	IF	CITATIONS
473	Theoretical Studies on Cycloaddition Reactions between 1-Aza-2-azoniaallene Cation and Olefins. <i>Journal of Organic Chemistry</i> , 2002, 67, 7432-7438.	1.7	16
474	Ab Initio Study of the Thiolysis of Trimethyl Phosphate Ester in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9078-9084.	1.1	23
475	The Reaction of Cu(I) (1S and 3D) with N <sub>2</sub> O: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5679-5685.	1.1	28
476	An ab Initio Study of the Reaction of Propargyl Cation with Ammonia. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4616-4622.	1.1	6
477	Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5697-5702.	1.1	49
478	Computational Study of the Reactions of H Atoms with Chlorinated Alkanes. Isodesmic Reactions for Transition States. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11603-11615.	1.1	21
479	High Level ab Initio Study of Thermal 1,3-Sigmatropic Shift in CH <sub>2</sub> CHCH <sub>2</sub> X with X = BH <sub>2</sub> , NH <sub>2</sub> , and CH <sub>3</sub> . <i>Journal of Physical Chemistry A</i> , 2002, 106, 5709-5715.	1.1	13
480	Direct Dynamics of an Alkoxy Radical (CH <sub>3</sub> O, C <sub>2</sub> H <sub>5</sub> O, and i-C <sub>3</sub> H <sub>7</sub> O) Reaction with an Oxygen Molecule. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8124-8132.	1.1	26
481	A Theoretical Study on Decomposition Pathways of N <sub>7</sub> <sup>+</sup> and N <sub>7</sub> <sup>-</sup> Clusters. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5928-5931.	1.1	21
482	Formation of CO in the Reaction of Oxygen Atoms with CH <sub>3</sub> : Reaction over a Barrier but Not through a Saddle Point. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8741-8756.	1.1	16
483	Dynamical Density Functional Study of Acetylene to Vinylidene Isomerization in (Cp)(CO) <sub>2</sub> Mn(HC≡CH). <i>Organometallics</i> , 2002, 21, 2715-2723.	1.1	48
484	Sequential Transition States and the Valley-Ridge Inflection Point in the Formation of a Semibullvalene. <i>Organic Letters</i> , 2002, 4, 3279-3282.	2.4	29
485	Unimolecular Rearrangement Reactions in Silylpyrazolones: A Theoretical Approach. <i>Organometallics</i> , 2002, 21, 864-870.	1.1	3
486	Kinetics of Reactions of Cl Atoms with Methane and Chlorinated Methanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10532-10542.	1.1	68
487	A Theoretical Analysis of Enantiomerization in Aromatic Amides. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2623-2628.	1.1	11
488	Photodissociation of Acetaldehyde, CH <sub>3</sub> CHO → CH <sub>4</sub> + CO: Direct ab Initio Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11415-11421.	1.1	38
489	Computational Study of the Mechanism and Product Yields in the Reaction Systems C <sub>2</sub> H <sub>3</sub> <sup>+</sup> + CH <sub>3</sub> <sup>+</sup> , C <sub>3</sub> H <sub>6</sub> <sup>+</sup> , H + C <sub>3</sub> H <sub>5</sub> and C <sub>2</sub> H <sub>3</sub> <sup>+</sup> + CH <sub>3</sub> <sup>+</sup> → CH <sub>4</sub> + C <sub>2</sub> H <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2002, 106, 6952-6966.	1.1	12
490	Theoretical Study of the Reaction of Boron with Methanol and the Decomposition Paths of the Reaction Products. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3181-3184.	1.1	6

#	ARTICLE	IF	CITATIONS
491	Unimolecular Dissociation of Formyl Halides $\text{HXCO} \rightarrow \text{CO} + \text{HX}$ (X = F, Cl): An Ab Initio Direct Classical Trajectory Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11623-11629.	1.1	19
492	Role of Diagonal Silicon-Carbon Interaction in the [2 + 2] Cycloaddition of Silene and Acetylene. <i>Organometallics</i> , 2002, 21, 3271-3277.	1.1	24
493	Reaction Mechanism of Chlorosiloxane Ring Formation from $\text{SiCl}_4$ and $\text{O}_2$ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 6802-6809.	1.1	5
494	A Density Functional Theory Study Clarifying the Reactions of Conjugated Ketenes with Formaldimine. A Plethora of Pericyclic and Pseudopericyclic Pathways. <i>Journal of the American Chemical Society</i> , 2002, 124, 5231-5241.	6.6	91
495	Carbene Formation in Its Lower Singlet State from Photoexcited 3H-Diazirine or Diazomethane. A Combined CASPT2 and ab Initio Direct Dynamics Trajectory Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 1728-1735.	6.6	57
496	Ab Initio Study of the Reaction Mechanisms of NiO and NiS with $\text{H}_2$ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 520-528.	1.1	15
497	On the Mechanism of (PCP)Ir-Catalyzed Acceptorless Dehydrogenation of Alkanes: A Combined Computational and Experimental Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 11404-11416.	6.6	115
498	Kinetics and Mechanism of the $\text{OH} + \text{C}_6\text{H}_6$ Reaction: A Detailed Analysis with First-Principles Calculations. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11309-11326.	1.1	89
499	Thermal and Photochemical Rearrangement of Bicyclo[3.1.0]hex-3-en-2-one to the Ketonic Tautomer of Phenol. Computational Evidence for the Formation of a Diradical Rather than a Zwitterionic Intermediate. <i>Journal of the American Chemical Society</i> , 2002, 124, 15375-15384.	6.6	18
500	Theoretical Prediction on the Synthesis Reaction Pathway of $\text{N}_6$ ( $\text{C}_{2h}$ ). <i>Journal of Physical Chemistry A</i> , 2002, 106, 2748-2752.	1.1	29
501	Possible Reaction Pathway of $\text{HN}_3^+$ , $\text{N}_5^+$ and Stability of the Products' Isomers. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1872-1876.	1.1	19
502	Theoretical Study of the Potential Energy Surfaces of Nitrogen-Rich Ion $\text{N}_4\text{H}_2\text{F}^+$ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 10391-10395.	1.1	12
503	Theoretical Study of Potential Energy Surfaces for $\text{N}_{12}$ Clusters. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5367-5372.	1.1	59
504	The Rearrangement of Fluorenylideneallene Oxide. A DFT Study. <i>Organic Letters</i> , 2002, 4, 35-38.	2.4	4
505	Factors Governing Intrinsic Chemical Reactivity Differences between Clavulanic and Penicillanic Acids. <i>Journal of the American Chemical Society</i> , 2002, 124, 12042-12053.	6.6	8
506	Comparisons between Density Functional Theory and Conventional ab Initio Methods for 1,2-Elimination of HF from 1,1,1-Trifluoroethane: Test Case Study for HF Elimination from Fluoroalkanes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8471-8478.	1.1	25
507	Insights into the Metathesis Reaction Involving $\text{M} \equiv \text{M}$ , $\text{C} \equiv \text{C}$ , and $\text{M} \equiv \text{C}$ Triple Bonds from Computations Employing Density Functional Theory on Model Compounds $\text{M}_2(\text{OH})_6$ and $\text{M}_2(\text{SH})_6$ , Where M = Mo and W. <i>Journal of the American Chemical Society</i> , 2002, 124, 15351-15358.	6.6	21
508	An Experimental and Computational Study of the Thermal Oxidation of $\text{C}_6\text{H}_5\text{NO}$ by $\text{NO}_2$ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 2903-2907.	1.1	4

#	ARTICLE	IF	CITATIONS
509	Chlorination Chemistry 4. Ab Initio Study of the Addition, Metathesis, and Isomerization Channels Governing the Reaction of Chlorine Atom with Propargyl Chloride. Journal of Physical Chemistry A, 2002, 106, 6143-6153.	1.1	5
510	Theoretical Studies on Cycloaddition Reactions between 2-Azoniallene Cations and Olefins. Journal of Organic Chemistry, 2002, 67, 3841-3846.	1.7	9
511	Ab Initio Rate Constants for Unimolecular Reactions: Eliminations of HX from CH <sub>3</sub> CH <sub>2</sub> X and DX from CD <sub>3</sub> CD <sub>2</sub> X (X = Cl, Br). Journal of Physical Chemistry A, 2002, 106, 8191-8200.	1.1	16
512	Theoretical Study of Gas Phase Tautomerization Reactions for the Ground and First Excited Electronic States of Adenine. Journal of Physical Chemistry A, 2002, 106, 4251-4256.	1.1	55
513	Direct Evidence for Base-Mediated Decomposition of Alkyl Hydroperoxides (ROOH) in the Gas Phase. Journal of the American Chemical Society, 2002, 124, 3196-3197.	6.6	42
514	Following Reaction Pathways Using a Damped Classical Trajectory Algorithm. Journal of Physical Chemistry A, 2002, 106, 165-169.	1.1	63
515	H-Coupled Electron Transfer in Alkane C-H Activations with Halogen Electrophiles. Journal of the American Chemical Society, 2002, 124, 10718-10727.	6.6	59
516	FIRST PRINCIPLES MOLECULAR DYNAMICS INVOLVING EXCITED STATES AND NONADIABATIC TRANSITIONS. Journal of Theoretical and Computational Chemistry, 2002, 01, 319-349.	1.8	136
517	Isomers of S <sub>2</sub> O: Infrared absorption spectra of cyclic S <sub>2</sub> O in solid Ar. Journal of Chemical Physics, 2002, 117, 6655-6661.	1.2	30
518	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
519	Activation of Methane by Neutral Transition Metal Oxides (ScO, NiO, and PdO): A Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 12072-12083.	1.1	39
520	Addition of Nucleophiles to Silenes. A Theoretical Study of the Effect of Substituents on Their Kinetic Stability. Organometallics, 2002, 21, 3930-3939.	1.1	32
521	Thermodynamics, Kinetics, and Dynamics of the Two Alternative Anionomeric Fragmentations of C-H-O Bonds: An Electrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 4708-4715.	6.6	28
522	[4+3] versus [4+2] Mechanisms in the Dimerization of 2-Boryl-1,3-butadienes. A Theoretical and Experimental Study. Journal of Organic Chemistry, 2002, 67, 9153-9161.	1.7	26
523	Cycloaddition Reactions of Acrylonitrile on the Si(100)-2x1 Surface. Journal of the American Chemical Society, 2002, 124, 6162-6167.	6.6	43
524	Density functional theory investigation of the reactions of CH <sub>2</sub> BrI, CH <sub>2</sub> BrBr, CH <sub>2</sub> ClI, and CH <sub>2</sub> ClCl isopolyhalomethanes with ethylene. Physical Chemistry Chemical Physics, 2002, 4, 5059-5065.	1.3	6
525	Ab initio investigations of the potential energy surfaces of the XO+HO <sub>2</sub> reaction (X=chlorine or bromine). Journal of Physical Chemistry A, 2002, 106, 11800-11808.	1.3	18
526	A solid state and theoretical study of the solvent effects controlling the mono- and di-lithiation of aromatic primary amines. Dalton Transactions RSC, 2002, , 2505.	2.3	12

#	ARTICLE	IF	CITATIONS
527	Comparison of $\dot{\text{I}}\pm$ CH and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. <i>Molecular Physics</i> , 2002, 100, 533-540.	0.8	21
528	An ab initio direct classical trajectory study of s-tetrazine photodissociation. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 2554-2559.	1.3	8
529	syn-Sesquinorbornenyl carbocations and their boron analogues: an ab initio and DFT study. <i>Perkin Transactions II RSC</i> , 2002, , 2057-2063.	1.1	5
530	Theoretical study on the reaction between 4,6-dimethyl-1,2,3-triazine and enamines. <i>Perkin Transactions II RSC</i> , 2002, , 1257-1263.	1.1	6
531	Passive and Active Oxidation of Si(100) by Atomic Oxygen: A Theoretical Study of Possible Reaction Mechanisms. <i>Journal of the American Chemical Society</i> , 2002, 124, 8730-8740.	6.6	49
532	Size-dependent oxidation of hydrogenated silicon clusters. <i>Applied Physics Letters</i> , 2002, 80, 4223-4225.	1.5	13
533	The Hetero-Diels-Alder Addition of Sulfur Dioxide to 1-Fluorobuta-1,3-dienes: The Sofa Conformations Preferred by 6-Fluorosultines (6-Fluoro-3,6-dihydro-1,2-oxathiin-2-oxides) Enjoy Enthalpic and Conformational Anomeric Effects. <i>Chemistry - A European Journal</i> , 2002, 8, 1336-1355.	1.7	27
534	Theoretical study on the mechanism of the gas-phase reaction of diborane(3) anion with carbon disulfide. <i>Journal of Computational Chemistry</i> , 2002, 23, 414-419.	1.5	4
535	DFT study of ethene metathesis proceeding on monomeric MoVI centres of MoO <sub>3</sub> /Al <sub>2</sub> O <sub>3</sub> catalyst. <i>Journal of Molecular Catalysis A</i> , 2002, 184, 371-377.	4.8	18
536	Methane elimination from ionized 1-butene. <i>International Journal of Mass Spectrometry</i> , 2002, 214, 315-326.	0.7	5
537	1,3-H-shift pathways in C <sub>2</sub> H <sub>4</sub> O <sup>+</sup> and C <sub>2</sub> H <sub>4</sub> O. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 295-303.	0.7	15
538	Reaction mechanism of thymine dimer formation in DNA induced by UV light. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2002, 152, 95-101.	2.0	80
539	CH <sub>3</sub> CH <sub>3</sub> <sup>+</sup> . formation from some C <sub>3</sub> H <sub>6</sub> O <sup>+</sup> . isomers according to theory. <i>Journal of the American Society for Mass Spectrometry</i> , 2002, 13, 1235-1241.	1.2	7
540	Protonated cyclopropane as an intermediate in cationic olefin cyclizations. Ab initio and density functional theory investigations. <i>Computational and Theoretical Chemistry</i> , 2002, 589-590, 7-26.	1.5	3
541	Density functional theory characterization of the structure and gas-phase, mid-infrared absorption spectrum of 2-azido-N,N-dimethylethanamine (DMAZ). <i>Computational and Theoretical Chemistry</i> , 2002, 587, 199-218.	1.5	20
542	Formation of bis (chloromethyl) ether in the vapor phase: a computational investigation. <i>Computational and Theoretical Chemistry</i> , 2002, 619, 207-228.	1.5	5
543	Computational chemistry study of the environmentally important acid-catalyzed hydrolysis of atrazine and related 2-chloro-s-triazines. <i>Pest Management Science</i> , 2002, 58, 759-768.	1.7	12
544	Density functional theory study of the Lewis acid-catalyzed Diels-Alder reaction of nitroalkenes with vinyl ethers using aluminum derivatives. <i>Journal of Physical Organic Chemistry</i> , 2002, 15, 660-666.	0.9	50

#	ARTICLE	IF	CITATIONS
545	An investigation on the reaction mechanism of the F <sub>2</sub> +Cl <sub>2</sub> ?2ClF using the B3LYP method. International Journal of Quantum Chemistry, 2002, 87, 192-197.	1.0	0
546	Ab initio quantum chemical studies of reactions in astrophysical ices. 4. Reactions in ices involving HCOOH, CH <sub>2</sub> NH, HCN, HNC, NH <sub>3</sub> , and H <sub>2</sub> O. International Journal of Quantum Chemistry, 2002, 88, 226-235.	1.0	35
547	1,5-hydrogen shifts in methyl-1,3-cycloheptadienes. International Journal of Quantum Chemistry, 2002, 90, 1064-1070.	1.0	5
548	Density functional complete study of hydrogen bonding between the water molecule and the hydroxyl radical (H <sub>2</sub> O · HO). International Journal of Quantum Chemistry, 2002, 89, 550-558.	1.0	52
549	An AM1 theoretical study on the effect of Zn <sup>2+</sup> Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. Tetrahedron, 2002, 58, 2695-2700.	1.0	15
550	A density functional theory study for the Diels-Alder reaction between N-acyl-1-aza-1,3-butadienes and vinylamines. Lewis acid catalyst and solvent effects. Tetrahedron, 2002, 58, 3765-3774.	1.0	81
551	Is 2-oxabicyclobutane formed during the reaction of peroxyacids with cyclopropene? A high-level ab initio study. Tetrahedron, 2002, 58, 8751-8758.	1.0	6
552	Etude DFT du mécanisme des réactions de cycloaddition dipolaire-1,3 de la C,N-diphénylnitrone avec des dipolarophiles fluorés de type éthylénique et acétylénique. Journal of Fluorine Chemistry, 2002, 114, 81-89.	0.9	14
553	Theoretical investigation on reactivity of singlet radical phosphinidene: reaction mechanism of its reacting with polar hydrogen chloride molecule. Journal of Molecular Structure, 2002, 609, 11-18.	1.8	1
554	A computational study of cyclopropyl nitrene. Tetrahedron Letters, 2002, 43, 745-748.	0.7	3
555	Theoretical study of photochemical processes involving singlet excited states of formaldehyde carbonyl oxide in the atmosphere. Chemical Physics, 2002, 285, 221-231.	0.9	42
556	Theoretical study on the mechanism of the reaction between CN and O <sub>2</sub> . Chemical Physics Letters, 2002, 353, 304-309.	1.2	10
557	Three-stage character of ring inversion in cyclohexene. Chemical Physics Letters, 2002, 354, 428-434.	1.2	29
558	Theoretical investigation on the reaction of ionized water with ethylene. Chemical Physics Letters, 2002, 354, 498-502.	1.2	5
559	Dissociation pathways of benzene trication. Chemical Physics Letters, 2002, 359, 253-261.	1.2	20
560	Theoretical study of C <sub>20</sub> fullerene dimerization: a facile [2+2] cycloaddition. Chemical Physics Letters, 2002, 359, 446-452.	1.2	22
561	Density functional investigation on the cycloreversion of cyclobutane radical cation: new reaction mechanism. Chemical Physics Letters, 2002, 360, 283-288.	1.2	7
562	Theoretical study on the singlet potential energy surface of CHOP system. Chemical Physics Letters, 2002, 361, 62-70.	1.2	24

#	ARTICLE	IF	CITATIONS
563	Theoretical studies of the solvent decomposition by lithium atoms in lithium-ion battery electrolyte. <i>Chemical Physics Letters</i> , 2002, 360, 359-366.	1.2	44
564	Density functional theory study of CS <sub>2</sub> /Cl adducts and their isomerization reactions. <i>Chemical Physics Letters</i> , 2002, 362, 205-209.	1.2	7
565	Reactions in the SbF <sub>5</sub> /HF/PF <sub>3</sub> system: a DFT and ab initio study. <i>Chemical Physics Letters</i> , 2002, 363, 328-336.	1.2	4
566	Theoretical study of decomposition pathways for HArF and HKrF. <i>Chemical Physics Letters</i> , 2002, 364, 628-633.	1.2	71
567	Theoretical study of the reaction mechanism of platinum oxide with methane. <i>Chemical Physics Letters</i> , 2002, 365, 140-147.	1.2	20
568	Theoretical study of the reaction of Fe <sup>+</sup> with CS <sub>2</sub> in gas phase. <i>Chemical Physics Letters</i> , 2002, 366, 253-259.	1.2	26
569	Cyclooctatetraene Computational Photo- and Thermal Chemistry: A Reactivity Model for Conjugated Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2002, 124, 13770-13789.	6.6	75
570	Overtone-Induced Chemistry of Trifluoroacetic Acid: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8651-8657.	1.1	14
571	Cycloaddition Reactions of Metalloaromatic Complexes of Iridium and Rhodium: A Mechanistic DFT Investigation. <i>Journal of the American Chemical Society</i> , 2003, 125, 11702-11709.	6.6	53
572	Ethane hydrogenolysis on silica-supported tantalum hydride. Quantum-chemical study. <i>Russian Chemical Bulletin</i> , 2003, 52, 1928-1932.	0.4	5
573	Title is missing!. <i>Russian Chemical Bulletin</i> , 2003, 52, 30-35.	0.4	11
574	Theoretical Study on the Molecular Mechanism for the Reaction of VO <sub>2</sub> <sup>+</sup> with C <sub>2</sub> H <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , 2003, 107, 3107-3120.	1.1	68
575	Reaction Pathways of the Simmons-Smith Reaction. <i>Journal of the American Chemical Society</i> , 2003, 125, 2341-2350.	6.6	99
576	Theoretical study on the mechanism of the HF+H <sub>2</sub> O reaction. <i>Chemical Physics Letters</i> , 2003, 379, 105-112.	1.2	1
577	Isomerization pathways of singlet Ga <sub>2</sub> H <sub>2</sub> : quantum-mechanical predictions. <i>Chemical Physics Letters</i> , 2003, 380, 304-312.	1.2	6
578	A computer-aided quantum chemical study of the N <sub>15</sub> cluster. <i>Journal of Molecular Modeling</i> , 2003, 9, 99-107.	0.8	8
579	Theoretical study of propene metathesis proceeding on monomeric Mo centers of molybdena-alumina catalysts. <i>Journal of Catalysis</i> , 2003, 220, 23-34.	3.1	27
580	DFT study on the electrophilic aromatic substitution catalyzed by Lewis Acids. <i>Journal of Catalysis</i> , 2003, 220, 333-346.	3.1	13

#	ARTICLE	IF	CITATIONS
581	Synthesis, Enantiomeric Conformations, and Stereodynamics of Aromatic ortho-Substituted Disulfones. <i>Helvetica Chimica Acta</i> , 2003, 86, 65-81.	1.0	11
582	Ab Initio Structure/Reactivity Investigations of Illudin-Based Antitumor Agents: A Model for Reaction in vivo. <i>Helvetica Chimica Acta</i> , 2003, 86, 4133-4151.	1.0	7
583	Extended method for adiabatic mode reordering. <i>Journal of Computational Chemistry</i> , 2003, 24, 386-395.	1.5	1
584	Implementation of a general multireference configuration interaction procedure with analytic gradients in a semiempirical context using the graphical unitary group approach. <i>Journal of Computational Chemistry</i> , 2003, 24, 714-726.	1.5	176
585	Exploring potential energy surfaces for chemical reactions: An overview of some practical methods. <i>Journal of Computational Chemistry</i> , 2003, 24, 1514-1527.	1.5	311
586	A flexible nudged elastic band program for optimization of minimum energy pathways using ab initio electronic structure methods. <i>Journal of Computational Chemistry</i> , 2003, 24, 990-996.	1.5	34
587	Ab initio investigation on the reaction path and rate for the gas-phase reaction of HO + H <sub>2</sub> O → H <sub>2</sub> O + OH. <i>Journal of Computational Chemistry</i> , 2003, 24, 1538-1548.	1.5	40
588	Theoretical approach to the mechanism of reactions between halogen atoms and unsaturated hydrocarbons: The Cl + propene reaction. <i>Journal of Computational Chemistry</i> , 2003, 24, 2044-2062.	1.5	29
589	Kinetics and mechanism for the CH <sub>2</sub> O + NO <sub>2</sub> reaction: A computational study. <i>International Journal of Chemical Kinetics</i> , 2003, 35, 184-190.	1.0	22
590	Theoretical Studies on the Metathesis Processes, [Tp(PH <sub>3</sub> )MR(2-Hiξ <sub>i</sub> CH <sub>3</sub> )] <sup>+</sup> [Tp(PH <sub>3</sub> )M(CH <sub>3</sub> )(2-Hiξ <sub>i</sub> R)] <sup>-</sup> (M=Fe, Ti) ETQq1	1.7	65
591	Chemical Reactivity Controlled by Negative Hyperconjugation: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2003, 9, 3143-3153.	1.7	31
592	An ab Initio/RRKM Study of Product Branching Ratios in the Photodissociation of Buta-1,2- and -1,3-dienes and But-2-yne at 193 nm. <i>Chemistry - A European Journal</i> , 2003, 9, 726-740.	1.7	45
593	Theoretical Study of the [2+3] Cycloaddition of Nitrones to Nitriles—Influence of Nitrile Substituent, Solvent and Lewis Acid Coordination. <i>Chemistry - A European Journal</i> , 2003, 9, 1503-1510.	1.7	38
594	Basic and acidic bifunctional catalysis: application to the tautomeric equilibrium of formamide. <i>Chemical Physics</i> , 2003, 295, 151-158.	0.9	12
595	Structures and kinetic stability of N <sub>7</sub> cluster. <i>Chemical Physics Letters</i> , 2003, 368, 12-19.	1.2	10
596	Ab initio study of reaction mechanism of C <sub>2</sub> +H <sub>2</sub> S. <i>Chemical Physics Letters</i> , 2003, 368, 139-146.	1.2	6
597	A computational study of the Diels–Alder reactions involving acenes: reactivity and aromaticity. <i>Chemical Physics Letters</i> , 2003, 368, 630-638.	1.2	49
598	Stable structures of nitrogen-rich sulfides: N <sub>3</sub> S <sub>N</sub> <sub>4</sub> and S(N <sub>4</sub> ) <sub>m</sub> (m=1–4). <i>Chemical Physics Letters</i> , 2003, 369, 386-393.	1.2	12



#	ARTICLE	IF	CITATIONS
599	The reaction of formaldehyde with chlorine atom. <i>Chemical Physics Letters</i> , 2003, 371, 29-34.	1.2	8
600	Photodissociation of acetaldehyde, $\text{CH}_3\text{CHO} \rightarrow \text{CH}_3 + \text{HCO}$ : direct ab initio molecular dynamics study. <i>Chemical Physics Letters</i> , 2003, 371, 568-575.	1.2	30
601	Internal rotation and charge transfer study of 2-nitrophenol. <i>Chemical Physics Letters</i> , 2003, 372, 147-155.	1.2	9
602	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. <i>Chemical Physics Letters</i> , 2003, 375, 591-597.	1.2	12
603	Theoretical study of the reaction mechanism of boron atom with carbon dioxide. <i>Chemical Physics Letters</i> , 2003, 375, 670-675.	1.2	10
604	Quantum chemical study of alcoholysis mechanism of 1,2-thiazetidine 1,1-dioxide. <i>Chemical Physics Letters</i> , 2003, 377, 13-19.	1.2	11
605	A theoretical study of structure and stability of various $\text{Ge}_2\text{H}_m^+$ ( $m=0-5$ ) ions. <i>Computational and Theoretical Chemistry</i> , 2003, 663, 1-7.	1.5	6
606	Intramolecular rearrangement of organosilyl groups between oxygen and nitrogen in aminosiloxanes: A joint experimental-theoretical study. <i>Journal of Organometallic Chemistry</i> , 2003, 686, 16-23.	0.8	4
607	Enhancement of 1,2-dehydration of alcohols by alkali cations and protons: a model for dehydration of carbohydrates. <i>Journal of Analytical and Applied Pyrolysis</i> , 2003, 66, 3-27.	2.6	55
608	A density functional study on the Pt(0)-catalysed hydrosilylation of ethylene. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 277-288.	1.5	11
609	A Gaussian-3 study of the $\text{C}_3\text{H}_6\text{S}$ isomers and the dissociation channels of diradical $\text{CH}_2\text{CH}_2\text{SCH}_2$ and its radical cation $\text{CH}_2\text{CH}_2\text{SCH}_2^+$ . <i>Computational and Theoretical Chemistry</i> , 2003, 629, 237-250.	1.5	7
610	DFT and CASPT2 study of two thermal reactions of nitromethane: C-N bond cleavage and nitro-to-nitrite isomerization. An example of the inverse symmetry breaking deficiency in density functional calculations of an homolytic dissociation. <i>Computational and Theoretical Chemistry</i> , 2003, 630, 17-23.	1.5	32
611	An ab initio investigation of sulfur diimides: stability of various conformers and conformational analysis part II. Dimethyl sulfur diimides (DMSD). <i>Computational and Theoretical Chemistry</i> , 2003, 636, 229-240.	1.5	6
612	Theoretical interpretation of the observed diastereoisomeric differentiation of cis- and trans-2-methylcyclohexanol in the gas phase mediated by scandium(I). <i>International Journal of Mass Spectrometry</i> , 2003, 222, 383-396.	0.7	4
613	Development of classical trajectory methodology for the study of dissociation dynamics of polyatomic ions. <i>International Journal of Mass Spectrometry</i> , 2003, 225, 191-212.	0.7	11
614	Theoretical studies of methane elimination from $\text{C}_4\text{H}_9^+$ and $\text{H}_2$ elimination from $\text{C}_3\text{H}_7^+$ . <i>International Journal of Mass Spectrometry</i> , 2003, 228, 955-967.	0.7	10
615	Theoretical study of the thermolysis reaction of $\beta$ -hydroxynitriles in the gas phase. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 618-625.	1.0	16
616	Mechanism of the thermal decomposition of bisphenol C polycarbonate: nature of its fire resistance. <i>Polymer</i> , 2003, 44, 5469-5475.	1.8	12

#	ARTICLE	IF	CITATIONS
617	Theoretical Studies on the Hydrolysis of Mono-Phosphate and Tri-Phosphate in Gas Phase and Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2003, 125, 13265-13273.	6.6	43
618	Decarboxylation of carbonyloxy radicals: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3891-3896.	1.3	10
619	Aromaticity of Square Planar N42- in the M2N4 (M = Li, Na, K, Rb, or Cs) Species. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2882-2889.	1.1	49
620	Theoretical Studies of the Reaction Mechanisms of Dimethylsulfide and Dimethylselenide with Peroxynitrite. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5862-5873.	1.1	21
621	A Computational Study of Conformations and Conformers of 1,3-Dithiane (1,3-Dithiacyclohexane). <i>Journal of Physical Chemistry A</i> , 2003, 107, 2908-2918.	1.1	40
622	An intrinsic reaction coordinate calculation of the torsional potential in ethane: Comparison of the computationally and experimentally derived torsional transitions and the rotational barrier. <i>Journal of Chemical Physics</i> , 2003, 119, 11186-11191.	1.2	20
623	Towards understanding the molecular internal rotations and vibrations and chemical reactions through the profiles of reactivity and selectivity indices: an ab initio SCF and DFT study. <i>Molecular Physics</i> , 2003, 101, 2841-2853.	0.8	42
624	RRKM Theory and Its Implementation. <i>Comprehensive Chemical Kinetics</i> , 2003, , 55-103.	2.3	11
625	Catalytic Reduction of Acetone by [(bpy)Rh] <sup>+</sup> : A Theoretical Mechanistic Investigation and Insight into Cooperativity Effects in This System. <i>Journal of the American Chemical Society</i> , 2003, 125, 11430-11441.	6.6	19
626	A Seemingly Well Understood Light-Induced Peroxide Decarboxylation Reaction Reinvestigated with Femtosecond Time Resolution. <i>Journal of the American Chemical Society</i> , 2003, 125, 13274-13278.	6.6	18
627	Theoretical Study of the Reactivity of Fe <sup>+</sup> toward OCS. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8955-8960.	1.1	18
628	NMR and Theoretical Investigations on the Structures and Dynamics of Octahedral Bis(chelate)dichloro VIII Compounds Isolated by an Unusual Reduction of Non-Oxo VIV Species. <i>Inorganic Chemistry</i> , 2003, 42, 4640-4649.	1.9	10
629	Ab Initio/RRKM Study of the Potential Energy Surface of Triplet Ethylene and Product Branching Ratios of the C(3P) + CH <sub>4</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1788-1796.	1.1	35
630	Reaction of Propargyl with Oxygen. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9374-9379.	1.1	8
631	Light-Induced Aminocarbene to Imine Dyotropic Rearrangement in a Chromium(0) Center: An Unprecedented Reaction Pathway. <i>Journal of the American Chemical Society</i> , 2003, 125, 9572-9573.	6.6	37
632	Stable Structures of Nitrogen-Rich Sulfides: S(N <sub>3</sub> ) <sub>m</sub> (m = 1-4). <i>Journal of Physical Chemistry A</i> , 2003, 107, 2080-2084.	1.1	24
633	Direct ab Initio Dynamics Study on the Hydrogen Abstraction Reaction of CH <sub>3</sub> CCl <sub>3</sub> + OH → CH <sub>2</sub> CCl <sub>3</sub> + H <sub>2</sub> O. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6231-6235.	1.1	9
634	A DFT Study on the Regioselectivity of the Reaction of Dichloropropynylborane with Isoprene. <i>Journal of Organic Chemistry</i> , 2003, 68, 4059-4066.	1.7	26

#	ARTICLE	IF	CITATIONS
635	Experimental and Computational Studies of the Kinetics and Mechanisms for C <sub>6</sub> H <sub>5</sub> Reactions with Acetone-h <sub>6</sub> and -d <sub>6</sub> . <i>Journal of Physical Chemistry A</i> , 2003, 107, 7755-7761.	1.1	19
636	Ab Initio Studies of ClO <sub>x</sub> Reactions. 3. Kinetics and Mechanism for the OH + OClO Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1040-1049.	1.1	19
637	Dehydrogenation of Methane by Gas-Phase Os <sup>+</sup> : A Density Functional Study. <i>Organometallics</i> , 2003, 22, 3820-3830.	1.1	57
638	Reactivity of Ebtellur Derivatives with the Peroxynitrite Anion: A Comparison with Their Ebselen Analogues. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5631-5639.	1.1	9
639	Theoretical Studies on Cycloaddition Reactions between the 2-Aza-1,3-butadiene Cation and Olefins. <i>Journal of Organic Chemistry</i> , 2003, 68, 4382-4387.	1.7	12
640	1,3-Dipolar Cycloaddition of Nitrones to Free and Pt-Bound Nitriles. A Theoretical Study of the Activation Effect, Reactivity, and Mechanism. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6108-6120.	1.1	56
641	Reactivity of [1,2-Benzisotellurazol-3(2H)-one] with Peroxynitrous Acid: A Comparison with Ebselen Analogues. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9984-9990.	1.1	8
642	Structural and Energetics Studies of Tri- and Tetra-tert-butylmethane. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5492-5498.	1.1	14
643	Scratching the Surface of Buckminsterfullerene: The Barriers for Stone-Wales Transformation through Symmetric and Asymmetric Transition States. <i>Journal of the American Chemical Society</i> , 2003, 125, 5572-5580.	6.6	122
644	Computational Study of the Aminolysis of 2-Benzoxazolinone. <i>Journal of Organic Chemistry</i> , 2003, 68, 3406-3412.	1.7	27
645	Rates of Catalyzed Processes in Enzymes and Other Cooperative Media. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4437-4443.	1.2	8
646	Methylamine Adsorption on and Desorption from Si(100). <i>Journal of Physical Chemistry B</i> , 2003, 107, 5491-5502.	1.2	46
647	Experimental and Theoretical Studies of the Methylidyne CH(X <sup>2</sup> ) Radical Reaction with Ethane (C <sub>2</sub> H <sub>6</sub> ): Overall Rate Constant and Product Channels. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5419-5426.	1.1	40
648	Ab Initio Study of the Thermal Isomerization of Tricyclo[3.1.0.0 <sup>2,6</sup> ]hexane to (Z,Z)-1,3-Cyclohexadiene through the (E,Z)-1,3-Cyclohexadiene Intermediate. <i>Journal of Physical Chemistry A</i> , 2003, 107, 198-203.	1.1	14
649	Ultrafast Decarboxylation of Carbonyloxy Radicals: Influence of Molecular Structure. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9499-9510.	1.1	43
650	Gaussian-3 Molecular Orbital Study of the Reaction of Boron with Methylamine and the Decomposition Paths of the Reaction Products. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1819-1824.	1.1	2
651	Theoretical Study of the Insertion Reactions of Zr <sup>+</sup> into HF, HCl, H <sub>2</sub> O, H <sub>2</sub> S, NH <sub>3</sub> , PH <sub>3</sub> , CH <sub>4</sub> , and SiH <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , 2003, 107, 6681-6687.	1.1	8
652	Theoretical Study of the Mechanism of the Formation of 3-Unsubstituted 4,4-Disubstituted $\beta$ -Lactams by Silver-Induced Ring Expansion of Alkoxypropylamines: A New Synthetic Route to 4-Alkoxyacyl-4-alkyl-2-azetidiones. <i>Journal of Organic Chemistry</i> , 2003, 68, 6685-6689.	1.7	13

#	ARTICLE	IF	CITATIONS
653	Theoretical Study of the $C_2(1\sigma_g^+, 3\sigma_u) + H_2O$ Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9825-9833.	1.1	11
654	A Theoretical Study of the Mechanism of Selective Fluorination of Saturated Hydrocarbons by Molecular Fluorine. Participation of $CHCl_3$ Solvent Molecules in the Ionic Process. <i>Journal of Organic Chemistry</i> , 2003, 68, 8170-8178.	1.7	11
655	Experimental and Theoretical Investigations of the Ultrafast Photoinduced Decomposition of Organic Peroxides in Solution: $\alpha$ Formation and Decarboxylation of Benzoyloxy Radicals. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5157-5167.	1.1	33
656	Fundamental Reaction Mechanism for Cocaine Hydrolysis in Human Butyrylcholinesterase. <i>Journal of the American Chemical Society</i> , 2003, 125, 2462-2474.	6.6	131
657	Formation of the Silicon Analogues of Isocyanic Acid, $HNSiO$ , and Its Isomers by Neutral-Neutral Reactions of the Fragments: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11497-11504.	1.1	7
658	Thermal Fragmentation of 3-Vinylloxetane: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2919-2928.	1.1	5
659	Theoretical Study of $[N_3X]^+$ ( $X = O, S, Se, Te$ ) Systems. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5561-5565.	1.1	11
660	Theoretical Investigation of the Reaction of $Co^+$ with $OCS$ . <i>Journal of Physical Chemistry A</i> , 2003, 107, 8618-8622.	1.1	19
661	Can the Ebselen Derivatives Catalyze the Isomerization of Peroxynitrite to Nitrate?. <i>Journal of the American Chemical Society</i> , 2003, 125, 3877-3888.	6.6	27
662	Differences and Similarities in the Reactivity of Peroxynitrite Anion and Peroxynitrous Acid with Ebselen. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1563-1573.	1.1	28
663	The Change of Aromaticity along a Diels-Alder Reaction Path. <i>Organic Letters</i> , 2003, 5, 1127-1130.	2.4	29
664	Trimethylene Sulfide- $(HCl)_n$ ( $n = 1, 2$ ) Complexes: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 899-907.	1.1	9
665	The Rearrangement of Dicarboranyl Methyl Cation: A Possible Synthetic Strategy Toward Cationic closo-Tricarbaboranes. <i>Inorganic Chemistry</i> , 2003, 42, 7725-7727.	1.9	10
666	Thermal Isomerization of Tricyclo[4.1.0.0 <sup>2,7</sup> ]heptane and Bicyclo[3.2.0]hept-6-ene through the (E,Z)-1,3-Cycloheptadiene Intermediate. <i>Journal of Organic Chemistry</i> , 2003, 68, 9081-9087.	1.7	10
667	Cycloaddition Reactions of 1-Pyrazoline on the $Si(100) 2 \times 1$ Surface: A Possible Route to an SiN Interfacial Double Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 6853-6858.	1.2	3
668	Ab Initio Studies of $ClO_x$ Radical Reactions: V. Evidence for a New Path in the $Cl + ClOCl$ Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3836-3840.	1.1	13
669	The $C_7$ - $C_{10}$ Cycloalkanes Revisited. <i>Journal of Organic Chemistry</i> , 2003, 68, 9322-9329.	1.7	86
670	Enhancing Reactivity of Carbonyl Compounds via Hydrogen-Bond Formation. A DFT Study of the Hetero-Diels-Alder Reaction between Butadiene Derivative and Acetone in Chloroform. <i>Journal of Organic Chemistry</i> , 2003, 68, 8662-8668.	1.7	91

#	ARTICLE	IF	CITATIONS
671	The hydrolysis process of the cis-dichloro(ethylenediamine)platinum(II): A theoretical study. <i>Journal of Chemical Physics</i> , 2003, 118, 10584-10592.	1.2	67
672	Mechanism of a Chemical Classic: A Quantum Chemical Investigation of the Autocatalyzed Reaction of the Serendipitous Wöhler Synthesis of Urea. <i>Journal of the American Chemical Society</i> , 2003, 125, 2307-2318.	6.6	42
673	Rearrangement Pathways of Five-Membered Ring Enlargement in Carbocations: A Quantum Chemical Calculations and Deuterium Kinetic Isotope Effects. <i>Journal of Organic Chemistry</i> , 2003, 68, 1859-1866.	1.7	16
674	Intramolecular 1,3-Dipolar Ene Reactions of Nitrile Oxides Occur by Stepwise 1,1-Cycloaddition/Retro-Ene Mechanisms. <i>Journal of the American Chemical Society</i> , 2003, 125, 13825-13830.	6.6	117
675	Activation Barriers in the Homolytic Cleavage of Radicals and Ion Radicals. <i>Journal of the American Chemical Society</i> , 2003, 125, 105-112.	6.6	30
676	Plateau Reactions: Double Proton-Transfer Processes with Structureless Transition States. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9668-9678.	1.1	34
677	Isodesmic Reactions for Transition States: Reactions of Cl Atoms with Methane and Halogenated Methanes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11082-11091.	1.1	20
678	Isomerization and Dissociation of CHNS: A Quantum Mechanical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11209-11216.	1.1	37
679	Kinetics of the Reaction of C <sub>2</sub> Cl <sub>3</sub> with Cl <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2003, 107, 1776-1778.	1.1	6
680	The Solid State Structure of [B <sub>10</sub> H <sub>11</sub> ] <sup>-</sup> and Its Dynamic NMR Spectra in Solution. <i>Inorganic Chemistry</i> , 2003, 42, 1175-1186.	1.9	30
681	Reaction path description of the vinylidene acetylene isomerization. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4604-4611.	1.3	13
682	Theozyme for antibody aldolases. Characterization of the transition-state analogue Electronic supplementary information (ESI) available: MP2/6-31G** energies, imaginary frequencies and cartesian coordinates. See <a href="http://www.rsc.org/suppdata/ob/b2/b209636f/">http://www.rsc.org/suppdata/ob/b2/b209636f/</a> . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 637-643.	1.5	13
683	Theoretical study of the reaction mechanism of the uncatalyzed epoxidation of alkenes by iodosylbenzene Electronic supplementary information (ESI) available: B3LYP optimized geometries (Cartesian coordinates) and total energies for compounds 1 to 9. See <a href="http://www.rsc.org/suppdata/nj/b2/b203861g/">http://www.rsc.org/suppdata/nj/b2/b203861g/</a> . <i>New Journal of Chemistry</i> , 2003, 27, 811-817.	1.4	18
684	Theoretical Study of Ni(N <sub>4</sub> ) <sub>2</sub> , Ni(C <sub>4</sub> H <sub>4</sub> ) <sub>2</sub> , and Ni(C <sub>2</sub> O <sub>2</sub> ) <sub>2</sub> Complexes. <i>Journal of Physical Chemistry A</i> , 2003, 107, 8584-8593.	1.1	18
685	Ab Initio Studies of ClO <sub>x</sub> Reactions: VI. Theoretical Prediction of Total Rate Constant and Product Branching Probabilities for the HO <sub>2</sub> + ClO Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 3841-3850.	1.1	28
686	Activation and Adsorption of Multiple H <sub>2</sub> Molecules on a Pd <sub>5</sub> Cluster: A Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4929-4939.	1.1	30
687	Calculation of accurate imaginary frequencies and tunnelling coefficients for hydrogen abstraction reactions using IRCmax. <i>Molecular Physics</i> , 2003, 101, 1329-1338.	0.8	37
688	Trends in alkyl substituent effects on nucleophilic reactions of carbonyl compounds: Gas phase reactions between ammonia and R <sub>1</sub> R <sub>2</sub> COCH <sub>3</sub> <sup>+</sup> oxonium ions Electronic 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(k <sub>rel</sub> /k <sub>sub</sub> ) against a-stabilisation constants. See <a href="http://www.rsc.org/suppdata/ob/b2/b209955c/">http://www.rsc.org/suppdata/ob/b2/b209955c/</a> . <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 705-713.	1.5	8

#	ARTICLE	IF	CITATIONS
689	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1392-1399.	1.3	51
690	Formation of Î <sup>2</sup> -O-4 Lignin Models -A Theoretical Study. <i>Holzforschung</i> , 2003, 57, 466-478.	0.9	35
691	Observation of a HI leaving group following ultraviolet photolysis of CH <sub>2</sub> I <sub>2</sub> in water and anab initioinvestigation of the Oâ€“H insertion/HI elimination reactions of the CH <sub>2</sub> Iâ€“I isopolyhalomethane species with H <sub>2</sub> O and 2H <sub>2</sub> O. <i>Journal of Chemical Physics</i> , 2003, 119, 4671-4681.	1.2	17
692	Thermal decomposition of ethanol. II. A computational study of the kinetics and mechanism for the H+C <sub>2</sub> H <sub>5</sub> OH reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 9990-9996.	1.2	56
693	Wave packet dynamics along bifurcating reaction paths. <i>Journal of Chemical Physics</i> , 2003, 118, 5831-5840.	1.2	30
694	A theoretical study on the stability of N <sub>15</sub> <sup>+</sup> cluster. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1116-1122.	1.3	6
695	A spinâ€“orbit coupling study on the spin inversion processes in the direct methane-to-methanol conversion by FeO <sup>+</sup> . <i>Journal of Chemical Physics</i> , 2003, 118, 5872-5879.	1.2	97
696	THEORETICAL PREDICTION OF POTENTIAL ENERGY SURFACE FOR N <sub>14</sub> CLUSTER. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 7-14.	1.8	8
697	Ab Initio/RRKM Study of Dissociation Mechanism of Benzene Trication. <i>Journal of Theoretical and Computational Chemistry</i> , 2003, 02, 205-231.	1.8	9
698	<i>Ab Initio</i> Study on the Potential Energy Surfaces of B <sub>4</sub> Cluster. <i>Journal of the Chinese Chemical Society</i> , 2003, 50, 1115-1122.	0.8	3
699	On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive?Â¶. <i>Photochemistry and Photobiology</i> , 2003, 78, 159.	1.3	47
700	CH <sub>4</sub> Loss from (CH <sub>3</sub> ) <sub>4</sub> N <sup>+</sup> Revisited: How Does This High Energy Elimination Compete with â€“CH <sub>3</sub> Loss?. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 767-773.	0.5	3
701	Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13831-13838.	1.2	20
702	Fluorination-induced back-bond weakening and hydrogen passivation on HF-etched Si surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	21
703	Ab initiomolecular orbital study of structures and energetics of Si <sub>3</sub> H <sub>2</sub> , Si <sub>3</sub> H <sub>2</sub> <sup>+</sup> , and Si <sub>3</sub> H <sub>2</sub> <sup>âˆ—</sup> . <i>Journal of Chemical Physics</i> , 2004, 120, 11071-11081.	1.2	7
704	Anchoring the potential energy surface of the cyclic water trimer. <i>Journal of Chemical Physics</i> , 2004, 121, 11023.	1.2	68
705	Directab initiodynamics study on the rate constants and kinetics isotope effects of CH <sub>3</sub> O+Hâ†’CH <sub>2</sub> O+H <sub>2</sub> reaction. <i>Journal of Chemical Physics</i> , 2004, 121, 9474-9480.	1.2	9
706	Effect of absolute laser phase on reaction paths in laser-induced chemical reactions. <i>Journal of Chemical Physics</i> , 2004, 121, 7764.	1.2	68

#	ARTICLE	IF	CITATIONS
707	Molecular elimination of Br <sub>2</sub> in 248 nm photolysis of bromoform probed by using cavity ring-down absorption spectroscopy. <i>Journal of Chemical Physics</i> , 2004, 121, 5253-5260.	1.2	45
708	An ab initio correlated study of the potential energy surface for the HOBr.H <sub>2</sub> O complex. <i>Journal of Chemical Physics</i> , 2004, 121, 141.	1.2	6
709	Theoretical study on the reaction mechanism of (CH <sub>3</sub> ) <sub>3</sub> CO <sup>•</sup> radical with NO. <i>Science in China Series B: Chemistry</i> , 2004, 47, 289.	0.8	0
710	3,5-PyridyneA Heterocyclicmeta-Benzyne Derivative. <i>Journal of the American Chemical Society</i> , 2004, 126, 6135-6149.	6.6	66
711	Structures and stability of N <sub>13</sub> <sup>+</sup> and N <sub>13</sub> <sup>•</sup> clusters. <i>Journal of Molecular Modeling</i> , 2004, 10, 13-18.	0.8	3
712	A computational approach to the synthesis of dirithromycin. <i>Journal of Molecular Modeling</i> , 2004, 10, 94-101.	0.8	3
713	Theoretical study on thermal decomposition of azoisobutyronitrile in ground state. <i>Science in China Series B: Chemistry</i> , 2004, 47, 373-380.	0.8	2
714	Theoretical characterizations of novel C <sub>2</sub> H <sub>5</sub> O <sup>+</sup> reactions. <i>International Journal of Mass Spectrometry</i> , 2004, 232, 17-24.	0.7	13
715	The nucleophilic addition of nitrones to carbonyl compounds: insights on the nature of the mechanism of the l-proline induced asymmetric reaction from a DFT analysis. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 1541-1549.	1.8	20
716	Degenerate propene metathesis on Mo-alkylidene centres of molybdena "alumina catalyst" a DFT study. <i>Journal of Molecular Catalysis A</i> , 2004, 218, 91-100.	4.8	16
717	Computational study of the chair-chair interconversion and stereoelectronic interactions in 1,2,3-trithiacyclo-hexane (1,2,3-trithiane). <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 32-41.	0.9	12
718	Theoretical study of protonated xylenes: ethene elimination and H,C scrambling reactions. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 1023-1032.	0.9	29
719	MCSCF study of the thermal isomerization of tricyclo[2.1.0.0 <sup>2,5</sup> ]pentane to 1,3-cyclopentadiene. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 411-415.	1.0	3
720	Conformational conversion of the boat and chair structures of bicyclo[3.2.0]hept-6-ene. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 432-435.	1.0	2
721	Computational study of the conformational interconversion of 5,5-dimethyl-1,2,3-trithiacyclohexane (5,5-dimethyl-1,2,3-trithiane). <i>International Journal of Quantum Chemistry</i> , 2004, 96, 443-455.	1.0	8
722	Ab initio study of the CH <sub>3</sub> O <sub>2</sub> self-reaction in gas phase: Elucidation of the CH <sub>3</sub> O <sub>2</sub> CH <sub>3</sub> O <sub>2</sub> → 2CH <sub>3</sub> O O <sub>2</sub> pathway. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 605-615.	1.0	18
723	A kinetic stability study of MN <sup>+</sup> 5 (M=Be, Mg, Ca, Sr, and Ba). <i>International Journal of Quantum Chemistry</i> , 2004, 98, 485-494.	1.0	15
724	Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 465-472.	1.0	12

#	ARTICLE	IF	CITATIONS
725	Bicyclopropylidene radical cation: A rehybridization ring opening to tetramethyleneethane. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 473-483.	1.0	5
726	Relative energies, stereoelectronic interactions, and conformational interconversion in silacycloalkanes. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 720-732.	1.0	26
727	Cycloaddition of Benzonitrile Oxide to Acetonitrile, Propyne and Propene – A Comparative Theoretical Study of the Reaction Mechanism and Regioselectivity. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 2046-2052.	1.2	16
728	Theoretical Studies on Cycloaddition Reactions between 1-Aza-2-azoniaallene Cations and Isocyanates. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 4070-4076.	1.2	9
729	Why do Electron-Deficient Dienes React Rapidly in Diels-Alder Reactions with Electron-Deficient Ethylenes? A Density Functional Theory Analysis. <i>European Journal of Organic Chemistry</i> , 2004, 2004, 4788-4793.	1.2	49
730	Kinetics and Mechanisms for the Reactions of Phenyl Radical with Ketene and its Deuterated Isotopomer: An Experimental and Theoretical Study. <i>ChemPhysChem</i> , 2004, 5, 225-232.	1.0	8
731	Kinetics and Mechanism of the C <sub>6</sub> H <sub>5</sub> <sup>+</sup> CH <sub>3</sub> CHO Reaction: Experimental Measurement and Theoretical Prediction of the Reactivity toward Four Molecular Sites. <i>ChemPhysChem</i> , 2004, 5, 661-668.	1.0	13
732	Oxygenolysis of Flavonoid Compounds: DFT Description of the Mechanism for Quercetin. <i>ChemPhysChem</i> , 2004, 5, 1726-1733.	1.0	40
733	Density functional investigation of reaction of borohydride cation BH <sub>2</sub> <sup>+</sup> with propylene. <i>Journal of Computational Chemistry</i> , 2004, 25, 258-264.	1.5	0
734	A computational study of the kinetics and mechanism for the reaction of HCO with HNO. <i>International Journal of Chemical Kinetics</i> , 2004, 36, 205-215.	1.0	16
735	Computational study on the kinetics and mechanisms for the reactions of HCO with HONO and HNOH. <i>International Journal of Chemical Kinetics</i> , 2004, 36, 178-187.	1.0	11
736	Density Functional Calculations on the Conversion of Azide and Carbon Monoxide to Isocyanate and Dinitrogen by a Nickel to Sulfur Rebound Mechanism. <i>Chemistry - A European Journal</i> , 2004, 10, 1805-1814.	1.7	13
737	Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. <i>Chemistry - A European Journal</i> , 2004, 10, 3404-3410.	1.7	63
738	Computational Investigation of Hydrogen Abstraction from 2-Aminoethanol by the 1,5-Dideoxyribose-5-yl Radical: A Model Study of a Reaction Occurring in the Active Site of Ethanolamine Ammonia Lyase. <i>Chemistry - A European Journal</i> , 2004, 10, 2781-2788.	1.7	10
739	Theoretical Study of the Electrocyclic Ring Closure of Hydroxypentadienyl Cations. <i>Chemistry - A European Journal</i> , 2004, 10, 4324-4333.	1.7	95
740	Understanding the Nature of the Molecular Mechanisms Associated with the Competitive Lewis Acid Catalyzed [4+2] and [4+3] Cycloadditions between Arylidinoxazolone Systems and Cyclopentadiene: A DFT Analysis. <i>Chemistry - A European Journal</i> , 2004, 10, 4742-4749.	1.7	27
741	From Allylic Alcohols to Aldols by Using Iron Carbonyls as Catalysts: Computational Study on a Novel Tandem Isomerization-Aldolization Reaction. <i>Chemistry - A European Journal</i> , 2004, 10, 5795-5803.	1.7	32
742	A theoretical investigation of the Chalk-Harrod and modified Chalk-Harrod mechanisms involved in hybrid integrated circuit building. <i>Future Generation Computer Systems</i> , 2004, 20, 781-791.	4.9	5



#	ARTICLE	IF	CITATIONS
743	sp <sup>3</sup> C-H and sp <sup>2</sup> C-H agostic ruthenium complexes: a combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2004, 357, 1854-1864.	1.2	49
744	C <sub>4</sub> H <sub>8</sub> <sup>+</sup> isomerizations by theory. <i>International Journal of Mass Spectrometry</i> , 2004, 236, 105-116.	0.7	5
745	A density functional study of the gas-phase pyrolytic reaction of ethyl-2-pyridine sulfonate. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 39-43.	1.5	0
746	Theoretical study on mechanism of the gas-phase pyrolytic reaction of ethyl-2-pyridine sulfonate. <i>Computational and Theoretical Chemistry</i> , 2004, 668, 133-137.	1.5	0
747	The domino reaction between 4,6-dinitrobenzofuroxan and cyclopentadiene. Insights on the nature of the molecular mechanism. <i>Computational and Theoretical Chemistry</i> , 2004, 709, 45-52.	1.5	37
748	A Gaussian-2 study on the structures, energetics, and reactions of C <sub>2</sub> H <sub>3</sub> S <sup>-</sup> anions. <i>Computational and Theoretical Chemistry</i> , 2004, 671, 221-228.	1.5	1
749	Quantum chemical study of alcoholysis mechanism of N-methyl-1,2-thiazetidine-1,1-dioxide. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 199-205.	1.5	6
750	Theoretical investigations on the conformational alterations of tetraarylporphyrins: toward understanding conformational alterations resulting from adsorption onto solid surfaces. <i>Computational and Theoretical Chemistry</i> , 2004, 676, 141-147.	1.5	5
751	Hydrogen activation and aldehyde elimination promoted by homogeneous Pt-Sn catalyst: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2004, 677, 133-143.	1.5	21
752	A DFT study on the intramolecular dissociation pathways of ethyl fluoroformate radical cation in the gas phase; I. Enol path. <i>Computational and Theoretical Chemistry</i> , 2004, 677, 97-104.	1.5	1
753	Theoretical study on the thermal decomposition of azoisobutyronitrile. <i>Computational and Theoretical Chemistry</i> , 2004, 679, 89-94.	1.5	16
754	Theoretical investigation of reaction mechanism for CH <sub>2</sub> (X)B <sub>1</sub> with NO radical. <i>Computational and Theoretical Chemistry</i> , 2004, 679, 121-125.	1.5	20
755	An ab initio study of the reaction of propargyl cation with water. <i>Computational and Theoretical Chemistry</i> , 2004, 683, 81-87.	1.5	2
756	DFT study of the [Ru(NO)Cl <sub>5</sub> ] <sup>2-</sup> ion: metastable states and isomerization path. <i>Computational and Theoretical Chemistry</i> , 2004, 683, 97-102.	1.5	10
757	Insight into the stability and structural properties of HPS <sub>3</sub> isomers from density functional theory computations. <i>Computational and Theoretical Chemistry</i> , 2004, 712, 1-7.	1.5	0
758	Theoretical study on gas-phase conformations and isomerization reaction mechanism of cyclic 3',5'-adenosine monophosphate. <i>Computational and Theoretical Chemistry</i> , 2004, 711, 19-24.	1.5	2
759	A G3(MP2) study on the electrocyclic reactions of [12]annulene. <i>Computational and Theoretical Chemistry</i> , 2004, 711, 133-139.	1.5	0
760	Ab initio study of the cycloaddition reaction between hexatriene and ethylene. <i>Computational and Theoretical Chemistry</i> , 2004, 712, 49-66.	1.5	3

#	ARTICLE	IF	CITATIONS
761	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. <i>Tetrahedron</i> , 2004, 60, 11503-11509.	1.0	150
762	A theoretical investigation of electronic ground state of parent sulfur diimide. <i>Journal of Molecular Spectroscopy</i> , 2004, 223, 195-204.	0.4	3
763	Dimerization of electrochemically generated ion radicals: mechanisms and reactivity factors. <i>Journal of Electroanalytical Chemistry</i> , 2004, 564, 99-113.	1.9	29
764	Circumvention of orbital symmetry restraints by 1,3-H-shifts of enolic radical cations. <i>Journal of the American Society for Mass Spectrometry</i> , 2004, 15, 972-981.	1.2	7
765	Theoretical study on the reaction path and rate constants of the hydrogen atom abstraction reaction of CH <sub>2</sub> O with CH <sub>3</sub> /OH. <i>Chemical Physics</i> , 2004, 307, 35-43.	0.9	17
766	Synthesis and biological evaluation of oxindoles and benzimidazolinones derivatives. <i>European Journal of Medicinal Chemistry</i> , 2004, 39, 453-458.	2.6	38
767	The reaction of formyl radical with chlorine atom. <i>Chemical Physics Letters</i> , 2004, 386, 384-389.	1.2	5
768	Direct ab initio dynamics studies of the reactions of HNO with H and OH radicals. <i>Chemical Physics Letters</i> , 2004, 388, 94-99.	1.2	25
769	A theoretical study on the mechanism of the reaction between Cl atoms and nitrobenzene. <i>Chemical Physics Letters</i> , 2004, 392, 236-241.	1.2	7
770	A DFT study of nitration of benzene by acyl nitrate catalyzed by zeolites. <i>Chemical Physics Letters</i> , 2004, 393, 173-178.	1.2	11
771	On the stability of HKrOH: a theoretical study. <i>Chemical Physics Letters</i> , 2004, 395, 182-185.	1.2	14
772	The role of lithium in hydrogen storage in aromatic carbon materials. <i>Chemical Physics Letters</i> , 2004, 398, 62-67.	1.2	17
773	DFT and MP2 investigation of the $\langle \text{mml:math altimg="si4.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://. Chemical Physics$	1.2	3
774	On the microscopic mechanism of carbon gasification: A theoretical study. <i>Carbon</i> , 2004, 42, 2921-2928.	5.4	58
775	Structure and bonding in the isoelectronic series C <sub>n</sub> H <sub>n</sub> P <sub>5</sub> <sup>n+</sup> : is phosphorus a carbon copy?. <i>Dalton Transactions</i> , 2004, , 2080-2086.	1.6	37
776	On the role of s-cis conformers in the reaction of dienes with OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2237-2244.	1.3	21
777	AIM Studies on Reactions FNCX + FXCN (X = O, S, and Se). <i>Journal of Physical Chemistry A</i> , 2004, 108, 10527-10534.	1.1	14
778	Ab initio MO and DFT study of syn-sesquinorbomatrienyl dication and its isoelectronic boron analogue. Electronic 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 <a href="http://www.rsc.org/suppdata/ni/b4/b403802a/">http://www.rsc.org/suppdata/ni/b4/b403802a/</a> . <i>New Journal of Chemistry</i> , 2004, 28, 880.	1.4	7

#	ARTICLE	IF	CITATIONS
779	Acetylene to vinylidene rearrangements on electron rich d6 metal centers: a density functional study. Dalton Transactions, 2004, , 3225.	1.6	32
780	Formation of the heterocumulene anion SCCCN <sup>-</sup> by a cyano migration from the radical anion of 1,2-dicyanoethylenedithiolate Dedicated 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
781	Analysis and dynamics of unusual double proton transfer reactions based on the reaction path Hamiltonian. Physical Chemistry Chemical Physics, 2004, 6, 3341.	1.3	13
782	On the Stability of Hydride Configurations on Silicon Cluster Surfaces: A First-Principle Theoretical Study. Journal of Physical Chemistry B, 2004, 108, 1967-1973.	1.2	11
783	Mechanism and Ligand-Transfer Selectivity of 1,2-Addition of Organozincate Complexes to Aldehyde. Journal of the American Chemical Society, 2004, 126, 10897-10903.	6.6	54
784	Density Functional Studies on Conformational Behaviors of Glycinamide in Solution. Journal of Physical Chemistry B, 2004, 108, 1405-1413.	1.2	20
785	Computational Study of the Oxygen Initiated Decomposition of 2-Oxepinoxy Radical: A Key Intermediate in the Oxidation of Benzene. Journal of Physical Chemistry A, 2004, 108, 8419-8433.	1.1	20
786	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
787	Unimolecular Decomposition of $\beta$ -Hydroxyethylperoxy Radicals in the HO $\cdot$ -Initiated Oxidation of Ethene: A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 11651-11663.	1.1	23
788	Experimental and Theoretical Studies of the Dimerizations of Imidoalkynes. Journal of Organic Chemistry, 2004, 69, 86-94.	1.7	32
789	A Joint Experimental and Theoretical Study on the Mechanisms of Methyl 2-Hydroxypropionate and Methyl 2-Hydroxyisobutyrate Decomposition in the Gas Phase. Journal of Physical Chemistry A, 2004, 108, 996-1007.	1.1	7
790	Cooperative Bimetallic Reactivity: Hydrogen Activation in Two-Electron Mixed-Valence Compounds. Journal of the American Chemical Society, 2004, 126, 9760-9768.	6.6	66
791	Double Proton Transfer and One-Electron Oxidation Behaviors in Double H-Bonded Glycinamide <sup>-</sup> Formamidinium Complex and Comparison with Biological Base Pair. Journal of Physical Chemistry B, 2004, 108, 16976-16982.	1.2	5
792	A Theoretical Study of the Reaction of GeH <sub>2</sub> with CO <sub>2</sub> and the Dissociation Paths of the Reaction Products. Journal of Physical Chemistry A, 2004, 108, 4002-4007.	1.1	7
793	Experimental and Quantum Chemical Study of the Mechanism of an Unexpected Intramolecular Reductive Coupling of a Bridging Phosphido Ligand and a C <sub>6</sub> F <sub>5</sub> Group and the Reversible Oxidative Addition of PPh <sub>2</sub> C <sub>6</sub> F <sub>5</sub> <sup>-</sup> . Organometallics, 2004, 23, 1797-1810.	1.1	35
794	Density Functional Studies on Dicobalt Octacarbonyl Mediated Urea Formation from Primary Amine. Organometallics, 2004, 23, 718-729.	1.1	13
795	Reaction of Benzene and Boron Atom: Mechanism of Formation of Benzoborirene and Hydrogen Atom. Journal of Physical Chemistry A, 2004, 108, 4576-4586.	1.1	31
796	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

#	ARTICLE	IF	CITATIONS
797	Matrix Isolation Infrared Spectroscopic and Theoretical Study of the Reactions of Beryllium Atoms with Methanol. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3390-3395.	1.1	16
798	Ab Initio Study of the Formation of Glycine via Amino Acetonitrile and Amino-Cyano-Acetic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 3798-3805.	1.1	21
799	Unusual Isomerization Reactions in 1,3-Diaza-2-silacyclopentanes. <i>Organometallics</i> , 2004, 23, 1180-1182.	1.1	4
800	Theoretical Determination of Activation Free Energies for Alkaline Hydrolysis of Cyclic and Acyclic Phosphodiester in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6407-6413.	1.1	38
801	Density Functional Study on the Mechanisms of the Reactions of Gas-Phase OsOn <sup>+</sup> (n = 1-4) with Methane. <i>Organometallics</i> , 2004, 23, 3656-3667.	1.1	27
802	Fragmentation Mechanisms of Product Ions from Protonated Tripeptides. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18743-18749.	1.2	43
803	Density Functional Theory Studies on Structure, Spectra, and Electronic Properties of 3,7-Dinitrodibenzobromolium Cation and Chloride. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7596-7602.	1.1	1
804	Theoretical and Experimental Study on the In-Plane SN <sub>2</sub> -Type Substitution Reaction of Haloalkenes with Inversion of Configuration at the sp <sup>2</sup> Carbon. <i>Organic Letters</i> , 2004, 6, 2461-2463.	2.4	28
805	Ab Initio Classical Trajectory Calculations of Acetylene Dication Dissociation. <i>Journal of Physical Chemistry A</i> , 2004, 108, 468-472.	1.1	10
806	Investigations of Double Proton Transfer Behavior between Glycinamide and Formamide Using Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10288-10295.	1.1	15
807	Formation of Silicon Analogues of Thio-isocyanic Acid, HNSiS, and Its Isomers by Neutral-Neutral Reactions of the Fragments: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9218-9225.	1.1	6
808	Theoretical Study of the Reaction Mechanism of BO, B <sub>2</sub> O <sub>2</sub> , and BS with H <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2004, 108, 473-483.	1.1	27
809	Combined Experimental and Computational Investigation of the Mechanism of Nickel-Catalyzed Three-Component Addition Processes. <i>Organometallics</i> , 2004, 23, 4636-4646.	1.1	106
810	Modeling Catalytic Effects of Clay Mineral Surfaces on Peptide Bond Formation. <i>Journal of Physical Chemistry B</i> , 2004, 108, 10120-10130.	1.2	36
811	Reaction Pathways and Free Energy Barriers for Alkaline Hydrolysis of Insecticide 2-Trimethylammonioethyl Methylphosphonofluoridate and Related Organophosphorus Compounds: A Theoretical Analysis. <i>Journal of Organic Chemistry</i> , 2004, 69, 8451-8458.	1.7	24
812	Unusual Intramolecular [2 + 2] Cycloaddition of Allyl and Vinylidene CC Bonds under Mild Conditions: A Theoretical Analysis. <i>Journal of Organic Chemistry</i> , 2004, 69, 2544-2550.	1.7	18
813	Structures of Nitrogen-Rich Sulfides: SN <sub>5</sub> and SN <sub>6</sub> . <i>Journal of Physical Chemistry A</i> , 2004, 108, 4679-4684.	1.1	7
814	Quantum Dynamical Study of H <sup>2</sup> -Hydrogen Transfer in Two Selected Late-Transition-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11116-11126.	1.1	13

#	ARTICLE	IF	CITATIONS
815	Potential Energy Surfaces for the Reactions Si + O <sub>2</sub> . Journal of Physical Chemistry A, 2004, 108, 8395-8399.	1.1	8
816	Studies on Reactions INCX + ICN (X = O, S, and Se). Inorganic Chemistry, 2004, 43, 5311-5320.	1.9	26
817	Multewater-Assisted Proton Transfer Study in Glycinamide Using Density Functional Theory. Journal of Physical Chemistry B, 2004, 108, 18088-18097.	1.2	18
818	A Theoretical Study on the Gas Phase Reactions of the Anions NbO <sub>3</sub> <sup>-</sup> , NbO <sub>5</sub> <sup>-</sup> , and NbO <sub>2</sub> (OH) <sub>2</sub> <sup>-</sup> with H <sub>2</sub> O and O <sub>2</sub> . Journal of Physical Chemistry A, 2004, 108, 10850-10860.	1.1	26
819	Adsorption and Decomposition Pathways of Cyanogen Halides on Si(100) (2 × 1). Journal of Physical Chemistry B, 2004, 108, 303-309.	1.2	10
820	Theoretical Study of TiO-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Journal of Physical Chemistry A, 2004, 108, 10245-10251.	1.1	9
821	Insights into Photodissociation Dynamics of Benzamide and Formanilide from ab Initio Calculations. Journal of the American Chemical Society, 2004, 126, 8976-8980.	6.6	32
822	Diastereoselective Synthesis of the Indenylruthenium(II) Complexes [Ru(1-5-C <sub>9</sub> H <sub>7</sub> ){I <sup>3</sup> (P,C,C)-Ph <sub>2</sub> P(CH <sub>2</sub> CRCH <sub>2</sub> )}(PPh <sub>3</sub> )] [PF <sub>6</sub> ] (R = H, Me): Enantiofacial Coordination, Hemilabile Properties, and Diastereoselective Nucleophilic Additions to I <sup>3</sup> (P,C,C)-Allylphosphine Ligands. Organometallics, 2004, 23, 2956-2966.	1.1	26
823	Fundamental Reaction Pathways and Free-Energy Barriers for Ester Hydrolysis of Intracellular Second-Messenger 3',5'-Cyclic Nucleotide. Journal of Physical Chemistry A, 2004, 108, 3789-3797.	1.1	34
824	Theoretical Study on the Structures and Stability of SiC <sub>3</sub> P Isomers. Journal of Physical Chemistry A, 2004, 108, 11828-11837.	1.1	9
825	Complex Mechanism of the Gas Phase Reaction between Formic Acid and Hydroxyl Radical. Proton Coupled Electron Transfer versus Radical Hydrogen Abstraction Mechanisms. Journal of the American Chemical Society, 2004, 126, 9809-9820.	6.6	86
826	Theoretical Study of Nitrogen-Rich BeN <sub>4</sub> Compounds. Journal of Physical Chemistry A, 2004, 108, 665-670.	1.1	12
827	Theoretical Study of the Nucleophilic 5-Endo-Trigonal Cyclization of 1,1-Difluoro-1-alkenes. Journal of Organic Chemistry, 2004, 69, 4203-4209.	1.7	18
828	Analysis of two intramolecular proton transfer processes in terms of the reaction force. Journal of Chemical Physics, 2004, 121, 4570-4576.	1.2	78
829	On the Mechanisms of Oxidation of Organic Sulfides by H <sub>2</sub> O <sub>2</sub> in Aqueous Solutions. Journal of the American Chemical Society, 2004, 126, 900-908.	6.6	98
830	Rearrangement Reactions of the Transient Lewis Acids (CF <sub>3</sub> ) <sub>3</sub> B and (CF <sub>3</sub> ) <sub>3</sub> BCF <sub>2</sub> : An Experimental and Theoretical Study. Inorganic Chemistry, 2004, 43, 490-505.	1.9	60
831	An intrinsic reaction coordinate calculation of the torsion-internal rotation potential of hydrogen peroxide and its isotopomers. Journal of Chemical Physics, 2004, 121, 273.	1.2	9
832	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

#	ARTICLE	IF	CITATIONS
833	Theoretical Study of Thermal Isomerization of Silacyclobutene to Cyclopropene. <i>Organometallics</i> , 2004, 23, 4744-4749.	1.1	15
834	Dyotropic Rearrangements of Dihalogenated Hydrocarbons: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5649-5654.	1.1	20
835	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement: Mechanism, Torquoselectivity and Solvent Effects. <i>Journal of Organic Chemistry</i> , 2004, 69, 3635-3644.	1.7	35
836	FORMATION OF NOVEL RARE-GAS MOLECULES IN LOW-TEMPERATURE MATRICES. <i>Annual Review of Physical Chemistry</i> , 2004, 55, 55-78.	4.8	176
837	Accurate reaction paths using a Hessian based predictor-corrector integrator. <i>Journal of Chemical Physics</i> , 2004, 120, 9918-9924.	1.2	796
838	Photo-induced decomposition of organic peroxides: Ultrafast formation and decarboxylation of carbonyloxy radicals. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5441.	1.3	27
839	Mechanisms of Staudinger Reactions within Density Functional Theory. <i>Journal of Organic Chemistry</i> , 2004, 69, 4299-4308.	1.7	96
840	Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide. <i>Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 13-33.	1.0	12
841	Theoretical Study on the Transformation of Bis(acetylene)cobalt to Cobaltacyclopentadiene and the Regioselectivity in this Transformation. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 781-791.	2.0	55
842	Theoretical Study of the Formation of a Benzene Cobalt Complex from Cobaltacyclopentadiene and Acetylene. <i>Bulletin of the Chemical Society of Japan</i> , 2005, 78, 792-803.	2.0	61
843	Decomposition of Tertiary Alkoxy Radicals. <i>Zeitschrift Fur Physikalische Chemie</i> , 2005, 219, 1205-1222.	1.4	22
844	An ab initio molecular orbital study of the reduction of carbonyls by alkylaluminum complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 24, 195-202.	1.3	3
845	A new look at the nido-undecaborate system. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 2736-2744.	0.8	16
846	A quantum chemical study on the mechanism of S-coordinated tetrazole-thiolato formation by the reaction of organic isothiocyanates with metal azido complexes of Pt(II), Pd(II), and Sn. <i>Journal of Organometallic Chemistry</i> , 2005, 690, 4319-4329.	0.8	10
847	Theoretical studies of the reaction of hydroperoxy radicals (HO <sub>2</sub> ) with ethyl peroxy (CH <sub>3</sub> CH <sub>2</sub> O <sub>2</sub> ), acetyl peroxy (CH <sub>3</sub> C(O)O <sub>2</sub> ), and acetonyl peroxy (CH <sub>3</sub> C(O)CH <sub>2</sub> O <sub>2</sub> ) radicals. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 176, 218-230.	2.0	57
848	Density functional theory study of the 5-pyrrolidin-2-yltetrazole-catalyzed aldol reaction. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 2764-2770.	1.8	37
849	1,3-Dipolar cycloaddition of azomethine ylide with ethene and 2-butene: a computational study. <i>Tetrahedron Letters</i> , 2005, 46, 1993-1995.	0.7	8
850	Theoretical study on the mechanism of N-heterocyclic carbene catalyzed transesterification reactions. <i>Tetrahedron Letters</i> , 2005, 46, 6265-6270.	0.7	81

#	ARTICLE	IF	CITATIONS
851	Density functional complete study of hydrogen bonding between the dichlorine monoxide and the hydroxyl radical (Cl <sub>2</sub> O•HO). Computational and Theoretical Chemistry, 2005, 714, 7-12.	1.5	7
852	Computational experiment on hydroformylation and hydrogenation of propenal catalyzed by Rh complex: a competitive study. Computational and Theoretical Chemistry, 2005, 714, 61-72.	1.5	5
853	Computational experiment on hydroformylation and hydrogenation of ethyne catalyzed by Rh complex: a competitive study. Computational and Theoretical Chemistry, 2005, 714, 179-188.	1.5	4
854	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
855	Stability of the tin analogues of isocyanic acid, [HNSnO], and its isomers: a computational study. Computational and Theoretical Chemistry, 2005, 716, 199-205.	1.5	2
856	A potential route to the formation of alkylidene ligand from two mutually cis alkene ligands: a DFT study. Computational and Theoretical Chemistry, 2005, 718, 191-201.	1.5	8
857	Ab initio and DFT gas phase investigations of the C <sub>7</sub> H <sub>11</sub> <sup>+</sup> potential energy surfaces of bicyclobutonium species and related carbocations. Computational and Theoretical Chemistry, 2005, 718, 93-104.	1.5	7
858	Theoretical study on the ring-opening hydrolysis reaction of cAMP. Computational and Theoretical Chemistry, 2005, 719, 149-152.	1.5	3
859	Theoretical study of the OH reaction with cytosine. Computational and Theoretical Chemistry, 2005, 723, 123-129.	1.5	30
860	Theoretical study of the reactivity of X(3P) (X=Ge, Sn, Pb) with N <sub>2</sub> O(X11). Computational and Theoretical Chemistry, 2005, 724, 185-193.	1.5	9
861	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
862	Investigations of double proton transfer and one-electron oxidation behavior in double H-bonded glycine•formamide complex in the gas phase. Computational and Theoretical Chemistry, 2005, 726, 17-24.	1.5	2
863	Ab initio study of the thermal isomerization of quadricyclane to norbornadiene. Computational and Theoretical Chemistry, 2005, 728, 67-70.	1.5	12
864	Theoretical studies of oxygen atom transfer from flavin to electron-rich substrates. Computational and Theoretical Chemistry, 2005, 757, 175-181.	1.5	8
865	DFT study on the reaction mechanisms of polyfluorosulfonate ester with F•. Computational and Theoretical Chemistry, 2005, 730, 143-150.	1.5	1
866	Theoretical studies on neutral hydrolysis of N-benzyl 3-oxo-2-sultam. Computational and Theoretical Chemistry, 2005, 757, 61-68.	1.5	1
867	Theoretical study on insertion of silylenoid H <sub>2</sub> SiLiF into X•H bonds (X=CH <sub>3</sub> , SiH <sub>3</sub> , NH <sub>2</sub> , PH <sub>2</sub> , OH, SH and) Tj ETQq0 0 0 rgBT /Overlock	1.5	10
868	DFT study on the mechanisms of the CH <sub>2</sub> CO+NCX (X=O, S) reactions. Computational and Theoretical Chemistry, 2005, 757, 143-148.	1.5	11

#	ARTICLE	IF	CITATIONS
869	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. <i>Tetrahedron</i> , 2005, 61, 417-422.	1.0	33
870	Theoretical studies on formal hetero [3+3] cycloaddition reaction between vinylogous amide and $\beta,\gamma$ -unsaturated imine cation. <i>Tetrahedron</i> , 2005, 61, 5663-5669.	1.0	6
871	Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis. <i>Tetrahedron</i> , 2005, 61, 7538-7545.	1.0	20
872	A DFT study of the polar Diels-Alder reaction between 4-aza-6-nitrobenzofuroxan and cyclopentadiene. <i>Tetrahedron</i> , 2005, 61, 7359-7365.	1.0	57
873	Experimental and DFT study of the aza-Diels-Alder reaction between cyclopentadiene and protonated benzylimine derivated from glyoxylates. <i>Tetrahedron</i> , 2005, 61, 10951-10957.	1.0	25
874	Modeling of biliverdin reduction process: regio-specificity and H-bonding. <i>Chemical Physics</i> , 2005, 310, 179-187.	0.9	2
875	GaussDal: An open source database management system for quantum chemical computations. <i>Computer Physics Communications</i> , 2005, 171, 133-153.	3.0	4
876	Influence of C5-methylation of cytosine on the formation of cyclobutane pyrimidine dimers. <i>Chemical Physics Letters</i> , 2005, 401, 99-103.	1.2	21
877	A density-functional theory study on double-bond isomerization of 1-butene to cis-2-butene catalyzed by zeolites. <i>Chemical Physics Letters</i> , 2005, 404, 384-388.	1.2	23
878	From OBeHe to H3BOBeHe: Enhancing the stability of a neutral helium compound. <i>Chemical Physics Letters</i> , 2005, 406, 179-183.	1.2	43
879	Tautomerism of 1,3-diphospholes. <i>Chemical Physics Letters</i> , 2005, 406, 173-178.	1.2	7
880	The importance of tunneling effect to the decomposition of 2,2-dimethoxypropane and 2,2-diethoxypropane. <i>Chemical Physics Letters</i> , 2005, 406, 489-494.	1.2	3
881	Ab initio kinetic study on the low-energy paths of the HO+C2H4 reaction. <i>Chemical Physics Letters</i> , 2005, 408, 25-30.	1.2	52
882	A direct ab initio dynamics study of the initial decomposition steps of gas phase 1,3,3-trinitroazetidine. <i>Chemical Physics Letters</i> , 2005, 412, 317-321.	1.2	14
883	Does the Co <sup>+</sup> -assisted decarbonylation of acetaldehyde occur via C=C or C-H activation? A theoretical investigation using density functional theory. <i>Chemical Physics Letters</i> , 2005, 414, 28-33.	1.2	34
884	Direct dynamics studies on the isomerization and H2 elimination reactions of H3PS. <i>Chemical Physics Letters</i> , 2005, 415, 370-374.	1.2	9
885	Electrostatic control on endo/exo selectivity in ionic cycloaddition. <i>Chemical Physics Letters</i> , 2005, 416, 354-357.	1.2	5
886	Simulation of the isomerization of an anionic hydroxo complex of rhodium(V). <i>Mendeleev Communications</i> , 2005, 15, 81-83.	0.6	1



#	ARTICLE	IF	CITATIONS
887	Photoreaction of Skin-sensitizing Trimethyl Psoralen with Lipid Membrane Models. <i>Photochemistry and Photobiology</i> , 2005, 81, 1153.	1.3	7
888	Mechanistic Insights in Charge-Transfer-Induced Luminescence of 1,2-Dioxetanones with a Substituent of Low Oxidation Potential. <i>Journal of the American Chemical Society</i> , 2005, 127, 8667-8679.	6.6	109
889	Stereodynamics of bond rotation in tertiary 1-naphthoic acid amides: A computational study. <i>Journal of Computational Chemistry</i> , 2005, 26, 365-373.	1.5	2
890	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. <i>Journal of Computational Chemistry</i> , 2005, 26, 569-583.	1.5	27
891	Double proton transfer and one-electron oxidation behavior in double H-bonded glycine-glycine complex in the gas phase. <i>Journal of Computational Chemistry</i> , 2005, 26, 552-560.	1.5	1
892	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. <i>Journal of Computational Chemistry</i> , 2005, 26, 980-986.	1.5	50
893	The Formation of Silylated $\hat{1}^2$ -Lactams from Silylketenes through Lewis Acid Promoted [2+2] Cycloaddition: A Combined Theoretical and Experimental Study. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 2599-2606.	1.2	16
894	Unimolecular Fragmentation of $\text{CH}_3\text{NH}_2$ : Towards a Mechanistic Description of HCN Formation. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3304-3313.	1.2	9
895	Reactivity of 3-Styrylchromones as Dienes in Diels-Alder Reactions under Microwave Irradiation: A New Synthesis of Xanthenes. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 2973-2986.	1.2	19
896	Lewis Acid Induced [2+2] Cycloadditions of Silyl Enol Ethers with $\hat{1}^2$ -Unsaturated Esters: A DFT Analysis. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 3973-3979.	1.2	13
897	Lewis Acid Mediated Domino Reaction between 2-Cyclohexenone and Methyl Azide - A DFT Study. <i>European Journal of Organic Chemistry</i> , 2005, 2005, 4705-4709.	1.2	16
898	Tropone Is a Mere Ketone for Cycloadditions to Ketenes. <i>Helvetica Chimica Acta</i> , 2005, 88, 1519-1539.	1.0	19
899	Experimental and Computational Studies of the Phenyl Radical Reaction with Propyne. <i>ChemPhysChem</i> , 2005, 6, 2075-2085.	1.0	24
900	Generation of the Elusivemeta-Benzoquinone in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3092-3096.	7.2	25
901	Proton Sandwiches: Nonclassical Carbocations with Tetracoordinate Protons. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 2719-2723.	7.2	45
904	Kinetics and mechanisms for reactions of HNO with $\text{CH}_3$ and $\text{C}_6\text{H}_5$ studied by quantum-chemical and statistical-theory calculations. <i>International Journal of Chemical Kinetics</i> , 2005, 37, 261-274.	1.0	23
905	Gas-phase tautomers of protonated 1-methylcytosine. Preparation, energetics, and dissociation mechanisms. <i>Journal of Mass Spectrometry</i> , 2005, 40, 1417-1428.	0.7	25
906	A DFT-Based Theoretical Investigation of the Mechanism of the $\text{PtCl}_2$ -Mediated Cycloisomerization of Allenynes. <i>Chemistry - A European Journal</i> , 2005, 11, 521-533.	1.7	29

#	ARTICLE	IF	CITATIONS
907	Water-Catalyzed Dehalogenation Reactions of the Isomer of CBr <sub>4</sub> and Its Reaction Products and a Comparison to Analogous Reactions of the Isomers of Di- and Trihalomethanes. Chemistry - A European Journal, 2005, 11, 1093-1108.	1.7	18
908	Decomposition of Neutral, Singly and Doubly Protonated Benzoquinone in the Gas Phase. Chemistry - A European Journal, 2005, 11, 628-638.	1.7	21
909	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. Chemistry - A European Journal, 2005, 11, 1734-1738.	1.7	71
910	Functionalized Nanodiamonds Part I. An Experimental Assessment of Diamantane and Computational Predictions for Higher Diamondoids. Chemistry - A European Journal, 2005, 11, 7091-7101.	1.7	113
911	The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. Chemistry - A European Journal, 2005, 11, 6743-6753.	1.7	90
912	Preparation and Reactivity of [D <sub>3</sub> d]-Octahedrane: The Most Stable (CH) <sub>12</sub> Hydrocarbon. Chemistry - A European Journal, 2005, 11, 6175-6184.	1.7	29
913	Mechanistic Investigation of the 2,5-Diphenylpyrrolidine-Catalyzed Enantioselective $\hat{\pm}$ -Chlorination of Aldehydes. Chemistry - A European Journal, 2005, 11, 7083-7090.	1.7	76
914	One-dimensional models of internal rotation in CX <sub>3</sub> NO molecules (X=H, D, F). Journal of Molecular Spectroscopy, 2005, 230, 43-53.	0.4	0
915	Intramolecular rearrangement of organosilyl groups between oxygen and nitrogen in aminosiloxanes – a joint experimental–theoretical study, part II. Journal of Organometallic Chemistry, 2005, 690, 1100-1119.	0.8	7
916	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
917	Theoretical Study for Alcoholysis of N-Benzyl 3-Oxo- $\gamma$ -Sultam. Structural Chemistry, 2005, 16, 149-154.	1.0	2
918	Molecular mechanism of direct alkene oxidation with nitrous oxide: DFT analysis. Kinetics and Catalysis, 2005, 46, 177-188.	0.3	29
919	Lithiation of tricarbonylchromium complexes with polyaromatic carbo-and heterocyclic ligands. DFT study. Russian Chemical Bulletin, 2005, 54, 2055-2066.	0.4	1
920	Theoretical study of stabilizing function of the NO to the (CH <sub>3</sub> ) <sub>3</sub> CO $\hat{\cdot}$ radical. International Journal of Quantum Chemistry, 2005, 101, 113-117.	1.0	2
921	Interaction of singlet oxygen and superoxide radical anion with guanine and formation of its mutagenic modification 8-oxoguanine. International Journal of Quantum Chemistry, 2005, 102, 282-301.	1.0	24
922	Reactions of $\hat{\cdot}$ -OH with thymine studied using density functional theory. International Journal of Quantum Chemistry, 2005, 101, 211-218.	1.0	26
923	Potential energy surfaces in Coulomb explosion of polyatomic molecules: Benzene and cyclohexane trications and acetylene dication. International Journal of Quantum Chemistry, 2005, 102, 506-519.	1.0	19
924	Theoretical study of the ring-closing reaction of 5 $\hat{\cdot}$ -AMP to cAMP and H <sub>2</sub> O in the gas phase. International Journal of Quantum Chemistry, 2005, 104, 373-378.	1.0	1

#	ARTICLE	IF	CITATIONS
925	Theoretical study of the mechanism for spin-forbidden quenching process $O(1D) + CO_2(1\hat{\Sigma}+g) \hat{\rightarrow} O(3P) + CO_2(1\hat{\Sigma}+g)$ . International Journal of Quantum Chemistry, 2005, 105, 154-159.	1.0	1
926	Relative energies, stereoelectronic interactions and conformational interconversions in silathiacyclohexanes. Journal of Physical Organic Chemistry, 2005, 18, 35-48.	0.9	15
927	The role of the transfer group in the intramolecular [5+2] cycloadditions of substituted $\hat{1}^2$ -hydroxy- $\hat{1}^3$ -pyrones: a DFT analysis. Journal of Physical Organic Chemistry, 2005, 18, 610-615.	0.9	8
928	Acetylene Cyclotrimerization by Early Second-Row Transition Metals in the Gas Phase. A Theoretical Study. Inorganic Chemistry, 2005, 44, 9807-9816.	1.9	36
929	Reaction Processes of Germane Molecules with Catalytic Water. Japanese Journal of Applied Physics, 2005, 44, 4133-4141.	0.8	2
930	A 193nm laser photofragmentation time-of-flight mass spectrometric study of chloriodomethane. Journal of Chemical Physics, 2005, 123, 174316.	1.2	9
931	CS <sub>2</sub> O <sup>+</sup> and CS <sub>2</sub> O in the gas phase: An experimental and computational study. Journal of Chemical Physics, 2005, 123, 164307.	1.2	1
932	Ab initio kinetics of the reaction of HCO with NO: Abstraction versus association/elimination mechanism. Journal of Chemical Physics, 2005, 122, 234308.	1.2	19
933	Computational study of the reaction of N(D <sub>2</sub> ) atoms with CH <sub>2</sub> F radicals: An example of a barrier-free reaction involving very high internal energies. Journal of Chemical Physics, 2005, 123, 114312.	1.2	29
934	The all-Cartesian reaction plane Hamiltonian: Formulation and application to the H-atom transfer in tropolone. Journal of Chemical Physics, 2005, 123, 054315.	1.2	33
935	Reaction path determination for quantum mechanical/molecular mechanical modeling of enzyme reactions by combining first order and second order $\hat{\omega}$ chain-of-replicas $\hat{\omega}$ methods. Journal of Chemical Physics, 2005, 122, 114502.	1.2	36
936	The potential energy landscape of noradrenaline: An electronic structure study. Molecular Physics, 2005, 103, 1641-1654.	0.8	14
937	Rate theory of yield in boron nitride nanotubes. Physical Review B, 2005, 72, .	1.1	45
938	COMPUTATIONAL STUDIES OF THE AMMONOLYSIS FOR N-METHYL $\hat{1}^2$ -SULTAM. Journal of Theoretical and Computational Chemistry, 2005, 04, 383-395.	1.8	1
939	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
940	A Theoretical Study on the Reaction Mechanism for the Bergman Cyclization from the Perspective of the Electron Localization Function and Catastrophe Theory. Journal of Physical Chemistry A, 2005, 109, 3687-3693.	1.1	57
941	Cyano- and Isocyanotris(trifluoromethyl)borates: Syntheses, Spectroscopic Properties, and Solid State Structures of K[(CF <sub>3</sub> ) <sub>3</sub> BCN] and K[(CF <sub>3</sub> ) <sub>3</sub> BNC]. Journal of the American Chemical Society, 2005, 127, 10712-10722.	6.6	59
942	Theoretical Insight into the C $\hat{\sigma}$ -C Coupling Reactions of the Vinyl, Phenyl, Ethynyl, and Methyl Complexes of Palladium and Platinum. Organometallics, 2005, 24, 715-723.	1.1	164

#	ARTICLE	IF	CITATIONS
943	Protic Conversion of Nitrile into Azavinylidene Complexes of Rhenium, a Mechanistic Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8187-8198.	1.1	14
944	Global Investigation on the Potential Energy Surface of CH <sub>3</sub> CN: Application of the Scaled Hypersphere Search Method. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7319-7328.	1.1	57
945	On Possible Pitfalls in ab Initio Quantum Mechanics/Molecular Mechanics Minimization Approaches for Studies of Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15645-15650.	1.2	164
946	Theoretical Studies on the Intramolecular Hydrogen Bond and Tautomerism of 8-Mercaptoquinoline in the Gaseous Phase and in Solution Using Modern DFT Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4137-4148.	1.1	34
947	Dynamics of the Staudinger Reaction. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 353-362.	2.3	23
948	Influence of the number of water molecules on the mechanism of N-sulfinylaniline hydrolysis. <i>Canadian Journal of Chemistry</i> , 2005, 83, 1588-1596.	0.6	5
949	Reaction mechanism and kinetics of the NCN+NO reaction: Comparison of theory and experiment. <i>Journal of Chemical Physics</i> , 2005, 122, 184321.	1.2	18
950	Mechanistic and kinetic study of the O + CH <sub>3</sub> OCH <sub>2</sub> reaction and the unimolecular decomposition of CH <sub>3</sub> OCH <sub>2</sub> O. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3980.	1.3	18
951	Theoretical Study of the Mechanism of Hydrogenation of Side-On Coordinated Dinitrogen Activated by Zr Binuclear Complexes ([( <i>i</i> -5-C <sub>5</sub> Me <sub>4</sub> H) <sub>2</sub> Zr] <sub>2</sub> ( <i>l</i> <sub>1</sub> /4,2, <i>l</i> <sub>2</sub> , <i>l</i> <sub>2</sub> -N <sub>2</sub> )). <i>Journal of Physical Chemistry A</i> , 2005, 109, 8800-8808.	1.1	32
952	Computation of Photochemical Reaction Mechanisms in Organic Chemistry. <i>Theoretical and Computational Chemistry</i> , 2005, 16, 191-223.	0.2	9
953	Ab initio and density functional theory study of lead complexes of atmospheric interest Pb(H <sub>2</sub> ), Pb(OH), Pb(H <sub>2</sub> O), Pb(HO <sub>2</sub> ) and Pb(OH) <sub>2</sub> . <i>Molecular Physics</i> , 2005, 103, 317-335.	0.8	15
954	Carbonate, carbamate, urea, and guanidine as model species for functional groups in biological molecules— A combined density functional theory and mass spectrometry examination of polysodiation and gas-phase dissociation. <i>Canadian Journal of Chemistry</i> , 2005, 83, 1941-1952.	0.6	7
955	The Reaction of Phenyl Radical with Molecular Oxygen: A G <sub>2</sub> M Study of the Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6114-6127.	1.1	126
956	The Kinetics of the Reactions of C <sub>2</sub> (a <sup>3</sup> Σ <sub>g</sub> <sup>-</sup> ) with Alcohols. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3921-3925.	1.1	10
957	Theoretical Study of Cisplatin Binding to DNA: The Importance of Initial Complex Stabilization. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11006-11015.	1.2	104
958	A Computational Study of the Reaction of Ground-State Nitrogen Atoms with Chloromethyl Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6540-6548.	1.1	4
959	Solvent-Assisted New Reaction Pathways for the (THF)W(CO) <sub>5</sub> -Promoted endo- and exo-Cycloisomerization of 4-Pentyn-1-ol: A Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 2005, 127, 944-952.	6.6	47
960	G <sub>3</sub> (MP <sub>2</sub> ) Study of the C <sub>3</sub> H <sub>6</sub> O+ Isomers Fragmented from 1,4-Dioxane. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7296-7308.	1.1	1

#	ARTICLE	IF	CITATIONS
961	SN2-like Reaction in Hydrogen-Bonded Complexes: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9353-9355.	1.1	1
962	Dissociation of Benzene Dication [C <sub>6</sub> H <sub>6</sub> ] <sup>2+</sup> : Exploring the Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11551-11559.	1.1	27
963	Spin-Coupled Study of the Electronic Mechanism of the Hetero-Diels-Alder Reaction of Acrolein and Ethene. <i>Journal of Physical Chemistry A</i> , 2005, 109, 231-235.	1.1	10
964	Potential Energy Surfaces of SimOnCluster Formation and Isomerization. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6294-6302.	1.1	37
965	Surface SN2 Reaction by H <sub>2</sub> O on Chlorinated Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 10909-10914.	1.2	7
966	A theoretical study of the structures and stabilities of N <sub>4</sub> O <sub>2</sub> isomers. <i>Molecular Physics</i> , 2005, 103, 249-256.	0.8	0
967	Water-Catalyzed O-H Insertion/HI Elimination Reactions of Isodihalomethanes (CH <sub>2</sub> X <sup>n</sup> I, Where X = Cl, F) of Physical Chemistry A, 2005, 109, 981-998.	1.1	22
968	Glycolaldehyde + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. <i>Journal of Physical Chemistry A</i> , 2005, 109, 169-180.	1.1	65
969	Thiolysis and Alcoholysis of Phosphate Tri- and Monoesters with Alkyl and Aryl Leaving Groups. An ab Initio Study in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5625-5635.	1.1	35
970	Insertion Reactions of Silylenoid Ph <sub>2</sub> SiLi(OBu-t) into X-H Bonds (X = F, OH, and NH <sub>2</sub> ). <i>Journal of Physical Chemistry A</i> , 2005, 109, 10563-10570.	1.1	7
971	Computational Study on the Mechanism and Rate Constant for the C <sub>6</sub> H <sub>5</sub> + C <sub>6</sub> H <sub>5</sub> NO Reaction. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9054-9060.	1.1	9
972	Experimental and Theoretical Studies of the C <sub>2</sub> F <sub>4</sub> + O Reaction: Nonadiabatic Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9786-9794.	1.1	7
973	Synthesis of β-Lactams by Ag <sup>+</sup> -Induced Ring Expansion of 1-Hydroxycyclopropylamines: A Theoretical Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7822-7831.	1.1	2
974	Comparative DFT Study of the Spin Trapping of Methyl, Mercapto, Hydroperoxy, Superoxide, and Nitric Oxide Radicals by Various Substituted Cyclic Nitrones. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1662-1674.	1.1	36
975	Solvent Effects on the SN2 Reaction: Application of the Density Functional Theory-Based Effective Fragment Potential Method. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1629-1636.	1.1	71
976	Dichlorocarbene Addition to Cyclopropenes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 1630-1635.	1.7	27
977	Comparative Study of Surface Cycloadditions of Ethylene and 2-Butene on the Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5067-5072.	1.2	23
978	New Selective Haloform-type Reaction Yielding 3-Hydroxy-2,2-difluoroacids: A Theoretical Study of the Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 2620-2627.	6.6	12

#	ARTICLE	IF	CITATIONS
979	Quantum Chemical and Master Equation Simulations of the Oxidation and Isomerization of Vinyloxy Radicals. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2514-2524.	1.1	43
980	Modeling Multiple Species of Nicotine and Deschloroepibatidine Interacting with $\pm 4^2$ Nicotinic Acetylcholine Receptor: A From Microscopic Binding to Phenomenological Binding Affinity. <i>Journal of the American Chemical Society</i> , 2005, 127, 14401-14414.	6.6	46
981	Mechanism of Cycloaddition Reactions between Ketene and N-Silyl-, N-Germyl-, and N-Stannylimines: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11022-11026.	1.1	9
982	A Possible Mechanism for Furan Formation in the Tropospheric Oxidation of Dienes. <i>Environmental Science &amp; Technology</i> , 2005, 39, 8797-8802.	4.6	22
983	Mechanistic and Kinetic Study of the O + CH <sub>2</sub> OH Reaction. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4796-4803.	1.1	11
984	Thermal Decomposition of Ethylene Oxide: A Potential Energy Surface, Master Equation Analysis, and Detailed Kinetic Modeling. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8016-8027.	1.1	38
985	Reactions of Methane with Hafnium Atoms: $\text{CH}_2\text{HfH}_2$ , Agostic Bonding, and $(\text{CH}_3)_2\text{HfH}_2$ . <i>Organometallics</i> , 2005, 24, 2854-2861.	1.1	42
986	On the Pyrolysis Mechanism of 2-Pyranones and 2-Pyranthiones: A Thermally Induced Ground Electronic State Chemistry of Pyran-2-thione. <i>Journal of Organic Chemistry</i> , 2005, 70, 7701-7710.	1.7	14
987	Theoretical Determinations of the Ambient Conformational Distribution and Unimolecular Decomposition of n-Propylperoxy Radical. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3637-3646.	1.1	36
988	The Kinetics of Addition and Fragmentation in Reversible Addition Fragmentation Chain Transfer Polymerization: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1230-1239.	1.1	88
989	Computational <sup>59</sup> Co NMR Spectroscopy: Beyond Static Molecules. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 181-193.	2.3	30
990	Computational Study of the $\sigma$ -Stable $\sigma$ -Bis(amino)silylene Reaction with Halomethanes. A Radical or Concerted Mechanism?. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3728-3738.	1.1	14
991	Mechanistic Insights into the Bazarov Synthesis of Urea from NH <sub>3</sub> and CO <sub>2</sub> Using Electronic Structure Calculation Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8560-8567.	1.1	43
992	A Comparison of the Cope Rearrangements of cis-1,2-Divinyloxypropane, cis-2,3-Divinyloxyaziridine, cis-2,3-Divinyloxirane, cis-2,3-Divinylophosphirane, and cis-2,3-Divinylothiirane: A DFT Study. <i>Journal of Organic Chemistry</i> , 2005, 70, 6018-6026.	1.7	34
993	Density Functional Theoretical Study of a Series of Binary Azides M(N <sub>3</sub> ) <sub>n</sub> (n = 3, 4). <i>Journal of Physical Chemistry A</i> , 2005, 109, 9089-9094.	1.1	20
994	Computational Study on the Reaction CH <sub>2</sub> CH <sub>2</sub> + F $\rightarrow$ CH <sub>2</sub> CHF + H. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4816-4823.	1.1	23
995	Theoretical Study of General Base-Catalyzed Hydrolysis of Aryl Esters and Implications for Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5259-5266.	1.2	11
996	Theoretical Study of the Suicide Inhibition Mechanism of the Enzyme Pyruvate Formate Lyase by Methacrylate. <i>Journal of the American Chemical Society</i> , 2005, 127, 6902-6909.	6.6	8

#	ARTICLE	IF	CITATIONS
997	Cycloaddition Isomerizations of Adsorbed 1,3-Cyclohexadiene on Si(100)-2 $\times$ 1 Surface: First Neighbor Interactions. <i>Journal of the American Chemical Society</i> , 2005, 127, 8485-8491.	6.6	17
998	Modeling $\hat{I}^2$ -Scission Reactions of Peptide Backbone Alkoxy Radicals: $\hat{A}$ Backbone C $\hat{a}$ -C Bond Fission. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 889-899.	2.3	6
999	Using Hessian Updating To Increase the Efficiency of a Hessian Based Predictor-Corrector Reaction Path Following Method. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 61-69.	2.3	810
1000	Predicted High-Energy Molecules: $\hat{A}$ Helical All-Nitrogen and Helical Nitrogen-Rich Ring Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3241-3243.	1.1	23
1001	Time-resolved gas-phase kinetic and quantum chemical studies of the reaction of silylene with oxygen. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2900.	1.3	30
1002	The effects of substrate orientation on the mechanism of a phosphotriesterase. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 4343.	1.5	32
1003	O-Atom Transport Catalysis by Atomic Cations in the Gas Phase: $\hat{A}$ Reduction of N <sub>2</sub> O by CO. <i>Journal of the American Chemical Society</i> , 2005, 127, 3545-3555.	6.6	136
1004	The Final Catalytic Step of Cytochrome P450 Aromatase: $\hat{a}$ A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 5224-5237.	6.6	103
1005	N <sub>4</sub> Ring as a Square Planar Ligand in Novel MN <sub>4</sub> Species. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3182-3186.	1.1	20
1006	Hydrogen Abstraction Acetylene Addition and Diels $\hat{a}$ Alder Mechanisms of PAH Formation: $\hat{A}$ A Detailed Study Using First Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 908-924.	2.3	141
1007	Reactivity of Metaphosphate and Thiometaphosphate in Water: $\hat{a}$ A DFT Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11295-11303.	1.1	14
1008	Theoretical Studies of Dissociative Phosphoryl Transfer in Interconversion of Phosphoenolpyruvate to Phosphonopyruvate: $\hat{A}$ Solvent Effects, Thio Effects, and Implications for Enzymatic Reactions. <i>Journal of Physical Chemistry B</i> , 2005, 109, 13827-13834.	1.2	20
1009	Interaction of lead atom with atmospheric dioxygen and ozone: Quantic study of the structure and the stability of resulting Pb(On) (n=1,2,3) compounds. <i>Journal of Chemical Physics</i> , 2005, 122, 154304.	1.2	16
1010	Two Separable Conformers of TATP and Analogues Exist at Room Temperature. <i>Organic Letters</i> , 2005, 7, 2461-2464.	2.4	60
1011	A Fast Radical Chain Mechanism in the Polyfluoroalkoxylation of Aromatics through NO <sub>2</sub> Group Displacement. Mechanistic and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2005, 70, 1718-1727.	1.7	29
1012	Kinetics of the Hydrogen Abstraction $\hat{a}$ CH <sub>3</sub> + Alkane $\hat{a}$ CH <sub>4</sub> + Alkyl Reaction Class: $\hat{A}$ An Application of the Reaction Class Transition State Theory. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7742-7750.	1.1	57
1013	Double proton transfer reactions at the transition from a concerted to a stepwise mechanism: a comparative ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 493.	1.3	18
1014	Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces. , 2005, , 195-249.		266

#	ARTICLE	IF	CITATIONS
1015	Quantum Chemical and Master Equation Studies of the Methyl Vinyl Carbonyl Oxides Formed in Isoprene Ozonolysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10710-10725.	1.1	56
1016	C-H Bond Activation of Methane Promoted by (Î-5-Phospholyl)Rh(CO) <sub>2</sub> : A Theoretical Perspective. <i>Organometallics</i> , 2005, 24, 2262-2268.	1.1	12
1017	Theoretical Study of the Highly Diastereoselective 1,3-Dipolar Cycloaddition of 1,4-Dihydropyridine-Containing Azomethine Ylides to [60]Fullerene (Prato's Reaction). <i>Journal of Organic Chemistry</i> , 2005, 70, 3256-3262.	1.7	36
1018	SYNTHESIS AND THEORETICAL CALCULATIONS OF THE 1H-PYRAZOLE-3-CARBOXAMIDE AND -3-CARBOXYLATE DERIVATIVES. <i>Heterocyclic Communications</i> , 2005, 11, .	0.6	1
1019	Energetics of Xylose Decomposition as Determined Using Quantum Mechanics Modeling. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11824-11838.	1.1	140
1020	Dimerization and Double Proton Transfer-Induced Tautomerism of 4(3H)-Pyrimidinone in Solution Studied by IR Spectroscopy and Quantum Chemical Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 26388-26395.	1.2	12
1021	Reaction Mechanism between Carbonyl Oxide and Hydroxyl Radical: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4001-4011.	1.1	29
1022	Unusual Solvent Effect on a SN2 Reaction. A Quantum-Mechanical and Kinetic Study of the Menshutkin Reaction between 2-Amino-1-methylbenzimidazole and Iodomethane in the Gas Phase and in Acetonitrile. <i>Journal of Physical Chemistry B</i> , 2006, 110, 1877-1888.	1.2	20
1023	Does the Decomposition of Peroxydicarbonates and Diacyl Peroxides Proceed in a Stepwise or Concerted Pathway?. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2448-2454.	1.1	11
1024	Kinetic and Theoretical Studies on the Mechanism of Intramolecular Catalysis in Phenyl Ester Hydrolysis. <i>Journal of Organic Chemistry</i> , 2006, 71, 7650-7656.	1.7	15
1025	Theoretical Studies of the Transition-State Structures and Free Energy Barriers for Base-Catalyzed Hydrolysis of Amides. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12644-12652.	1.1	56
1026	Theoretical Mechanistic Study on the Radical-Radical Reaction of Ketenyl with Nitrogen Dioxide. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2527-2534.	1.1	9
1027	How are the ready and unready states of nickel-iron hydrogenase activated by H <sub>2</sub> ? A density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4086-4094.	1.3	20
1028	Oxygen insertion in a carbon-phosphorus bond of the phenylethynyl-di-(tert-butyl)-phosphine bridged dicobalt complex: exploring the nature of oxygen migration using DFT. <i>Dalton Transactions</i> , 2006, , 5454-5463.	1.6	3
1029	Kinetics and mechanism of the Î <sup>2</sup> -alanine + OH gas phase reaction: A quantum mechanical approach. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 285-292.	1.3	15
1030	Protonolysis of the Hg-C Bond of Chloromethylmercury and Dimethylmercury. A DFT and QTAIM Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9451-9458.	1.1	41
1031	Mechanistic Insights into the Reaction between VO <sub>2</sub> <sup>+</sup> and Propene Based on a DFT Study. <i>Organometallics</i> , 2006, 25, 1643-1653.	1.1	28
1032	Effect of the Metal Fragment in the Thermal Cycloaddition between Alkynyl Metal(0) Fischer Carbene Complexes and Nitrones. <i>Journal of Organic Chemistry</i> , 2006, 71, 6178-6184.	1.7	43



#	ARTICLE	IF	CITATIONS
1033	Nonradical Mechanisms for the Uncatalyzed Thermal Functionalization of Silicon Surfaces by Alkenes and Alkynes: A Density Functional Study. <i>Langmuir</i> , 2006, 22, 9949-9956.	1.6	46
1034	Better Understanding of the Ring-Cleavage Process of Cyanocyclopropyl Anionic Derivatives. A Theoretical Study Based on the Electron Localization Function. <i>Journal of Organic Chemistry</i> , 2006, 71, 754-762.	1.7	24
1035	Mechanism of Remote Conjugate Addition of Lithium Organocuprates to Polyconjugated Carbonyl Compounds. <i>Chemistry - an Asian Journal</i> , 2006, 1, 322-330.	1.7	29
1036	Stability and Thermal Rearrangement of (E,E)-1,3-Cycloheptadiene and trans-Bicyclo[3.2.0]hept-6-ene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2034-2038.	1.1	5
1037	Theoretical Study on the Decomposition of DMP and DEP in Condensed Phase: Solvent Effect and Tunneling Effect. <i>Acta Physico-chimica Sinica</i> , 2006, 22, 1047-1051.	0.6	3
1038	Reaction Mechanism and Tautomeric Equilibrium of 2-Mercaptopyrimidine in the Gas Phase and in Aqueous Solution: A Combined Monte Carlo and Quantum Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7253-7261.	1.1	42
1039	A computational study on the amine-oxidation mechanism of monoamine oxidase: Insight into the polar nucleophilic mechanism. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 646.	1.5	54
1040	Modeling the Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8979-8985.	1.1	35
1041	Theoretical Study of Reactant Activation in 1,3-Dipolar Cycloadditions of Cyclic Nitrones to Free and Pt-Bound Nitriles. <i>Journal of Organic Chemistry</i> , 2006, 71, 582-592.	1.7	52
1042	Stability and Electronic Properties of Nitrogen Nanoneedles and Nanotubes. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1965-1971.	2.5	13
1043	The oxidized soot surface: Theoretical study of desorption mechanisms involving oxygenated functionalities and comparison with temperature programmed desorption experiments. <i>Journal of Chemical Physics</i> , 2006, 125, 194706.	1.2	37
1044	Density functional theory and atoms-in-molecule study on the role of two-electron stabilizing interactions in retro Diels-Alder reaction of cycloadducts derived from substituted cyclopentadiene and p-benzoquinone. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 3923-3930.	1.5	10
1045	Analysis of the Reaction Force for a Gas Phase SN2 Process: $\text{CH}_3\text{Cl} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH} + \text{HCl}$ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 756-761.	1.1	59
1046	Theoretical Determination of the Rate Constant for OH Hydrogen Abstraction from Toluene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10155-10162.	1.1	69
1047	Study of the Carbon-13 and Deuterium Kinetic Isotope Effects in the Cl and OH Reactions of CH <sub>4</sub> and CH <sub>3</sub> Cl. <i>Journal of Physical Chemistry A</i> , 2006, 110, 141-152.	1.1	33
1048	Multicoordinate Driven Method for Approximating Enzymatic Reaction Paths: Automatic Definition of the Reaction Coordinate Using a Subset of Chemical Coordinates. <i>Journal of Physical Chemistry A</i> , 2006, 110, 772-778.	1.1	51
1049	Mechanistic Aspects of Proton Chain Transfer: A Computational Study for the Green Fluorescent Protein Chromophore. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5084-5093.	1.2	24
1050	Quantum Chemical and Statistical Rate Study of the Reaction of O(3P) with Allene: O-Addition and H-Abstraction Channels. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12166-12176.	1.1	24

#	ARTICLE	IF	CITATIONS
1051	Thermodynamic Functions of Conformational Changes: Conformational Network of Glycine Diamide Folding, Entropy Lowering, and Informational Accumulation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13325-13331.	1.1	8
1052	Reactions of endo-3-Diazotricyclo[3.2.1.0 <sup>2,4</sup> ]oct-6-ene, a Potential Precursor for the Generation of a Neutral C <sub>8</sub> H <sub>8</sub> Molecule with a Pyramidally Coordinated Carbon. <i>Journal of Organic Chemistry</i> , 2006, 71, 6975-6982.	1.7	7
1053	Is NO <sub>3</sub> Formed during the Decomposition of Nitramine Explosives?. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13974-13978.	1.1	24
1054	Theoretical Investigation of Luminescence Behavior as a Function of Alkyl Chain Size in 4-Aminobenzonitrile Alicyclic Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11455-11461.	1.1	36
1055	H-Atom Abstraction from CH <sub>3</sub> NHNH <sub>2</sub> by NO <sub>2</sub> : CCSD(T)/6-311++G(3df,2p)//MPWB1K/6-31+G(d,p) and CCSD(T)/6-311+G(2df,p)//CCSD/6-31+G(d,p) Calculations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6129-6138.	1.1	27
1056	Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase: Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1982-1990.	1.1	33
1057	Searching for Saddle Points by Using the Nudged Elastic Band Method: An Implementation for Gas-Phase Systems. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 895-904.	2.3	33
1058	A Barrier-Free Atomic Radical-Molecule Reaction: F + Propene. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1551-1564.	2.3	19
1059	Pentacoordinate 1H-Phosphirenes: Reactivity, Bonding Properties, and Substituent Effects on Their Structures and Thermal Stability. <i>Journal of Organic Chemistry</i> , 2006, 71, 5448-5456.	1.7	13
1060	On the Surface-Catalyzed Reaction between the Gases 2,2-Dimethylpropanal and Methanamine. Formation of Active-Site Imines. <i>Journal of Organic Chemistry</i> , 2006, 71, 3435-3443.	1.7	11
1061	Efficient Photochemical Merocyanine-to-Spiropyran Ring Closure Mechanism through an Extended Conical Intersection Seam. A Model CASSCF/CASPT2 Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3986-3991.	1.1	45
1062	Quantum Chemical and Theoretical Kinetics Study of the O(3P) + C <sub>2</sub> H <sub>2</sub> Reaction: A Multistate Process. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6696-6706.	1.1	48
1063	Adsorption Reactions of Dimethylaluminum Isopropoxide and Water on the H/Si(100)-2 × 1 Surface: Initial Reactions for Atomic Layer Deposition of Al <sub>2</sub> O <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2006, 110, 11277-11283.	1.2	18
1064	A Theoretical Study of the Reaction of O(3P) with Isobutene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7858-7866.	1.1	25
1065	Ab Initio Kinetics for the Unimolecular Reaction C <sub>6</sub> H <sub>5</sub> OH + CO + C <sub>5</sub> H <sub>6</sub> . <i>Journal of Physical Chemistry A</i> , 2006, 110, 1672-1677.	1.1	55
1066	Reactivity of the CHBr <sub>2</sub> <sup>+</sup> Dication toward Molecular Hydrogen. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6447-6453.	1.1	19
1067	Reaction Mechanism of Deamidation of Asparaginyl Residues in Peptides: Effect of Solvent Molecules. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8354-8365.	1.1	60
1068	Double Proton Transfer Reactions with Plateau-Like Transition State Regions: Pyrazole-Trifluoroacetic Acid Clusters. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2816-2820.	1.1	11

#	ARTICLE	IF	CITATIONS
1069	Water-Catalyzed Hydrolysis of the Radical Cation of Ketene in the Gas Phase: A Theory and Experiment. Journal of Physical Chemistry A, 2006, 110, 8266-8274.	1.1	12
1070	A Theoretical Study of Rhodium(I) Catalyzed Carbonylative Ring Expansion of Aziridines to $\beta$ -Lactams: A Crucial Activation of the Breaking C-N Bond by Hyperconjugation. Journal of Organic Chemistry, 2006, 71, 7315-7321.	1.7	31
1071	Aromatic Hydrocarbon Nitration under Tropospheric and Combustion Conditions. A Theoretical Mechanistic Study. Journal of Physical Chemistry A, 2006, 110, 13270-13282.	1.1	19
1072	Rozen's Epoxidation Reagent, $\text{CH}_3\text{CN}\cdot\text{HOF}$ : A Theoretical Study of Its Structure, Vibrational Spectroscopy, and Reaction Mechanism. Journal of Physical Chemistry A, 2006, 110, 8275-8281.	1.1	9
1073	The Reaction of Nitrogen Atoms with Methyl Radicals: Are Spin-Forbidden Channels Important? Journal of Physical Chemistry A, 2006, 110, 10912-10920.	1.1	17
1074	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396.	1.7	39
1075	Empirical Valence-Bond Models for Reactive Potential Energy Surfaces Using Distributed Gaussians. Journal of Chemical Theory and Computation, 2006, 2, 905-911.	2.3	62
1076	Mechanistic Study of the $\text{CH}_3\text{O}_2\cdot + \text{HO}_2\cdot \rightarrow \text{CH}_3\text{O}_2\text{H} + \text{O}_2$ Reaction in the Gas Phase. Computational Evidence for the Formation of a Hydrogen-Bonded Diradical Complex. Journal of Physical Chemistry A, 2006, 110, 6073-6082.	1.1	58
1077	The Loss of Carbon Dioxide from Activated Perbenzoate Anions in the Gas Phase: Unimolecular Rearrangement via Epoxidation of the Benzene Ring. Journal of Organic Chemistry, 2006, 71, 7996-8005.	1.7	19
1078	Isopropylcyclopropane + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. Journal of Physical Chemistry A, 2006, 110, 1917-1924.	1.1	17
1079	A Combined Density Functional Theory and Coupled Cluster Method Investigation of the Structural Properties and Stabilities of Radical $\text{CH}_2\text{CP}$ and Its Isomers. Journal of Physical Chemistry A, 2006, 110, 2411-2420.	1.1	1
1080	Direct Dynamics Study on the Reaction of $\text{N}_2\text{H}_4$ with F Atom: A Hydrogen Abstraction Reaction? Journal of Physical Chemistry A, 2006, 110, 11636-11644.	1.1	6
1081	On the Origin of the Stereoselectivity in the Alkylation of Oxazolopiperidone Enolates. Journal of the American Chemical Society, 2006, 128, 6581-6588.	6.6	17
1082	Origin of Rotational Barriers of the N-N Bond in Hydrazine: NBO Analysis. Journal of Physical Chemistry A, 2006, 110, 2065-2071.	1.1	10
1083	Theoretical Study of the Antioxidant Properties of Pyridoxine. Journal of Physical Chemistry A, 2006, 110, 13068-13072.	1.1	77
1084	Collision-Induced Dissociation of $\text{HS}^-(\text{HCN})$ : Unsymmetrical Hydrogen Bonding in a Proton-Bound Dimer Anion. Journal of Physical Chemistry A, 2006, 110, 1342-1349.	1.1	13
1085	Mechanism of Triplet Photosensitized Diels-Alder Reaction between Indoles and Cyclohexadienes: Theoretical Support for an Adiabatic Pathway. Journal of Organic Chemistry, 2006, 71, 6932-6941.	1.7	23
1086	Two-Metal-Ion Mechanism for Hammerhead-Ribozyme Catalysis. Journal of Physical Chemistry B, 2006, 110, 3395-3409.	1.2	34

#	ARTICLE	IF	CITATIONS
1087	A DFT Study on the Thermal Aryl Migration in Aryliodonium Ylides. Support for a Concerted Mechanism. <i>Journal of Organic Chemistry</i> , 2006, 71, 7060-7062.	1.7	26
1088	Structural Properties and Dynamics of Five-Coordinate Nickel(II)-Allyl Complexes Containing Monodentate Phosphorus Ligands. <i>Organometallics</i> , 2006, 25, 2308-2330.	1.1	12
1089	Theoretical Study of Electronic Structures of [Peroxoporphinato]manganate [Mn(P)(O <sub>2</sub> )] <sup>-</sup> Anion. <i>Bulletin of the Chemical Society of Japan</i> , 2006, 79, 1201-1210.	2.0	5
1090	Structures and stabilities of the donor-acceptor complexes HXPY (X=Al, B; Y=H, F, OH). <i>Molecular Physics</i> , 2006, 104, 447-452.	0.8	3
1091	Automatic integration of the reaction path using diagonally implicit Runge-Kutta methods. <i>Journal of Chemical Physics</i> , 2006, 125, 244108.	1.2	9
1092	Ab initio quantum chemical studies of reaction mechanism for CN with CH <sub>2</sub> CO. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1076-1085.	1.0	4
1093	Theoretical studies of the hydrolysis reaction of 5'-AMP. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1870-1877.	1.0	0
1094	Comment on "Relative Energies, Stereoelectronic Interactions, and Conformational Interconversion in Silacycloalkanes". <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1975-1978.	1.0	27
1095	Ab initio MO study of potential energy surface of NH <sub>2</sub> with CN reaction. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1827-1843.	1.0	6
1096	Kinetics and structural aspects of the cisplatin interactions with guanine: A quantum mechanical description. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2129-2144.	1.0	35
1097	Singlet-triplet gaps and insertion reactions of aminocyanocarbenes: A computational study of hydrogen cyanide covalent dimers. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2379-2389.	1.0	6
1098	[2,3]-sigmatropic rearrangements of hydrogen and alkyl 3-propenyl sulfoxides: A computational study. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2390-2397.	1.0	8
1099	Electronic structure study of the reaction C <sub>2</sub> H <sub>4</sub> <sup>+</sup> → C <sub>2</sub> H <sub>2</sub> <sup>+</sup> + H <sub>2</sub> . <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2763-2771.	1.0	6
1100	Transition states for deactivation reactions in the modeled 2,2,6,6-tetramethyl-1-piperidinyloxy-mediated free-radical polymerization of acrylonitrile. <i>Journal of Polymer Science Part A</i> , 2006, 44, 914-927.	2.5	15
1101	Theoretical study on the reaction of silylenoid H <sub>2</sub> SiLiF with HF. <i>Chemical Physics</i> , 2006, 323, 185-192.	0.9	6
1102	Theoretical study of intermolecular proton transfer reaction in isolated 5-hydroxyisoxazole-water complexes. <i>Chemical Physics</i> , 2006, 322, 387-391.	0.9	8
1103	Ab initio quantum chemical studies on the reactions of CF <sub>3</sub> O <sub>2</sub> with OH. <i>Chemical Physics</i> , 2006, 327, 10-14.	0.9	18
1104	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. <i>Chemical Physics</i> , 2006, 328, 307-317.	0.9	8

#	ARTICLE	IF	CITATIONS
1105	Theoretical study of $[XN_6]^{2-}$ (X=O, S, Se, Te) systems. <i>Chemical Physics Letters</i> , 2006, 418, 272-280.	1.2	1
1106	Global analysis of reaction pathways on the potential energy surface of cyanoacetylene by the scaled hypersphere search method. <i>Chemical Physics Letters</i> , 2006, 418, 208-216.	1.2	32
1107	Topological and natural population analyses of gas-phase identity $S_N2$ reactions of some methyl halides: Backside attack. <i>Chemical Physics Letters</i> , 2006, 419, 179-183.	1.2	5
1108	Theoretical evidence for the reaction of N-methyl-2-pyrrolidinone with carbon disulfide. <i>Chemical Physics Letters</i> , 2006, 420, 162-165.	1.2	9
1109	Theoretical study on three-membered silametallacycles toward MeOH: Mechanisms on formation of ring-opening products. <i>Chemical Physics Letters</i> , 2006, 422, 6-10.	1.2	4
1110	The initial mechanisms of $Al_2O_3$ atomic layer deposition on $OH/Si(100)-2 \times 1$ surface by tri-methylaluminum and water. <i>Chemical Physics Letters</i> , 2006, 426, 365-369.	1.2	31
1111	Density functional study of the Hoffmann elimination of (N-Cl),N-methylethanolamine in gas phase and in aqueous solution. <i>Chemical Physics Letters</i> , 2006, 429, 425-429.	1.2	4
1112	Transition states and charge analyses along the IRC for the singlet chlorocarbenes insertions into C-H bond of alkanes. <i>Chemical Physics Letters</i> , 2006, 430, 414-419.	1.2	13
1113	Oxidative addition of methane and benzene C-H bonds to rhodium center: A DFT study. <i>Chemical Physics Letters</i> , 2006, 431, 385-389.	1.2	9
1114	Theoretical investigation of the reactivity in the C-F bond activation of $CH_3F$ by $Lu^+$ in the gas phase. <i>Chemical Physics Letters</i> , 2006, 431, 223-226.	1.2	13
1115	Theoretical survey of the potential energy surface of $Ni^{++}$ acetone reaction. <i>Chemical Physics Letters</i> , 2006, 432, 27-32.	1.2	22
1116	A barrier-free atom-molecule reaction: $F + HONO$ . <i>Chemical Physics</i> , 2006, 324, 474-482.	0.9	6
1117	Why ketonization is favored over enolization in 5-membered ring H-transfers by $CH_3C(OH^+)CH_2CH_2$ and in 6-membered ring H-transfers by $CH_3(COH^+)CH_2CH_2CH_2$ . <i>International Journal of Mass Spectrometry</i> , 2006, 249-250, 120-129.	0.7	5
1118	Gas-phase ion chemistry of $Si^+$ and $NF_3$ : An experimental and theoretical study. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 225-231.	0.7	12
1119	Fragmentation of doubly charged metal-acetamide complexes: Second ionization energies and dissociation chemistries. <i>International Journal of Mass Spectrometry</i> , 2006, 255-256, 251-264.	0.7	17
1120	Insertion of the p-complex structure of silylenoid $H_2SiLiF$ into X-H bonds (X=C, Si, N, P, O, S, and F). <i>Journal of Organometallic Chemistry</i> , 2006, 691, 208-223.	0.8	13
1121	Site epimerization in ansa-zirconocene polymerization catalysts. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4367-4378.	0.8	15
1122	Reactions of $C_5H_5M^+$ (M=Fe, Ni) with substituted thiophenes. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4931-4936.	0.8	3

#	ARTICLE	IF	CITATIONS
1123	Structure and properties of the 5a,6-anhydrotetracyclineâ€“platinum(II) dichloride complex: A theoretical ab initio study. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 1594-1605.	1.5	27
1124	Efficient synthesis and structural analysis of new dioxopiperazine isoquinolines. <i>Tetrahedron</i> , 2006, 62, 4408-4418.	1.0	8
1125	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. <i>Tetrahedron</i> , 2006, 62, 5502-5509.	1.0	35
1126	A DFT study for the formation of imidazo[1,2-c]pyrimidines through an intramolecular Michael addition. <i>Tetrahedron</i> , 2006, 62, 10408-10416.	1.0	9
1127	Properties and isomerization mechanism of the singlet state imidazoleâ€“imidazolium system. <i>Computational and Theoretical Chemistry</i> , 2006, 758, 1-8.	1.5	1
1128	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. <i>Computational and Theoretical Chemistry</i> , 2006, 762, 25-31.	1.5	14
1129	Theoretical study of reaction mechanism for subsequent carcinogenic metabolites by nitrosodimethylamine. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 239-243.	1.5	4
1130	Structure, stability and chemical bonding character of covalent boron azides BX(N3)2 (X=F, Cl, Br). <i>Computational and Theoretical Chemistry</i> , 2006, 759, 171-176.	1.5	0
1131	Theoretical study on PCCCP and its isomers. <i>Computational and Theoretical Chemistry</i> , 2006, 759, 209-213.	1.5	4
1132	Ab initio quantum chemical studies of reaction mechanism for CH2CO with NCO. <i>Computational and Theoretical Chemistry</i> , 2006, 760, 131-140.	1.5	12
1133	Computational analysis of the selective cyclopropanation mode for the PtCl2-catalyzed cycloisomerization of a polyunsaturated precursor. <i>Computational and Theoretical Chemistry</i> , 2006, 761, 45-51.	1.5	12
1134	Theoretical study of fluorination reaction by diethylaminosulfur trifluoride (DAST). <i>Computational and Theoretical Chemistry</i> , 2006, 761, 73-81.	1.5	11
1135	Oxidation of catechol to muconic acid: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2006, 761, 209-215.	1.5	3
1136	Looking for the stable isomers of [N,C,C,O]+ system. <i>Computational and Theoretical Chemistry</i> , 2006, 763, 91-96.	1.5	0
1137	Secondary N-nitrosocarbamate anions: Structure and alkylation reactions. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2006, 764, 21-31.	1.5	3
1138	Theoretical study on structures and energetics of Ge2P2. <i>Computational and Theoretical Chemistry</i> , 2006, 764, 47-52.	1.5	3
1139	The carbonyl insertion reaction of ethylCo(CO)n(PH3)4â€“n and vinylCo(CO)n(PH3)4â€“n: A detailed DFT study. <i>Computational and Theoretical Chemistry</i> , 2006, 765, 21-26.	1.5	3
1140	Theoretical investigation of the reactivity in the Câ€“F bond activation of CH3F by La+ in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2006, 765, 27-34.	1.5	18

#	ARTICLE	IF	CITATIONS
1141	The study of isotope effects of chloroform and chloromethane using vibrational frequencies. Computational and Theoretical Chemistry, 2006, 765, 105-114.	1.5	4
1142	New insights into the interconversion mechanism between phenol and its isomers. Computational and Theoretical Chemistry, 2006, 767, 11-18.	1.5	17
1143	A theoretical treatment of the intersystem crossing in the spin-forbidden reaction. Computational and Theoretical Chemistry, 2006, 770, 1-6.	1.5	1
1144	Diaziridines thermal cleavage possibilities: Disrotatory or conrotatory?. Computational and Theoretical Chemistry, 2006, 770, 7-12.	1.5	7
1145	A theoretical study on the radical-neutral reaction mechanism of carbon monophosphide, CP, with acetylene, C <sub>2</sub> H <sub>2</sub> . Computational and Theoretical Chemistry, 2006, 772, 45-50.	1.5	6
1146	DFT study of the spin-forbidden reaction between Ti <sup>+</sup> and N <sub>2</sub> O. Computational and Theoretical Chemistry, 2006, 774, 59-65.	1.5	18
1147	Theoretical studies on the reactions of NO <sub>2</sub> with CH <sub>3</sub> SO, CH <sub>3</sub> SS, CH <sub>3</sub> SO <sub>2</sub> and CH <sub>3</sub> S(S)O. Computational and Theoretical Chemistry, 2006, 775, 101-106.	1.5	4
1148	Mechanism for the gas-phase reaction between N <sub>3</sub> and NO <sub>2</sub> : A theoretical study. Computational and Theoretical Chemistry, 2006, 801, 39-45.	1.5	1
1149	Theoretical study of 1,3-dipolar cycloaddition of nitrones to doubly activated nitriles. Russian Journal of Inorganic Chemistry, 2006, 51, 1602-1612.	0.3	5
1150	The mechanism of allyl isomerization of unsaturated compounds catalyzed by organomagnesium clusters. Russian Journal of Physical Chemistry A, 2006, 80, 702-705.	0.1	3
1151	Theoretical study on H <sub>2</sub> elimination pathways of silylenoid H <sub>2</sub> SiLiF with CH <sub>4</sub> , NH <sub>3</sub> , H <sub>2</sub> O, HF, SiH <sub>4</sub> , PH <sub>3</sub> , H <sub>2</sub> S, and HCl. Structural Chemistry, 2006, 17, 63-73.	1.0	7
1152	Ab initio computational insight into the ion-pair S <sub>N</sub> 2 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
1153	Theoretical study of [XN <sub>5</sub> ] <sup>-</sup> (X=O, S, Se, Te) systems. Journal of Molecular Modeling, 2006, 12, 805-811.	0.8	4
1154	Computational Organic Photochemistry: Strategy, Achievements and Perspectives. Theoretical Chemistry Accounts, 2006, 116, 87-105.	0.5	88
1155	Predicting Potential Stable Isomers on the Singlet Surface of the [H,P,C,S] System by the MP2 and QCISD(T) Methods. Theoretical Chemistry Accounts, 2006, 117, 49-56.	0.5	3
1156	Theoretical study on the reaction mechanism of CH <sub>4</sub> with CaO. Chemical Physics, 2006, 330, 343-348.	0.9	26
1157	The structure and energetics of singlet, closed-shell [B, C, F, H <sub>2</sub> ]: Simplicity resulting in diversity. Journal of Fluorine Chemistry, 2006, 127, 1355-1367.	0.9	3
1158	Methane loss from (CH <sub>3</sub> ) <sub>3</sub> O <sup>+</sup> : An asynchronous, concerted 1,2-alkane elimination. International Journal of Mass Spectrometry, 2006, 248, 103-107.	0.7	4

#	ARTICLE	IF	CITATIONS
1159	On the reaction of ground-state nitrogen atoms with bromomethyl radicals: A computational study. <i>International Journal of Mass Spectrometry</i> , 2006, 249-250, 451-461.	0.7	3
1160	Cationic germanium fluorides. <i>International Journal of Mass Spectrometry</i> , 2006, 257, 50-59.	0.7	8
1161	Benzene loss from trityl cations: A mechanistic study. <i>Journal of the American Society for Mass Spectrometry</i> , 2006, 17, 730-736.	1.2	9
1162	Low-Pressure Pyrolysis of $t\text{Bu}_2\text{SO}$ : Synthesis and IR Spectroscopic Detection of HSOH. <i>Chemistry - A European Journal</i> , 2006, 12, 832-844.	1.7	40
1163	New Insights into the Mechanism of Proton Transfer to Hydride Complexes: Kinetic and Theoretical Evidence Showing the Existence of Competitive Pathways for Protonation of the Cluster $[\text{W}_3\text{S}_4\text{H}_3(\text{dmpe})_3]^+$ with Acids. <i>Chemistry - A European Journal</i> , 2006, 12, 1413-1426.	1.7	44
1164	Density Functional Studies of Dicobalt Octacarbonyl-Mediated Azobenzene Formation from 4-Ethynylaniline. <i>Chemistry - A European Journal</i> , 2006, 12, 1403-1412.	1.7	1
1165	A Theoretical Proposal for the Synthesis of Carbapenems from 4-(2-Propynyl)azetidiones Promoted by $[\text{W}(\text{CO})_5]$ as an Alternative to the $\text{Ag}^+$ -Assisted Process. <i>Chemistry - A European Journal</i> , 2006, 12, 7929-7934.	1.7	5
1166	Density Functional Studies on the Nazarov Reaction Involving Cyclic Systems. <i>Chemistry - A European Journal</i> , 2006, 12, 2836-2845.	1.7	42
1167	Stereoelectronic Effects on Type I 1,2-Dyotropic Rearrangements in Vicinal Dibromides. <i>Chemistry - A European Journal</i> , 2006, 12, 6323-6330.	1.7	37
1168	Enantio- and Diastereoselective Michael Addition Reactions of Unmodified Aldehydes and Ketones with Nitroolefins Catalyzed by a Pyrrolidine Sulfonamide. <i>Chemistry - A European Journal</i> , 2006, 12, 4321-4332.	1.7	212
1169	Cyclic Carbodiphosphorane: Diphosphinocarbene Thermal Interconversion. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 7447-7450.	7.2	30
1170	Kinetic and Thermodynamic Aspects of the CT and T-Shaped Adduct Formation Between 1,3-Dimethylimidazoline-2-thione (or -2-selone) and Halogens. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 2166-2174.	1.0	19
1171	$\pi$ -Strain-Induced Electrophilicity in Small Cycloalkynes: A DFT Analysis of the Polar Cycloaddition of Cyclopentyne towards Enol Ethers. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 498-506.	1.2	28
1172	The Mechanism of Semibullvalene Bromination. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 738-745.	1.2	7
1173	Towards an Understanding of the Polar Diels-Alder Reactions of Nitrosoalkenes with Enamines: A Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 2570-2580.	1.2	44
1174	A DFT Study of the Molecular Mechanisms of the Nucleophilic Addition of Ester-Derived Lithium Enolates and Silyl Ketene Acetals to Nitrones: Effects of the Lewis Acid Catalyst. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3464-3472.	1.2	23
1175	Stereochemistry of the Tetrabutylammonium Cyanide-Catalyzed Cyanosilylation of Cyclic $\alpha,\beta$ -Epoxyketones: Dependence of the Diastereoselectivity on the Ring Size. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 3969-3976.	1.2	12
1176	Computation Revealed a Case where Kinetic Selectivity is Controlled by Dynamics: Isomerization of Benzylideneanilines. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 4327-4330.	1.2	14



#	ARTICLE	IF	CITATIONS
1177	Theoretical study on the [Si, C, N, O] potential energy surface. <i>Journal of Computational Chemistry</i> , 2006, 27, 749-761.	1.5	5
1178	Exploring Two-State Reaction Pathways in the Photodimerization of Cyclohexadiene. <i>ChemPhysChem</i> , 2006, 7, 614-618.	1.0	6
1179	The "Non-Reaction" of Ground-State Triplet Carbon Atoms with Water Revisited. <i>ChemPhysChem</i> , 2006, 7, 880-885.	1.0	34
1180	Mechanism of Cysteine Oxidation by a Hydroxyl Radical: A Theoretical Study. <i>ChemPhysChem</i> , 2006, 7, 912-919.	1.0	27
1181	Theoretical Investigation of the Decarbonylation of Acetaldehyde by Fe <sup>+</sup> and Cr <sup>+</sup> . <i>ChemPhysChem</i> , 2006, 7, 1345-1354.	1.0	27
1182	Formation of Trichlorinated Dibenzo-p-dioxins from 2,4-Dichlorophenol and 2,4,5-Trichlorophenolate: A Theoretical Study. <i>ChemPhysChem</i> , 2006, 7, 2331-2338.	1.0	5
1183	Direct Experimental Observation of CS <sub>2</sub> OH. <i>ChemPhysChem</i> , 2006, 7, 2352-2357.	1.0	2
1185	Chiral Thiourea-Based Bifunctional Organocatalysts in the Asymmetric Nitro-Michael Addition: A Joint Experimental-Theoretical Study. <i>Advanced Synthesis and Catalysis</i> , 2006, 348, 826-832.	2.1	198
1186	Thermodynamic and kinetic properties of the formation reactions of the donor-acceptor complexes HXPY (X=Al, B; Y=H, Cl, SH). <i>Europhysics Letters</i> , 2006, 75, 254-259.	0.7	4
1187	Quadratic string method for determining the minimum-energy path based on multiobjective optimization. <i>Journal of Chemical Physics</i> , 2006, 124, 054109.	1.2	93
1188	The water exchange process of tetraaquaplatinum(II): Density-functional theory and ab initio computational study. <i>Journal of Chemical Physics</i> , 2006, 124, 074511.	1.2	5
1189	Modeling Reaction Mechanism of Cocaine Hydrolysis and Rational Drug Design for Therapeutic Treatment of Cocaine Abuse. , 0, , 107-159.		2
1190	Theoretical analysis of transition states in the exchange reaction of hydrogen and methane involving $\sigma$ -bond metathesis. <i>Journal of Coordination Chemistry</i> , 2006, 59, 777-782.	0.8	5
1191	Direct dynamics study on the hydrogen abstraction reactions N <sub>2</sub> H <sub>4</sub> +R <sup>+</sup> N <sub>2</sub> H <sub>3</sub> +RH (R=NH <sub>2</sub> ,CH <sub>3</sub> ). <i>Journal of Chemical Physics</i> , 2006, 125, 064304.	1.2	10
1192	Adiabatic approximations to internal rotation. <i>Journal of Chemical Physics</i> , 2006, 124, 224310.	1.2	26
1193	THEORETICAL STUDY ON HYDROLYSIS MECHANISM OF Î <sup>2</sup> -PHOSPHOLACTAMS. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 421-431.	1.8	1
1194	Thermodynamic functions of conformational changes I. A comparative first principles study of 1,2-disubstituted ethanes. <i>Molecular Physics</i> , 2006, 104, 795-803.	0.8	5
1195	Chapter 6 Electronic structure and reactivity in double Rydberg anions: characterization of a novel kind of electron pair. <i>Theoretical and Computational Chemistry</i> , 2007, 19, 87-100.	0.2	10

#	ARTICLE	IF	CITATIONS
1196	Computing Reaction Pathways on Molecular Potential Energy Surfaces. <i>Reviews in Computational Chemistry</i> , 2007, , 35-65.	1.5	12
1197	A Computational Strategy for Organic Photochemistry. <i>Reviews in Computational Chemistry</i> , 2007, , 87-146.	1.5	138
1198	Ab initio study of the reaction of propionyl (C <sub>2</sub> H <sub>5</sub> CO) radical with oxygen (O <sub>2</sub> ). <i>Journal of Chemical Physics</i> , 2007, 127, 054306.	1.2	61
1199	Sequential quadratic programming method for determining the minimum energy path. <i>Journal of Chemical Physics</i> , 2007, 127, 164107.	1.2	28
1200	Theoretical Study of Decomposition Mechanism of Azoisobutyronitrile. <i>Chinese Journal of Chemical Physics</i> , 2007, 20, 224-232.	0.6	0
1201	Reaction of CH <sub>2</sub> Cl with O <sub>2</sub> . <i>Chinese Journal of Chemical Physics</i> , 2007, 20, 383-387.	0.6	2
1202	UNDERSTANDING REACTIVE HAZARDS USING MOLECULAR SIMULATION: MECHANISMS OF HYDROXYLAMINE DECOMPOSITION. <i>Chemical Engineering Communications</i> , 2007, 194, 579-585.	1.5	3
1203	Reaction of CH <sub>3</sub> with NO <sub>2</sub> . <i>Chinese Journal of Chemical Physics</i> , 2007, 20, 31-36.	0.6	5
1204	Theoretical Study on the Kinetic and Mechanism of H+HO <sub>2</sub> Reaction. <i>Bulletin of the Chemical Society of Japan</i> , 2007, 80, 1901-1913.	2.0	51
1205	Density Functional Study on the 1,4-Hydride Migration in the $\eta^5$ -Naphthalene Manganese Complex [( <i>exo</i> -R- $\eta^5$ -C <sub>10</sub> H <sub>8</sub> )Mn(CO) <sub>3</sub> ]. <i>Chemistry Letters</i> , 2007, 36, 268-269.	0.7	1
1206	The Interface Between Electronic Structure Theory and Reaction Dynamics by Reaction Path Methods. <i>Advances in Chemical Physics</i> , 2007, , 389-453.	0.3	21
1207	Quantum Mechanics for Organic Chemistry. , 0, , 1-41.		1
1208	The correlation between aromaticity and stability in planar N <sub>2</sub> X <sub>2</sub> (X = O, S, Se, and Te) Species. <i>Molecular Physics</i> , 2007, 105, 1883-1889.	0.8	5
1209	Density Functional Theory Study of the Reaction Mechanism and Energetics of the Reduction of Hydrogen Peroxide by Ebselen, Ebselen Diselenide, and Ebselen Selenol. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3152-3160.	1.1	51
1210	The Participation of Alkynylboronates in Inverse Electron Demand [4 + 2] Cycloadditions: A Mechanistic Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 2691-2699.	6.6	62
1211	Selective Formation of Triplet Alkyl Nitrenes from Photolysis of $\eta^2$ -Azido-Propiophenone and Their Reactivity. <i>Journal of the American Chemical Society</i> , 2007, 129, 16263-16272.	6.6	46
1212	From Azobenzene Coordination to Aryl-Halide Bond Activation by Platinum. <i>Organometallics</i> , 2007, 26, 4528-4534.	1.1	39
1213	Topological Analysis of the Electronic Charge Density in the Ethene Protonation Reaction Catalyzed by Acidic Zeolite. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7848-7859.	1.1	16

#	ARTICLE	IF	CITATIONS
1214	Investigation of the Typical Triangular Structure B <sub>3</sub> in Boron Chemistry: An Insight into Bare All-Boron Clusters Used as Ligands or Building Blocks. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9122-9129.	1.1	26
1215	Theoretical Investigation of the Hydrogen Abstraction Reaction of the OH Radical with CH <sub>2</sub> FCH <sub>2</sub> F (HFC-152): A Dual-Level Direct Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8095-8103.	1.1	10
1216	Antibiotic Deactivation by a Zinc <sup>II</sup> -Lactamase: Mechanistic Insights from QM/MM and DFT Studies. <i>Journal of the American Chemical Society</i> , 2007, 129, 10814-10822.	6.6	85
1217	The hydrolysis process of the anticancer complex [ImH][trans-RuCl <sub>4</sub> (Im) <sub>2</sub> ]: a theoretical study. <i>Dalton Transactions</i> , 2007, , 3507.	1.6	21
1218	Computational Chemistry of Polyatomic Reaction Kinetics and Dynamics: The Quest for an Accurate CH <sub>5</sub> Potential Energy Surface. <i>Chemical Reviews</i> , 2007, 107, 5101-5132.	23.0	58
1219	Computational Study of the Reaction between Biogenic Stabilized Criegee Intermediates and Sulfuric Acid. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3394-3401.	1.1	33
1220	DFT Study of the Mechanisms of In Water Au(I)-Catalyzed Tandem [3,3]-Rearrangement/Nazarov Reaction/[1,2]-Hydrogen Shift of Enynyl Acetates: A Proton-Transport Catalysis Strategy in the Water-Catalyzed [1,2]-Hydrogen Shift. <i>Journal of the American Chemical Society</i> , 2007, 129, 15503-15512.	6.6	280
1221	Comprehensive theoretical studies on the CF <sub>3</sub> H dissociation mechanism and the reactions of CF <sub>3</sub> H with OH and H free radicals. <i>Journal of Chemical Physics</i> , 2007, 126, 034307.	1.2	28
1222	Shock tube study of dissociation and relaxation in 1,1-difluoroethane and vinyl fluoride. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4164.	1.3	11
1223	Gas phase kinetic and quantum chemical studies of the reactions of silylene with the methylsilanes. Absolute rate constants, temperature dependences, RRKM modelling and potential energy surfaces. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2121.	1.3	21
1224	Theoretical Study of the Reaction from 6-Methylidene Penem to Seven-Membered Ring Intermediates. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4720-4725.	1.1	4
1225	Which One among Zn(II), Co(II), Mn(II), and Fe(II) is the Most Efficient Ion for the Methionine Aminopeptidase Catalyzed Reaction?. <i>Journal of the American Chemical Society</i> , 2007, 129, 7776-7784.	6.6	57
1226	Planar carbon radical's assembly and stabilization, a way to design spin-based molecular materials. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5304.	1.3	15
1227	Applications of analytic and geometry concepts of the theory of Calculus of Variations to the Intrinsic Reaction Coordinate model. <i>Molecular Physics</i> , 2007, 105, 2475-2492.	0.8	17
1228	Mechanistic aspects of proton chain transfer in the green fluorescent protein : Part II. A comparison of minimal quantum chemical models. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 452-458.	1.3	25
1229	A Theoretical Study of the Heck Reaction: N-Heterocyclic Carbene versus Phosphine Ligands. <i>Organometallics</i> , 2007, 26, 1317-1324.	1.1	64
1230	Theoretical Prediction of the p53 Gene Mutagenic Mechanism Induced by trans-4-Hydroxy-2-nonenal. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5362-5371.	1.2	10
1231	Theoretical Study on the Substitution Reactions of Silylenoid H <sub>2</sub> SiLiF with CH <sub>4</sub> , NH <sub>3</sub> , H <sub>2</sub> O, HF, SiH <sub>4</sub> , PH <sub>3</sub> , H <sub>2</sub> S, and HCl. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8475-8481.	1.1	14

#	ARTICLE	IF	CITATIONS
1232	Gas-Phase Ionic Syntheses of Amino Acids: $\hat{I}^2$ versus $\hat{I}^\pm$ . Journal of the American Chemical Society, 2007, 129, 9910-9917.	6.6	39
1233	Heterocyclic Analogues of Cyclohexene: Theoretical Studies of the Molecular Structures and Ring-Inversion Processes. Journal of Physical Chemistry A, 2007, 111, 2368-2375.	1.1	18
1234	Selenocysteine versus Cysteine Reactivity: A Theoretical Study of Their Oxidation by Hydrogen Peroxide. Journal of Physical Chemistry A, 2007, 111, 673-678.	1.1	54
1235	Lewis Acid and Substituent Effects on the Molecular Mechanism for the Nazarov Reaction of Penta-1,4-dien-3-one and Derivatives. A Topological Analysis Based on the Combined Use of Electron Localization Function and Catastrophe Theory. Journal of Chemical Theory and Computation, 2007, 3, 816-823.	2.3	31
1236	New Insight into the Gas-Phase Bimolecular Self-Reaction of the HOO Radical. Journal of Physical Chemistry A, 2007, 111, 1695-1704.	1.1	46
1237	A Theoretical Investigation of the Co(CO) <sub>4</sub> -Catalyzed Carbonylative Ring Expansion of N-Benzoyl-2-methylaziridine to $\hat{I}^2$ -Lactams: A Reaction Mechanism and Effect of Substituent at the Aziridine C-Atom. Journal of Organic Chemistry, 2007, 72, 3259-3267.	1.7	23
1238	The Importance of a Conformational Equilibrium on the Reactivity of Molybdenum and Rhenium Hydroxo $\hat{I}^2$ Carbonyl Complexes toward Phenyl Acetate: A Theoretical Investigation. Organometallics, 2007, 26, 5271-5277.	1.1	5
1239	Isotopomeric Conformational Changes in the Anisole $\hat{I}^2$ Water Complex: New Insights from HR-UV Spectroscopy and Theoretical Studies. Journal of Physical Chemistry A, 2007, 111, 12363-12371.	1.1	29
1240	Competition between $\hat{I}^\pm$ -Cleavage and Energy Transfer in $\hat{I}^\pm$ -Azidoacetophenones. Journal of Organic Chemistry, 2007, 72, 2757-2768.	1.7	40
1241	Theoretical Investigation on Stability and Isomerizations of CH <sub>3</sub> SO Isomers. Journal of Physical Chemistry A, 2007, 111, 2343-2350.	1.1	23
1242	Nature of Cp*MoO <sub>2</sub> <sup>+</sup> in Water and Intramolecular Proton-Transfer Mechanism by Stopped-Flow Kinetics and Density Functional Theory Calculations. Inorganic Chemistry, 2007, 46, 4103-4113.	1.9	39
1243	Computational Study on the Mechanisms and Energetics of Trimethylindium Reactions with H <sub>2</sub> O and H <sub>2</sub> S. Journal of Physical Chemistry A, 2007, 111, 6481-6488.	1.1	9
1244	Radical-Cationic Gaseous Amino Acids: A Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 7906-7914.	1.1	11
1245	Redox Regulation of Protein Tyrosine Phosphatase 1B (PTP1B): A Biomimetic Study on the Unexpected Formation of a Sulfenyl Amide Intermediate. Journal of the American Chemical Society, 2007, 129, 8872-8881.	6.6	49
1246	Density Functional Theory Investigations on Sulfur Ylide Promoted Cyclopropanation Reactions: Insights on Mechanism and Diastereoselection Issues. Journal of Organic Chemistry, 2007, 72, 331-341.	1.7	35
1247	CO <sub>2</sub> Activation by Nb <sup>+</sup> and NbO <sup>+</sup> in the Gas Phase. A Case of Two-State Reactivity Process. Journal of Chemical Theory and Computation, 2007, 3, 811-815.	2.3	20
1248	Sulfoxide-Induced Stereoselection in [1,5]-Sigmatropic Hydrogen Shifts of Vinylallenes. A Computational Study. Journal of Organic Chemistry, 2007, 72, 2617-2624.	1.7	13
1249	Photoinduced C-N Bond Cleavage in 2-Azido-1,3-diphenyl-propan-1-one Derivatives: Photorelease of Hydrazoic Acid. Journal of Organic Chemistry, 2007, 72, 6372-6381.	1.7	25

#	ARTICLE	IF	CITATIONS
1250	Mechanism of the Generation of Ketenimine $\hat{M}(\text{CO})_n$ Complexes (M = Cr, W, Fe) from Fischer Carbenes and Isocyanides. <i>Organometallics</i> , 2007, 26, 3010-3017.	1.1	44
1251	Theoretical Investigations of Isolated Mo(VI) and Mo(IV) Centers of a Molybdena $\hat{S}$ ilica Catalyst for Olefin Metathesis. <i>Journal of Physical Chemistry C</i> , 2007, 111, 9337-9348.	1.5	37
1252	Steric versus Electronic Effects in the Structure of Heteroatom (S and O)-Substituted Free and Metal (Cr and W)-Complexed Carbenes. <i>Organometallics</i> , 2007, 26, 5854-5858.	1.1	36
1253	SSOH and HSSO Radicals: An Experimental and Theoretical Study of $[\text{S}2\text{OH}]0/+/-$ Species. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6526-6533.	1.1	27
1254	Insights on Co-Catalyst-Promoted Enamine Formation between Dimethylamine and Propanal through Ab Initio and Density Functional Theory Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 8202-8215.	1.7	75
1255	Insight into Global Reaction Mechanism of $[\text{C}2, \text{H}4, \text{O}]$ System from ab Initio Calculations by the Scaled Hypersphere Search Method. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5099-5110.	1.1	48
1256	Kinetic and Thermodynamic Stability of Acenes: A Theoretical Study of Nucleophilic and Electrophilic Addition. <i>Journal of Organic Chemistry</i> , 2007, 72, 51-61.	1.7	36
1257	Computational Study of Reaction Pathways for the Formation of Indium Nitride from Trimethylindium with $\text{HN}_3$ : A Comparison of the Reaction with $\text{NH}_3$ and That on $\text{TiO}_2$ Rutile (110) Surface. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6781-6788.	1.1	11
1258	Competition between Hydrogen Abstraction and Halogen Displacement in the Reaction of Br with $\text{CH}_3\text{I}$ , $\text{CH}_3\text{Br}$ , and $\text{CH}_3\text{Cl}$ . <i>Journal of Physical Chemistry A</i> , 2007, 111, 6852-6859.	1.1	5
1259	Multidimensional Quantum Dynamical Study of $\hat{I}^2$ -Hydrogen Transfer in a Cationic Rhodium Complex. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2407-2419.	1.1	7
1260	Origin of Diastereoselectivity in the Synthesis of Chiral Bicyclic Lactams: A $\hat{I}$ -Facial Selective Attack of Singlet Oxygen Induced by Hindered Internal Rotation. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5855-5863.	1.1	7
1261	OH-Initiated Oxidation of Toluene. 1. Quantum Chemistry Investigation of the Reaction Path. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3686-3690.	1.1	32
1262	Ab Initio Study on the Kinetics of Hydrogen Abstraction for the $\text{H} + \text{Alkene} \hat{H}_2 + \text{Alkenyl}$ Reaction Class. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2156-2165.	1.1	29
1263	Comparison of Density Functionals for Reactions of Sulfur Ylides with Aldehydes and Olefins. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12019-12025.	1.1	9
1264	Reaction of Acetaldehyde with $\text{Ni}^+$ : An Extended Theoretical Study of the Decarbonylation Mechanism of Acetaldehyde by First-Row Transition Metal Ions. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3566-3570.	1.1	24
1265	Mechanistic Twist of the $[8+2]$ Cycloadditions of Dienylisobenzofurans and Dimethyl Acetylenedicarboxylate: Stepwise $[8+2]$ versus $[4+2]/[1,5]$ -Vinyl Shift Mechanisms Revealed through a Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2007, 129, 10773-10784.	6.6	63
1266	Mechanism of Thiol Oxidation by the Superoxide Radical. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13046-13052.	1.1	26
1267	Theoretical Reinvestigation of the $\text{O}(^3\text{P}) + \text{C}_6\text{H}_6$ Reaction: A Quantum Chemical and Statistical Rate Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3836-3849.	1.1	34

#	ARTICLE	IF	CITATIONS
1268	Theoretical Survey of the Gas-Phase Reactions of Allylamine with Co <sup>+</sup> . Journal of Physical Chemistry A, 2007, 111, 6208-6216.	1.1	15
1269	Mechanistic Studies of UV Assisted [4 + 2] Cycloadditions in Synthetic Efforts toward Vibsanin E. Journal of the American Chemical Society, 2007, 129, 10763-10772.	6.6	32
1270	Selective Ruthenium-Catalyzed Transformations of Enynes with Diazoalkanes into Alkenylbicyclo[3.1.0]hexanes. Journal of the American Chemical Society, 2007, 129, 6037-6049.	6.6	104
1271	Alkylation of the toluene methyl group: A DFT study. Catalysis Communications, 2007, 8, 1354-1360.	1.6	4
1272	Theoretical Study of Chemo-, Regio-, and Stereoselectivity in 1,3-Dipolar Cycloadditions of Nitrones and Nitrile Oxides to Free and Pt-Bound Bifunctional Dipolarophiles. Journal of Organic Chemistry, 2007, 72, 4475-4485.	1.7	47
1273	A Theoretical Study on the Hydrolysis Process of the Antimetastatic Ruthenium(III) Complex NAMI-A. Journal of Physical Chemistry B, 2007, 111, 7862-7869.	1.2	54
1274	A new perspective on chemical and physical processes: the reaction force. Molecular Physics, 2007, 105, 2619-2625.	0.8	142
1275	Theoretical Study on Mechanisms of the Epoxy <sup>+</sup> Amine Curing Reaction. Macromolecules, 2007, 40, 4370-4377.	2.2	155
1276	Modeling Mechanisms of Unusual Benzene Imine N6 Adduct Formation in Carcinogenic Reactions of Arylnitrenium Ions with Adenosine. Journal of Organic Chemistry, 2007, 72, 10058-10064.	1.7	5
1277	The Role of Reaction Force and Chemical Potential in Characterizing the Mechanism of Double Proton Transfer in the Adenine <sup>+</sup> Uracil Complex. Journal of Physical Chemistry A, 2007, 111, 5921-5926.	1.1	131
1278	Methylene Transfer or Carbometalation? A Theoretical Study to Determine the Mechanism of Lithium Carbenoid-Promoted Cyclopropanation Reactions in Aggregation and Solvation States. Journal of Organic Chemistry, 2007, 72, 848-860.	1.7	22
1279	Proton Walk in the Aqueous Platinum Complex [TpPtMeCO] via a Sticky $\eta^5$ -Methane Ligand. Chemistry - A European Journal, 2007, 13, 2812-2823.	1.7	13
1280	On a Possible Growth Mechanism for Polycyclic Aromatic Hydrocarbon Dications: C <sub>7</sub> H <sub>6</sub> <sup>2+</sup> +C <sub>2</sub> H <sub>2</sub> . Chemistry - A European Journal, 2007, 13, 2893-2902.	1.7	22
1281	Experimental and DFT Study of the Tautomeric Behavior of Cobalt-Containing Secondary Phosphine Oxides. Chemistry - A European Journal, 2007, 13, 1583-1593.	1.7	19
1282	The Preferred Reaction Path for the Oxidation of Methanol by PQQ-Containing Methanol Dehydrogenase: Addition <sup>+</sup> Elimination versus Hydride-Transfer Mechanism. Chemistry - A European Journal, 2007, 13, 2109-2117.	1.7	48
1283	Electrocyclic Ring Opening of cis-Bicyclo[m.n.0]alkenes: The Anti-Woodward <sup>+</sup> Hoffmann Quest. Chemistry - A European Journal, 2007, 13, 5009-5017.	1.7	22
1284	Theoretical Evidence for Pyramidalized Bicyclic Serine Enolates in Highly Diastereoselective Alkylations. Chemistry - A European Journal, 2007, 13, 4840-4848.	1.7	36
1285	Theoretical Study of the Reaction of Vitamin B <sub>6</sub> with O <sub>2</sub> . Chemistry - A European Journal, 2007, 13, 4636-4642.	1.7	41

#	ARTICLE	IF	CITATIONS
1286	On the Mechanism and Stereochemistry of Chiral Lithium-Carbenoid-Promoted Cyclopropanation Reactions. <i>Chemistry - A European Journal</i> , 2007, 13, 6724-6731.	1.7	21
1287	Computational Investigations on the General Reaction Profile and Diastereoselectivity in Sulfur Ylide Promoted Aziridination. <i>Chemistry - A European Journal</i> , 2007, 13, 4805-4815.	1.7	34
1288	Extended D <sub>A</sub> -Like Cyclization Reactions Towards the Synthesis of Eight-Membered Ring-Containing Polycycles: Scope and Theoretical Studies. <i>Chemistry - A European Journal</i> , 2007, 13, 7682-7700.	1.7	19
1289	Ligand-Activated Lithium-Mediated Zincation of <i>N</i> -Phenylpyrrole. <i>Chemistry - A European Journal</i> , 2007, 13, 9982-9989.	1.7	49
1290	Thermal Activation of Methane by Group-10 Metal Hydrides MH <sub>3</sub> : The Same and Not the Same. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 5614-5617.	7.2	58
1292	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. <i>Journal of Computational Chemistry</i> , 2007, 28, 1485-1502.	1.5	190
1293	Effects of entropy on the gas-phase pyrolysis of ethyl <i>N,N</i> -dimethylcarbamate. <i>Journal of Computational Chemistry</i> , 2007, 28, 625-631.	1.5	2
1294	Combined DFT, QCISD(T), and G2 mechanism investigation for the reactions of carbon monophosphide CP with unsaturated hydrocarbons allene CH <sub>2</sub> CCH <sub>2</sub> and methylacetylene CH <sub>3</sub> CCH. <i>Journal of Computational Chemistry</i> , 2007, 28, 1221-1233.	1.5	1
1295	Theoretical investigation on the protonation reactions and products of the stable [N,C,C,S] isomers. <i>Journal of Computational Chemistry</i> , 2007, 28, 2472-2482.	1.5	0
1296	Mechanisms of H <sub>2</sub> , H <sub>2</sub> C=CH <sub>2</sub> , and O=CH <sub>2</sub> Insertion into Cp <sub>2</sub> Zr(̂-2-SiMe <sub>2</sub> =NtBu)(PMe <sub>3</sub> ). <i>European Journal of Inorganic Chemistry</i> , 2007, 2007, 2046-2054.	1.0	9
1297	A Novel Direct Conversion of Primary Amides to Their Corresponding Methyl Esters. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 1026-1030.	1.2	19
1298	DFT Study on the Sn <sup>II</sup> -Catalyzed Diastereoselective Synthesis of Tetrahydrofuran from D <sup>A</sup> Cyclopropane and Benzaldehyde. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 4855-4866.	1.2	16
1299	Double Group Transfer Reactions as Indicators of Aromatic Stabilization. <i>European Journal of Organic Chemistry</i> , 2007, 2007, 5410-5415.	1.2	19
1300	Theoretical Study on the Reaction Mechanism of Ketene CH <sub>2</sub> CO with Isocyanate NCO Radical. <i>Chinese Journal of Chemistry</i> , 2007, 25, 1105-1111.	2.6	2
1301	A Density Functional Study on the Hydrolysis Process of Non-classical Transplatin(II) with Two Same Planar Heterocycle Amines. <i>Chinese Journal of Chemistry</i> , 2007, 25, 1604-1611.	2.6	2
1302	A DFT Study of the Nitric Oxide and Tyrosyl Radical Interaction: A Proposed Radical Mechanism. <i>ChemPhysChem</i> , 2007, 8, 2595-2602.	1.0	6
1303	Theoretical and experimental studies of the diketene system: Product branching decomposition rate constants and energetics of isomers. <i>International Journal of Chemical Kinetics</i> , 2007, 39, 580-590.	1.0	5
1304	Observation of an unusually facile fragmentation pathway of gas-phase peptide ions: a study on the gas-phase fragmentation mechanism and energetics of tryptic peptides modified with 4-sulphophenyl isothiocyanate (SPITC) and 4-chlorosulphophenyl isocyanate (SPC) and their 18-crown-6 complexes. <i>Journal of Mass Spectrometry</i> , 2007, 42, 380-388.	0.7	4

#	ARTICLE	IF	CITATIONS
1305	Conformational analysis of methyl 2-methyl-2-(1-naphthyl)propionate. <i>Tetrahedron</i> , 2007, 63, 615-624.	1.0	1
1306	Synthesis of hetero- and carbocycles by nucleophilic substitution at sp <sup>2</sup> carbon. <i>Tetrahedron</i> , 2007, 63, 5940-5953.	1.0	26
1307	Quantum-chemical study of the Lewis acid influence on the cycloaddition of benzonitrile oxide to acetonitrile, propyne and propene. <i>Tetrahedron</i> , 2007, 63, 5251-5260.	1.0	32
1308	Phosphine triggered [3+2] allenolate-acrylate annulation: a mechanistic enlightenment. <i>Tetrahedron Letters</i> , 2007, 48, 3617-3620.	0.7	172
1309	Theoretical studies on the formation of N-nitrosodimethylamine. <i>Computational and Theoretical Chemistry</i> , 2007, 802, 1-6.	1.5	23
1310	Theoretical study on the potential energy surface of SiC <sub>2</sub> O. <i>Computational and Theoretical Chemistry</i> , 2007, 802, 59-65.	1.5	4
1311	Theoretical study of hydroxylation reaction mechanism and subsequent carcinogenic metabolites for nitrosopyrrolidine. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 35-38.	1.5	1
1312	Reaction pathways of direct O and S atoms abstraction from oxirane and thiirane by silylidene: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2007, 805, 79-86.	1.5	4
1313	A theoretical study on the mechanism of the oxidation of hydroxylamine by. <i>Computational and Theoretical Chemistry</i> , 2007, 805, 143-152.	1.5	5
1314	Computational study on the conversion of an aziridine and iminium salt to a 1,2-diamine. <i>Computational and Theoretical Chemistry</i> , 2007, 806, 171-177.	1.5	6
1315	Mechanisms of decarboxylation of ortho-substituted benzoic acids. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 1-9.	1.5	35
1316	Dehydrogenation reactivities of bimetallic species (M=Pt,Rh) with different spin multiplicities toward NH <sub>3</sub> in the gas phase: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2007, 808, 9-16.	1.5	8
1317	The influence of the leaving group X (X=F, Cl, Br, I) on the carbenoid nature of the carbenoids X <sub>2</sub> AlCH <sub>2</sub> X. A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2007, 807, 173-178.	1.5	6
1318	Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitrene and a maleimide:bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 125-133.	1.5	38
1319	A theoretical study of the cleavage of the amide bond of formamide by attack of the hydroxyl ligand in [Mo(OH)(i-3-C <sub>3</sub> H <sub>5</sub> )(CO) <sub>2</sub> (N <sub>2</sub> C <sub>2</sub> H <sub>4</sub> )] and [Re(OH)(CO) <sub>3</sub> (N <sub>2</sub> C <sub>2</sub> H <sub>4</sub> )] complexes. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 241-247.	1.5	4
1320	A theoretical study on tautomerization processes of dehydrated and monohydrated cytosine. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 161-167.	1.5	29
1321	Thermal rearrangement of 2-acetoxy-2,6,6-trimethylbicyclo[3.1.0]hexane: Theoretical elucidation of the mechanism. <i>Computational and Theoretical Chemistry</i> , 2007, 814, 61-73.	1.5	2
1322	Computational studies on cycloaddition reactions between 1,3-diaza-2-azoniaallene cation and olefins. <i>Computational and Theoretical Chemistry</i> , 2007, 815, 127-133.	1.5	3



#	ARTICLE	IF	CITATIONS
1323	Reaction of NH(3Î£âˆ™) radical with C2H4: A theoretical study. Computational and Theoretical Chemistry, 2007, 816, 21-29.	1.5	2
1324	Methanol dehydrogenation promoted by a heterobimetallic Ru(II)â€“Sn(II) complex as catalyst: A density functional study. Computational and Theoretical Chemistry, 2007, 816, 77-84.	1.5	7
1325	Theoretical study on the hydrolytic deamination reaction mechanism of adenineâ€“(H2O)n (n=1â€“4). Computational and Theoretical Chemistry, 2007, 819, 95-101.	1.5	19
1326	Singlet and triplet potential energy surfaces of C3H2. Computational and Theoretical Chemistry, 2007, 820, 65-73.	1.5	19
1327	G3(MP2) study of the reaction of O(3P) with CF3CHCH2. Computational and Theoretical Chemistry, 2007, 821, 82-88.	1.5	2
1328	Fragmentations and proton-transfer mechanisms of gaseous radical-cationic tryptophan: A theoretical study. Computational and Theoretical Chemistry, 2007, 822, 21-27.	1.5	10
1329	Ionization of carbonyl sulphide/disulphur monoxide mixtures in atmospheric gases: A theoretical study of the formation of S3O+ ions. Computational and Theoretical Chemistry, 2007, 822, 153-157.	1.5	0
1330	OH + HONO reaction: A theoretical study. Computational and Theoretical Chemistry, 2007, 847, 10-22.	1.5	6
1331	Theoretical study of the cracking mechanisms of linear Î±-olefins catalyzed by zeolites. Applied Surface Science, 2007, 254, 604-609.	3.1	22
1332	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. Chemical Physics Letters, 2007, 435, 176-181.	1.2	7
1333	Experimental and theoretical studies of the CCl+O2 reaction. Chemical Physics Letters, 2007, 437, 8-13.	1.2	6
1334	A theoretical study of the pyrolysis of isopropyl acetate. Chemical Physics Letters, 2007, 439, 8-13.	1.2	13
1335	Cl+HONO reaction: Are the hydrogen abstraction and addition direct/indirect processes?. Chemical Physics Letters, 2007, 441, 198-203.	1.2	4
1336	Theoretical study of reaction mechanism for NCO+HCNO. Chemical Physics Letters, 2007, 442, 1-6.	1.2	17
1337	Computational study of the reaction mechanism of benzylperoxy radical with HO2 in the gas phase. Chemical Physics Letters, 2007, 445, 17-21.	1.2	7
1338	New highly enantioselective thiourea-based bifunctional organocatalysts for nitro-Michael addition reactions. Catalysis Today, 2007, 121, 151-157.	2.2	99
1339	DFT and CCSD(T) study of the (A=Al,Ga) isomerization, [Ga2(Î¼4-H)(Î¼4-H2)]âˆ™ and [Ga2(Î¼4-H3)]âˆ™ unprecedented hydrido-bimetallic structures. Chemical Physics, 2007, 333, 1-9.	0.9	2
1340	Collision-induced dissociation of fluoropyridinide anions. International Journal of Mass Spectrometry, 2007, 266, 166-179.	0.7	6

#	ARTICLE	IF	CITATIONS
1341	Gaseous nitril azide N4O2: A joint theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2007, 840, 59-65.	1.8	12
1342	Mechanistic competition variations due to the substituents in the lithium carbenoid promoted cyclopropanation reactions. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 3723-3731.	0.8	1
1343	Hydride abstraction of methylamine with Cu+(1S) in the gas phase: A density functional theory study. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 3796-3803.	0.8	8
1344	Propane activation by MC5H+5 (M=Ni and Co): An experimental and theoretical work. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 5563-5570.	0.8	5
1345	Exciting flavins: Absorption spectra and spin-orbit coupling in light-oxygen-voltage (LOV) domains. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 290-300.	2.0	43
1346	Water effect on the excited-state decay paths of singlet excited cytosine. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 283-289.	2.0	43
1347	Ab initio quantum chemical studies of the reactions of CF3CFHO2 with HO2. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 46-55.	1.0	6
1348	Modeling the cyclopolymerization of diallyl ether and methyl $\alpha$ -[(allyloxy)methyl]acrylate. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 894-906.	1.0	9
1349	Theoretical study of the Si2NO potential energy surface. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1181-1193.	1.0	2
1350	DFT study of rearrangements in cyclopentylheptyl carbocations. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1772-1781.	1.0	8
1351	Theoretical studies of sulbactam: Reactions after acylation. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1925-1934.	1.0	1
1352	DFT study of cycloaddition reaction of isothiocyanates with diazoazoles to 4-imino-4H-pyrazolo[5,1-d][1,2,3,5]thiadiazines. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2479-2488.	1.0	5
1353	Quantum chemical study of penicillin: Reactions after acylation. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 2032-2039.	1.0	2
1354	Gas-phase fragmentation of protonated benzodiazepines. <i>Rapid Communications in Mass Spectrometry</i> , 2007, 21, 2273-2281.	0.7	19
1355	Brother versus brother: competitive stabilization of carbocationic centers by flanking cyclopropanes and $\beta$ -systems. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 384-394.	0.9	10
1356	Catalytic isomerization of 1-pentene to cis-2-pentene over zeolites: A quantum mechanical study. <i>Materials Chemistry and Physics</i> , 2007, 106, 394-398.	2.0	3
1357	Renner-teller effect at the initial acetylene thermal transformation stages. <i>Russian Journal of Physical Chemistry B</i> , 2007, 1, 79-84.	0.2	1
1358	Conformational study on the structures and energies of the weakly bound complexes of AlCl3 with diatomic molecules. <i>Open Chemistry</i> , 2007, 5, 1007-1018.	1.0	3

#	ARTICLE	IF	CITATIONS
1359	A DFT Study on the Mechanism of Rh <sub>2</sub> Cl <sub>2</sub> -Catalyzed Intramolecular Amidation of Carbamates. <i>Chemistry - an Asian Journal</i> , 2007, 2, 1101-1108.	1.7	99
1360	Bicyclic proline analogues as organocatalysts for stereoselective aldol reactions: an in silico DFT study. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 1287.	1.5	65
1361	Local Modifications of Single-Wall Carbon Nanotubes Induced by Bond Formation with Encapsulated Fullerenes. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1099-1109.	1.2	32
1362	Mechanistic study of the ring-size modulation in Michael–Dieckmann type reactions of 2-acylaminoacrylates with ketene diethyl acetal. <i>New Journal of Chemistry</i> , 2007, 31, 224-229.	1.4	9
1363	On the Formation of Cyclobutane Pyrimidine Dimers in UV-irradiated DNA: Why are Thymines More Reactive? <i>Photochemistry and Photobiology</i> , 2007, 78, 159-167.	1.3	5
1364	Energetics of Cytosine Singlet Excited-State Decay Paths-A Difficult Case for CASSCF and CASPT2. <i>Photochemistry and Photobiology</i> , 2007, 83, 603-610.	1.3	79
1365	Atomic radical–molecule reactions F + CH <sub>3</sub> CH: mechanistic study. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 417-429.	0.5	4
1366	Theoretical study on the potential energy surface of NC <sub>3</sub> P isomers. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 501-520.	0.5	0
1367	Light driven molecular switches: exploring and tuning their photophysical and photochemical properties. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 1041-1059.	0.5	21
1368	A barrier-free molecular radical-molecule reaction: $C_2(a^3\Pi) + O_2(X^3\Sigma^-_g) \rightarrow CO_2 + O$ . <i>Theoretical Chemistry Accounts</i> , 2007, 117, 1041-1059.	0.5	3
1369	Theoretical study on the potential energy surface of NC <sub>3</sub> P isomers. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 739-754.	0.5	1
1370	Theoretical investigation of the decomposition mechanisms of N-(2-chloroethyl)-N-nitrosourea. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 973-978.	0.5	3
1371	Chromium tricarbonyl complexes of 1,2-and 1,4-dihydronaphthalene. Synthesis and metal-induced thermal isomerizations involving endo-hydrogen atoms. <i>Russian Chemical Bulletin</i> , 2007, 56, 242-254.	0.4	3
1372	Ab initio quantum-chemical study of vinylation of pyrrole and 2-phenylazopyrrole with acetylene in a KOH/DMSO system. <i>Journal of Structural Chemistry</i> , 2007, 48, S100-S110.	0.3	2
1373	Conformational Analysis, Infrared, and Fluorescence Spectra of 1-Phenyl-1,2-propanedione 1-oxime and Related Tautomers: Experimental and Theoretical Study. <i>Monatshefte für Chemie</i> , 2007, 138, 725-734.	0.9	13
1374	Theoretical study of N <sub>4</sub> X (X = O, S, Se) systems. <i>Journal of Molecular Modeling</i> , 2007, 13, 1073-1080.	0.8	4
1375	Insertion of singlet chlorocarbenes across C-H bonds in alkanes: Evidence for two phase mechanism. <i>Journal of Chemical Sciences</i> , 2007, 119, 467-473.	0.7	1
1376	Transition state ring sizes in H-transfers in closed shell aliphatic cations. <i>International Journal of Mass Spectrometry</i> , 2007, 266, 8-14.	0.7	2

#	ARTICLE	IF	CITATIONS
1377	Mass spectrometric characterization of small oxocarboxylic acids and gas phase ion fragmentation mechanisms studied by electrospray triple quadrupole-MS/MS-TOF system and DFT theory. <i>International Journal of Mass Spectrometry</i> , 2007, 266, 97-113.	0.7	17
1378	Characterization by theory of H-transfers and onium reactions of $\text{CH}_3\text{CH}_2\text{CH}_2\text{N}+\text{H}=\text{CH}_2$ . <i>Journal of the American Society for Mass Spectrometry</i> , 2007, 18, 270-278.	1.2	21
1379	DFT and CCSD(T) study of the disilicon trihydride ( $\text{Si}_2\text{H}_3$ ) isomerization, unprecedented isomeric structures. <i>Computational and Theoretical Chemistry</i> , 2008, 852, 30-35.	1.5	3
1380	Diatomic radical-molecule reactions $\text{CN} + \text{HONO}$ : Mechanistic study. <i>Computational and Theoretical Chemistry</i> , 2008, 857, 20-26.	1.5	1
1381	Theoretical investigation on the mechanism of $\text{LiH}+\text{NH}_3 \rightarrow \text{LiNH}_2+\text{H}_2$ reaction. <i>Computational and Theoretical Chemistry</i> , 2008, 857, 111-114.	1.5	15
1382	Theoretical investigation on the radical-neutral reaction mechanism of CP with $\text{CH}_2\text{CO}$ and the structural nature of several low-lying intermediates. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 46-56.	1.5	3
1383	Chemical reactivity analysis of the $\text{CO}+\text{OH}$ and $\text{CO}+\text{HO}_2$ reactions. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 138-147.	1.5	9
1384	Theoretical study on the multi-channel reaction of $\text{CH}_3\text{S}$ with $\text{ClO}$ . <i>Computational and Theoretical Chemistry</i> , 2008, 866, 46-51.	1.5	5
1385	Hydrogenation of conjugated CC and CO bonds: Quantum chemical preview before metal catalysis. <i>Computational and Theoretical Chemistry</i> , 2008, 870, 61-64.	1.5	4
1386	Isomerization and 1,3-dipolar cycloaddition of gem-difluorinated NH-azomethine ylides in the reaction of difluorocarbene with diarylmethanimines. <i>Russian Chemical Bulletin</i> , 2008, 57, 1070-1079.	0.4	5
1387	Quantitative $^2\text{H}$ NMR spectroscopy. <i>Russian Chemical Bulletin</i> , 2008, 57, 1689-1696.	0.4	0
1388	Theoretical study of the reaction from 7-alkylidenecephalosporin sulfone to bicyclic intermediates in inhibiting $\beta$ -lactamase. <i>Structural Chemistry</i> , 2008, 19, 509-515.	1.0	2
1389	Probing the imine silylenoid $\text{HN}=\text{SiNaF}$ and its insertions reaction with $\text{R}^{\ominus}\text{H}$ ( $\text{R}=\text{F}, \text{OH}, \text{NH}_2, \text{CH}_3$ ) using DFT. <i>Structural Chemistry</i> , 2008, 19, 527-533.	1.0	6
1390	Ab initio quantum-chemical study of the mechanism of methoxide ion formation in $\text{MOH}/\text{DMSO}/\text{CH}_3\text{OH}$ systems ( $\text{M} = \text{Li}, \text{Na}, \text{K}$ ). <i>Journal of Structural Chemistry</i> , 2008, 49, 595-599.	0.3	5
1391	Kinetics of the hydrogen abstraction $\text{CHO} + \text{Alkane} \rightarrow \text{HCHO} + \text{Alkyl}$ reaction class: an application of the reaction class transition state theory. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 107-118.	0.5	10
1392	A theoretical study of the reaction of $\text{Ti}^+$ with propane. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 243-261.	0.5	9
1393	Theoretical study on the structures, isomerization and stability of $\text{SiC}_3\text{H}$ isomers. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 501-509.	0.5	5
1394	Theoretical study of the gas-phase ethane $\text{C}^{\ominus}\text{H}$ and $\text{C}^{\ominus}\text{C}$ bonds activation by bare niobium cation. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 395-403.	0.5	9

#	ARTICLE	IF	CITATIONS
1395	The interconversion mechanism between TcO <sub>3</sub> <sup>+</sup> and TcO <sub>2</sub> + core of 99mTc labeled amine-oxime (AO) complexes. <i>Theoretical Chemistry Accounts</i> , 2008, 121, 271-278.	0.5	11
1396	Theoretical study on the reaction mechanism of CN radical with ketene. <i>Science in China Series B: Chemistry</i> , 2008, 51, 101-110.	0.8	3
1397	Experimental and theoretical studies of the reaction between cationic vanadium oxide clusters and acetylene. <i>Science Bulletin</i> , 2008, 53, 3829-3838.	4.3	10
1398	Regio and stereoselectivity in ionic cycloadditions. <i>Journal of Chemical Sciences</i> , 2008, 120, 225-236.	0.7	5
1399	Recent excursions to the borderlands between the realms of concerted and stepwise: carbocation cascades in natural products biosynthesis. <i>Journal of Physical Organic Chemistry</i> , 2008, 21, 561-570.	0.9	129
1400	Mass spectrometric characterization of 4-oxopentanoic acid and gas-phase ion fragmentation mechanisms studied using a triple quadrupole and time-of-flight analyzer hybrid system and density functional theory. <i>Rapid Communications in Mass Spectrometry</i> , 2008, 22, 2269-2279.	0.7	14
1401	A comparative DFT study of substrates and products of industrial enzyme nitrile hydratase. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 161-179.	1.0	4
1402	Conformational analysis of cycloheptane, oxacycloheptane, 1,2-dioxacycloheptane, 1,3-dioxacycloheptane, and 1,4-dioxacycloheptane. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 339-350.	1.0	26
1403	A theoretical investigation on the cycloaddition reaction between azocarbenium ions and nitriles. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1067-1075.	1.0	6
1404	Mechanism for the gas-phase reaction between OH and 3-methylfuran: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1232-1238.	1.0	24
1405	A barrier-free atomic radical-molecule reaction: N( <sup>2</sup> D) NO <sub>2</sub> ( <sup>2</sup> A <sub>1</sub> ) mechanistic study. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1309-1315.	1.0	2
1406	Isomerization of HNO to HON in the singlet state assisted by amino acid residues and/or water molecules. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1246-1256.	1.0	1
1407	A theoretical study of methanol vinylation reaction mechanism. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2630-2635.	1.0	13
1408	Simple formulas for improved point-charge electrostatics in classical force fields and hybrid quantum mechanical/molecular mechanical embedding. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1905-1912.	1.0	53
1409	Extended Hartree-Fock theory of chemical reactions. VIII. Hydroxylation reactions by P450. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2991-3009.	1.0	14
1410	Ion chemistry in germane/fluorocompounds gaseous mixtures: a mass spectrometric and theoretical study. <i>Journal of Mass Spectrometry</i> , 2008, 43, 1320-1333.	0.7	11
1411	Preparation of halogenated derivatives of thiazolo[5,4-d]thiazole via direct electrophilic aromatic substitution. <i>Journal of Heterocyclic Chemistry</i> , 2008, 45, 811-819.	1.4	16
1412	Amavadin and Other Vanadium Complexes as Remarkably Efficient Catalysts for One-Pot Conversion of Ethane to Propionic and Acetic Acids. <i>Chemistry - A European Journal</i> , 2008, 14, 1828-1842.	1.7	67

#	ARTICLE	IF	CITATIONS
1413	Remarkable Ligand Effect in Ni <sup>II</sup> - and Pd <sup>II</sup> -Catalyzed Bisthiolation and Bisselenation of Terminal Alkynes: Solving the Problem of Stereoselective Dialkylchalcogenide Addition to the C≡C Bond. <i>Chemistry - A European Journal</i> , 2008, 14, 2420-2434.	1.7	76
1414	Switchable C- and N-Bound Isomers of Transition-Metal Cyanocarbaniions: Synthesis and Interconversions of Cyclopentadienyl Ruthenium Complexes of Phenylsulfonylacetonitrile Anions. <i>Chemistry - A European Journal</i> , 2008, 14, 2482-2498.	1.7	17
1415	Mechanism, Regioselectivity, and the Kinetics of Phosphine-Catalyzed [3+2] Cycloaddition Reactions of Allenates and Electron-Deficient Alkenes. <i>Chemistry - A European Journal</i> , 2008, 14, 4361-4373.	1.7	346
1416	Density Functional Studies on Palladium-Catalyzed Suzuki-Miyaura Cross-Coupling Reactions Assisted by N- or P-Chelating Ligands. <i>Chemistry - A European Journal</i> , 2008, 14, 4426-4434.	1.7	74
1417	On the Mechanisms of Degenerate Ligand Exchange in [M(CH <sub>3</sub> ) <sub>3</sub> ] <sup>+</sup> /CH <sub>4</sub> Couples (M=Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt) as Explored by Mass Spectrometric and Computational Studies: Oxidative Addition/Reductive Elimination versus $\sigma$ -Complex-Assisted Metathesis. <i>Chemistry - A European Journal</i> , 2008, 14, 5229-5236.	1.7	47
1418	Efficient Synthesis of Methylenetetrahydrofurans and Methylenepyrrolidines by Formal [3+2] Cycloadditions of Propargyl Substrates. <i>Chemistry - A European Journal</i> , 2008, 14, 6026-6036.	1.7	32
1419	New Insights on the Mechanism of the Transition-Metal Stereoselective Olefin Cyclopropanation. <i>Chemistry - A European Journal</i> , 2008, 14, 6771-6779.	1.7	38
1420	Monomer versus Alcohol Activation in the 4-Dimethylaminopyridine-Catalyzed Ring-Opening Polymerization of Lactide and Lactic <i>O</i> -Carboxylic Anhydride. <i>Chemistry - A European Journal</i> , 2008, 14, 5304-5312.	1.7	108
1421	Synthesis and Reactivity of [Penta(4-halogenophenyl)cyclopentadienyl][hydrotris(indazolyl)borato]ruthenium(II) Complexes: Rotation-Induced Fosbury Flop in an Organometallic Molecular Turnstile. <i>Chemistry - A European Journal</i> , 2008, 14, 8147-8156.	1.7	50
1422	The Role of Noninnocent Solvent Molecules in Organocatalyzed Asymmetric Michael Addition Reactions. <i>Chemistry - A European Journal</i> , 2008, 14, 10472-10485.	1.7	51
1423	Reaction Mechanism of Molybdoenzyme Formate Dehydrogenase. <i>Chemistry - A European Journal</i> , 2008, 14, 8674-8681.	1.7	47
1424	Predicting Reactivity and Stereoselectivity in the Nazarov Reaction: A Combined Computational and Experimental Study. <i>Chemistry - A European Journal</i> , 2008, 14, 9292-9304.	1.7	27
1425	Antioxidant Activity of the Anti-Inflammatory Compound Ebselen: A Reversible Cyclization Pathway via Selenenic and Seleninic Acid Intermediates. <i>Chemistry - A European Journal</i> , 2008, 14, 10603-10614.	1.7	186
1426	Transmetalation Reactions from Fischer Carbene Complexes to Late Transition Metals: A DFT Study. <i>Chemistry - A European Journal</i> , 2008, 14, 11222-11230.	1.7	44
1427	$\sigma$ -Roll-Cover-Cyclometalation of 2,2'-Bipyridine Platinum(II) Complexes in the Gas Phase: A Combined Experimental and Computational Study. <i>Chemistry - A European Journal</i> , 2008, 14, 11050-11060.	1.7	54
1428	Theoretical insight into the influences of $\pm$ -substituents in aliphatic aldehydes on the enantioselectivities of aldol reactions. <i>Chirality</i> , 2008, 20, 54-61.	1.3	4
1429	Theoretical Study on Proton-Transfer Reaction of Intracellular Second-messenger 3',5'-Cyclic Nucleotide. <i>Chinese Journal of Chemistry</i> , 2008, 26, 1363-1366.	2.6	1
1430	Direct Ab Initio Dynamics Study on the Reaction of CH <sub>3</sub> CHF <sub>2</sub> (HFC-152a) with the Cl Atom. <i>ChemPhysChem</i> , 2008, 9, 847-853.	1.0	5

#	ARTICLE	IF	CITATIONS
1431	Theoretical Investigation of the OH <sup>•</sup> -Initiated Oxidation of Benzaldehyde in the Troposphere. <i>ChemPhysChem</i> , 2008, 9, 1453-1459.	1.0	19
1432	Insight into Markovnikov Reactions of Alkenes in Terms of Ab Initio and Molecular Face Theory. <i>ChemPhysChem</i> , 2008, 9, 2379-2389.	1.0	27
1433	IR Low-Temperature Matrix and ab Initio Study on Î²-Alanine Conformers. <i>ChemPhysChem</i> , 2008, 9, 2042-2051.	1.0	32
1434	Competitive Intramolecular Aryl- and Alkyl-C-H Bond Activation and Ligand Evaporation from Gaseous Bisimino Complexes [Pt(L)(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> S] <sup>+</sup> (L=C <sub>6</sub> H <sub>5</sub> Ni <sup>3/4</sup> C(CH <sub>3</sub> ) <sub>3</sub> ), <sup>14</sup> Helvetica Chimica Acta, 2008, 91, 1902-1915.	1.0	14
1435	Ligand Effects on the Mechanisms of Thermal Bond Activation in the Gas-Phase Reactions NiX <sup>+</sup> /CH <sub>4</sub> <sup>+</sup> Ni(CH <sub>3</sub> ) <sub>3</sub> <sup>+</sup> /HX (X=H, CH <sub>3</sub> , OH, F). Short Communication. <i>Helvetica Chimica Acta</i> , 2008, 91, 2203-2210.	1.0	33
1436	Reaction of hypochlorous acid with imidazole: Formation of 2-chloro- and 2-oxoimidazoles. <i>Journal of Computational Chemistry</i> , 2008, 29, 98-107.	1.5	18
1437	Improving the efficiency of the NEB reaction path finding algorithm. <i>Journal of Computational Chemistry</i> , 2008, 29, 139-143.	1.5	30
1438	Ring inversion in 1,4,7 cyclononatriene and analogues: Ab initio and DFT calculations and topological analysis. <i>Journal of Computational Chemistry</i> , 2008, 29, 280-290.	1.5	4
1439	Theoretical studies on pyridoxal 5-phosphate-dependent transamination of Î±-amino acids. <i>Journal of Computational Chemistry</i> , 2008, 29, 1919-1929.	1.5	32
1440	The dramatic effect of NH <sub>3</sub> coordination on the Fe <sup>+</sup> -assisted activation of carbon dioxide in the gas phase: From bare metal ions to complexes. <i>Journal of Computational Chemistry</i> , 2008, 29, 2382-2396.	1.5	2
1441	Theoretical Study on a Class of Organometallic Complexes Based on All-Metal Aromatic Ga <sub>3</sub> <sup>+</sup> Through Sandwiching Stabilization. <i>European Journal of Inorganic Chemistry</i> , 2008, 2099-2106.	1.0	6
1442	The Cyclooligomerisation of Acetylene at Metal Centres. <i>European Journal of Inorganic Chemistry</i> , 2008, 2874-2883.	1.0	19
1443	The Noncarbonylative Photochemistry of Group 6 Fischer Carbene Complexes. <i>European Journal of Inorganic Chemistry</i> , 2008, 2454-2462.	1.0	20
1444	A Novel Addition Mechanism for the Reaction of Frustrated Lewis Pairs with Olefins. <i>European Journal of Inorganic Chemistry</i> , 2008, 2501-2505.	1.0	85
1445	A Theoretical Study on the Reactivity of a Rhenium Hydroxo-Carbonyl Complex Towards Î²-Lactams. <i>European Journal of Inorganic Chemistry</i> , 2008, 4547-4554.	1.0	1
1446	Reactions of Arenediazonium Benzenedisulfonimides with Aliphatic Triorganoindium Compounds. <i>European Journal of Organic Chemistry</i> , 2008, 862-868.	1.2	14
1447	Ketene Formation or Phenyl-Group Migration as the Favorable Intramolecular Rearrangement in Phenyliodonium Ylides of Hydroxyquinones. <i>European Journal of Organic Chemistry</i> , 2008, 1783-1788.	1.2	13
1448	3,5-Bis(trifluoromethyl)phenyl Sulfones for the Highly Stereoselective Julia-Kocienski Synthesis of Î±,Î²-Unsaturated Esters and Weinreb Amides. <i>European Journal of Organic Chemistry</i> , 2008, 2915-2922.	1.2	25

#	ARTICLE	IF	CITATIONS
1449	On the Mechanism of Gold(I)-Catalyzed Ring Expansion of Cyclopropanols: Theoretical Calculations Uncover a Bottle-Neck 1,4-H Shift and Suggest Adequate Reaction Conditions. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 3004-3013.	1.2	28
1450	Mechanisms of Brønsted Acid Catalyzed Additions of Phenols and Protected Amines to Olefins: A DFT Study. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 4296-4303.	1.2	27
1451	Mechanism of the Nucleophilic Substitution of Acyl Electrophiles using Lithium Organocuprates. <i>Advanced Synthesis and Catalysis</i> , 2008, 350, 1063-1072.	2.1	27
1452	Elimination of H <sub>2</sub> from CH <sub>3</sub> CH=N <sup>+</sup> HCH <sub>3</sub> : A synchronous, concerted 1,4-H <sub>2</sub> elimination. <i>Journal of the American Society for Mass Spectrometry</i> , 2008, 19, 27-32.	1.2	2
1453	1,2-Eliminations from (CH <sub>3</sub> ) <sub>2</sub> NH <sup>+</sup> CH <sub>2</sub> CH <sub>3</sub> and (CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> <sup>+</sup> : Guided dissociations. <i>Journal of the American Society for Mass Spectrometry</i> , 2008, 19, 1491-1499.	1.2	6
1454	Bonding analysis and the mechanisms on the ring-opening of alkoxy-bridged bis(silylene) transition-metal complexes toward MeOH. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 639-645.	0.8	6
1455	Theoretical study on the hydrogen abstraction reaction of CH <sub>3</sub> CH <sub>2</sub> F (HFC-161) with Cl atom. <i>Chemical Physics Letters</i> , 2008, 450, 186-191.	1.2	7
1456	Gas-phase reactivities of charged platinum dimers with ammonia: A combined experimental/theoretical study. <i>Chemical Physics Letters</i> , 2008, 450, 268-273.	1.2	16
1457	Mechanism for the gas-phase reaction between NO <sub>3</sub> and furan: A theoretical study. <i>Chemical Physics Letters</i> , 2008, 455, 164-168.	1.2	7
1458	Selective IR-induced isomerization of 1,2-dichloropropane isolated in xenon matrix. <i>Chemical Physics Letters</i> , 2008, 456, 127-134.	1.2	10
1459	Initial adsorption mechanisms of TiCl <sub>4</sub> on OH/Si(100)-2 $\times$ 1. <i>Chemical Physics Letters</i> , 2008, 457, 69-73.	1.2	16
1460	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. <i>Chemical Physics Letters</i> , 2008, 456, 135-140.	1.2	80
1461	How does the Fe <sup>+</sup> -mediated demethanation of CH <sub>3</sub> OCH <sub>3</sub> occurs? A density functional theoretical study. <i>Chemical Physics Letters</i> , 2008, 459, 33-38.	1.2	12
1462	Theoretical study of the reaction mechanism of ethynyl radical with benzene and related reactions on the C <sub>8</sub> H <sub>7</sub> potential energy surface. <i>Chemical Physics Letters</i> , 2008, 459, 54-59.	1.2	22
1463	Adsorption of TiCl <sub>4</sub> on H/Si(1 0 0)-2 $\times$ 1 Surface. <i>Chemical Physics Letters</i> , 2008, 461, 249-253.	1.2	14
1464	Mechanistic and kinetic study of the OH+C <sub>2</sub> H <sub>5</sub> CN reaction. <i>Chemical Physics Letters</i> , 2008, 463, 315-321.	1.2	14
1465	Computational studies on the mechanisms for the gas-phase reaction between thiophene and NO <sub>3</sub> . <i>Chemical Physics Letters</i> , 2008, 467, 52-57.	1.2	7
1466	A theoretical analysis of the Ti(IV)-catalyzed glycoaminocyanation reaction. <i>Carbohydrate Research</i> , 2008, 343, 1835-1839.	1.1	0



#	ARTICLE	IF	CITATIONS
1467	A DFT study of methanol dissociation on isolated vanadate groups. <i>Catalysis Today</i> , 2008, 139, 214-220.	2.2	17
1468	Ab initio/DFT theory and multichannel RRKM study on the mechanisms and kinetics for the CH <sub>3</sub> S+CO reaction. <i>Chemical Physics</i> , 2008, 344, 221-226.	0.9	17
1469	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. <i>Chemical Physics</i> , 2008, 344, 273-280.	0.9	12
1470	Theoretical study of the cycloaddition of nitrones to cinnamitrile: effect of Lewis acid coordination on the selectivity of the reaction. <i>Tetrahedron</i> , 2008, 64, 477-486.	1.0	16
1471	Sigmatropic shifts and cycloadditions on neutral, cationic, and anionic pentadienyl+butadiene potential energy surfaces. <i>Tetrahedron</i> , 2008, 64, 5672-5679.	1.0	16
1472	Diastereo- and regioselective Diels-Alder reactions of 2-phosphaindolizines. <i>Tetrahedron</i> , 2008, 64, 6395-6401.	1.0	18
1473	On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. <i>Tetrahedron</i> , 2008, 64, 6215-6220.	1.0	19
1474	Mechanistic insights on the site selectivity in successive 1,3-dipolar cycloadditions to meso-tetraarylporphyrins. <i>Tetrahedron</i> , 2008, 64, 7937-7943.	1.0	28
1475	New chiral tetraaza ligands for the efficient enantioselective addition of dialkylzinc to aromatic aldehydes. <i>Tetrahedron</i> , 2008, 64, 9717-9724.	1.0	34
1476	Formation of novel thiazolomorphinans and thiazoloaporphines. <i>Tetrahedron</i> , 2008, 64, 10388-10394.	1.0	7
1477	Theoretical study of the reactions of AlF with HCl: Reaction pathways. <i>Computational and Theoretical Chemistry</i> , 2008, 848, 139-143.	1.5	2
1478	A DFT modelling of the Darzens reaction. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 1-7.	1.5	3
1479	Si <sub>2</sub> CS: A new sulfur-containing molecule with singlet cyclic ground state. <i>Computational and Theoretical Chemistry</i> , 2008, 848, 74-81.	1.5	2
1480	Theoretical study on the reaction of Mn <sup>+</sup> (7S and 5S states) with COS. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 127-133.	1.5	5
1481	Computational study on the mechanism for the reaction of OH with 2-methylfuran. <i>Computational and Theoretical Chemistry</i> , 2008, 851, 353-357.	1.5	22
1482	Mechanistic details of the domino reaction of nitronaphthalenes with the electron-rich dienes. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2008, 853, 68-76.	1.5	27
1483	Theoretical study on the mechanism and rate constants for the gas phase reaction of OH radicals with trans-CF <sub>3</sub> CHCHF. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 30-37.	1.5	8
1484	Theoretical study on the addition reactions of silylenoids H <sub>2</sub> SiLiX (X=F, Cl) to formaldehyde. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 96-104.	1.5	6

#	ARTICLE	IF	CITATIONS
1485	Oxidation of catechol to 2-hydroxymuconic semialdehyde. <i>Computational and Theoretical Chemistry</i> , 2008, 856, 71-78.	1.5	0
1486	Theoretical studies of samarium carbenoid promoted cyclopropanation reaction with allylic alcohol on the reaction pathways. <i>Computational and Theoretical Chemistry</i> , 2008, 858, 66-71.	1.5	4
1487	Ozonization of C70 and subsequent thermolysis of ozonide 1,2-C70O3: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2008, 860, 24-31.	1.5	17
1488	Theoretical study of the reaction of 2,4-dichlorophenol with 1O2. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 27-32.	1.5	14
1489	Theoretical study of the mechanism and regioselectivity of the 1,3-dipolar cycloaddition of diazomethane with methyl acrylate using theoretical approaches. <i>Computational and Theoretical Chemistry</i> , 2008, 862, 1-6.	1.5	19
1490	Quantum chemical study of thiosulfenic acids and their anions. <i>Computational and Theoretical Chemistry</i> , 2008, 863, 105-110.	1.5	6
1491	Theoretical study on the reaction of atomic oxygen radical anion with propene. <i>Computational and Theoretical Chemistry</i> , 2008, 867, 28-32.	1.5	2
1492	Quantum chemical study on the atmospheric photooxidation of methyl vinyl ether (MVE). <i>Computational and Theoretical Chemistry</i> , 2008, 868, 87-93.	1.5	11
1493	DFT study on C-C bond cleavage of nitriles by a silyl(silylene)iron complex. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 59-66.	1.5	10
1494	Theoretical investigation for the reaction of NO2(2A1) with CO(1 $\hat{\sigma}^+$ ) catalyzed by Ti+(X4F). <i>Computational and Theoretical Chemistry</i> , 2008, 869, 89-93.	1.5	10
1495	On the selective electrogeneration of 1-aryl-4,4-dichlorobut-3-en-1-ones from 2,2,2-trichloroethylideneacetophenones. <i>Electrochimica Acta</i> , 2008, 53, 7138-7145.	2.6	4
1496	Norbornadiene complexes of molybdenum(II) and their transformation to a catalyst for ring-opening metathesis polymerization: DFT calculations and X-ray crystal structure of a new norbornadiene complex [MoCl(GeCl3)(CO)3( $\hat{i}$ -4-nbd)]. <i>Inorganica Chimica Acta</i> , 2008, 361, 502-512.	1.2	20
1497	Density Functional Theory Studies of Negishi Alkyl-Alkyl Cross-Coupling Reactions Catalyzed by a Methylterpyridyl-Ni(I) Complex. <i>Journal of Organic Chemistry</i> , 2008, 73, 3680-3688.	1.7	174
1498	Mechanistic possibilities for oxetane formation in the biosynthesis of Taxol's D ring. <i>Russian Journal of General Chemistry</i> , 2008, 78, 723-731.	0.3	15
1499	Capture of hydroxymethylene and its fast disappearance through tunnelling. <i>Nature</i> , 2008, 453, 906-909.	13.7	264
1500	Mechanistic analogies and differences between gold- and palladium-supported Schiff base complexes as hydrogenation catalysts: A combined kinetic and DFT study. <i>Journal of Catalysis</i> , 2008, 254, 226-237.	3.1	29
1501	Catalytic mechanism of human DNA polymerase $\beta$ with Mg <sup>2+</sup> and Mn <sup>2+</sup> from ab initio quantum mechanical/molecular mechanical studies. <i>DNA Repair</i> , 2008, 7, 1824-1834.	1.3	52
1502	Experimental and Theoretical Study of the Carbon-13 and Deuterium Kinetic Isotope Effects in the Cl and OH Reactions of CH3F. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12416-12429.	1.1	10

#	ARTICLE	IF	CITATIONS
1503	Reaction Coordinates and the Transition-Vector Approximation to the IRC. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 920-928.	2.3	43
1504	Comparison of Nitroaldol Reaction Mechanisms Using Accurate Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10635-10649.	1.1	9
1505	Unusual Concerted Lewis Acid-Lewis Base Mechanism for Hydrogen Activation by a Phosphine-Borane Compound. <i>Inorganic Chemistry</i> , 2008, 47, 6212-6219.	1.9	123
1506	Theoretical and Experimental Studies on the Mechanism of Norbornadiene Pauson-Khand Cycloadducts Photorearrangement. Is There a Pathway on the Excited Singlet Potential Energy Surface?. <i>Journal of the American Chemical Society</i> , 2008, 130, 16898-16907.	6.6	5
1507	A Computational Study on Some Viable Targets for Gas-Phase Synthesis of Metal Complexes of the Cyclic (B <sub>6</sub> C) <sup>2+</sup> and Their Bonding Pattern. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10365-10377.	1.1	13
1508	Computational Study on Nonenzymatic Peptide Bond Cleavage at Asparagine and Aspartic Acid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8752-8761.	1.1	57
1509	Reaction Electronic Flux: A New Concept To Get Insights into Reaction Mechanisms. Study of Model Symmetric Nucleophilic Substitutions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11801-11807.	1.1	100
1510	Theoretical Analysis of the Reaction Mechanism of Biotin Carboxylase. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 366-374.	2.3	7
1511	Asymmetric Aza-Henry Reaction Under Phase Transfer Catalysis: An Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2008, 130, 7955-7966.	6.6	151
1512	Transition State Theory and Molecular Orbital Calculations Applied to Rates and Reaction Mechanisms in Geochemical Kinetics. , 2008, , 39-72.		1
1513	Partial Oxidation of Propylene Catalyzed by VO <sub>3</sub> Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5984-5993.	1.1	45
1514	Substituent Effects on Singlet-Triplet Gaps and Mechanisms of 1,2-Rearrangements of 1,3-Oxazol-2-ylidenes to 1,3-Oxazoles. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8775-8784.	1.1	19
1515	Intermolecular Cope-Type Hydroamination of Alkenes and Alkynes using Hydroxylamines. <i>Journal of the American Chemical Society</i> , 2008, 130, 17893-17906.	6.6	84
1516	Kinetic Modeling of Methyl Butanoate in Shock Tube. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13470-13480.	1.1	70
1517	Regulation Mechanism of Spin-Orbit Coupling in Charge-Transfer-Induced Luminescence of Imidazopyrazinone Derivatives. <i>Journal of the American Chemical Society</i> , 2008, 130, 132-149.	6.6	53
1518	Pericyclic versus Pseudopericyclic Reactions. What the Laplacian of the Charge Density, $\nabla^2 \rho(\mathbf{r})$ , Has To Say about It? The Case of Cycloaddition Reactions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8164-8178.	1.1	22
1519	The H <sub>2</sub> O <sub>2</sub> +OH <sup>+</sup> HO <sub>2</sub> +H <sub>2</sub> O reaction in aqueous solution from a charge-dependent continuum model of solvation. <i>Journal of Chemical Physics</i> , 2008, 129, 014506.	1.2	13
1520	High Level ab Initio Exploration on the Conversion of Carbon Dioxide into Oxazolidinones: The Mechanism and Regioselectivity. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6708-6714.	1.1	26

#	ARTICLE	IF	CITATIONS
1521	An Understanding of the Electrophilic/Nucleophilic Behavior of Electro-Deficient 2,3-Disubstituted 1,3-Butadienes in Polar Diels-Alder Reactions. A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4046-4053.	1.1	100
1522	Computational Studies on Biosynthetic Carbocation Rearrangements Leading to Sativene, Cyclosativene, Î±-Ylangene, and Î²-Ylangene. <i>Journal of Organic Chemistry</i> , 2008, 73, 6570-6579.	1.7	57
1523	Elucidation of the natural artemisinin decomposition route upon iron interaction: a fine electronic redistribution promotes reactivity. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5083.	1.3	11
1525	Understanding the Reactivity of Captodative Ethylenes in Polar Cycloaddition Reactions. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 4615-4624.	1.7	846
1526	Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 49-63.	2.3	21
1527	Theoretical study of two pathways of double-bond isomerization of pentene catalyzed by zeolites. <i>Computational Materials Science</i> , 2008, 42, 179-185.	1.4	9
1528	Reactions of the hydroperoxide anion with dimethyl methylphosphonate in an ion trap mass spectrometer: evidence for a gas phase Î±-effect. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 2316.	1.5	49
1529	Experimental and Theoretical Study of the Reactions between Small Neutral Iron Oxide Clusters and Carbon Monoxide. <i>Journal of the American Chemical Society</i> , 2008, 130, 15879-15888.	6.6	156
1530	Branching Ratios of Aliphatic Amines + OH Gas-Phase Reactions: A Variational Transition-State Theory Study. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 322-327.	2.3	43
1531	New Algorithms for Optimizing and Linking Conical Intersection Points. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 257-266.	2.3	97
1532	Crystalline packings of diketoarylhydrazones controlled by a methyl for trifluoromethyl structural change. <i>CrystEngComm</i> , 2008, 10, 541.	1.3	22
1533	Theoretical investigation of the reaction mechanism for the phosphate diester hydrolysis using an asymmetric dinuclear metal complex as a biomimetic model of the purple acid phosphatase enzyme. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7039.	1.3	30
1534	Reactivity of Pt- and Pd-bound nitriles towards nitrile oxides and nitrones: substitution vs. cycloaddition. <i>Dalton Transactions</i> , 2008, , 1312.	1.6	25
1535	DFT calculations of 1H and 13C NMR chemical shifts in transition metal hydrides. <i>Dalton Transactions</i> , 2008, , 3959.	1.6	37
1536	Ring opening at N1-C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study. <i>Dalton Transactions</i> , 2008, , 6427.	1.6	1
1537	Theoretical study of multiphoton ionization of cyclohexadienes and unimolecular decomposition of their mono- and dications. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2321.	1.3	12
1538	Propensity for local folding induced by the urea fragment in short-chain oligomers. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 2596.	1.5	37
1539	An efficient synthesis of chiral phosphinyl oxide pyrrolidines and their application to asymmetric direct aldol reactions. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 3997.	1.5	49

#	ARTICLE	IF	CITATIONS
1540	Catalytic Oxidation of H <sub>2</sub> by N <sub>2</sub> O in the Gas Phase: O-Atom Transport with Atomic Metal Cations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10141-10146.	1.1	21
1541	Reaction Mechanism of HCN+ + C <sub>2</sub> H <sub>4</sub> : A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12252-12262.	1.1	6
1542	Cascade Reactions of Dialkynyl Fischer Carbene Complexes Involving Intramolecular Alkyne Insertions Oriented to the Synthesis of Functionalized Polycycles. <i>Organometallics</i> , 2008, 27, 3593-3600.	1.1	13
1543	Interplay of Hydrogenation and Dehydrogenation in Isoindoline and Indoline Isomers: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5278-5285.	1.1	5
1544	Theoretical Survey of the Potential Energy Surface of Methyl Nitrite + Cu <sup>+</sup> Reaction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 533-541.	1.1	2
1545	Variability of Chain Transfer to Monomer Step in Olefin Polymerization. <i>Organometallics</i> , 2008, 27, 4098-4107.	1.1	59
1546	Soot Platelets and PAHs with an Odd Number of Unsaturated Carbon Atoms and $\pi$ Electrons: A Theoretical Study of Their Spin Properties and Interaction with Ozone. <i>Journal of Physical Chemistry A</i> , 2008, 112, 973-982.	1.1	20
1547	Acetylene Cyclotrimerization Catalyzed by TiO <sub>2</sub> and VO <sub>2</sub> in the Gas Phase: A DFT Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3731-3741.	1.1	36
1548	Gas-Phase Reactions of Co <sup>+</sup> with Ethylamine: A Theoretical Approach to the Reaction Mechanisms of Transition Metal Ions with Primary Amines. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5312-5321.	1.1	15
1549	Directing Aryl-I versus Aryl-Br Bond Activation by Nickel via a Ring Walking Process. <i>Inorganic Chemistry</i> , 2008, 47, 5114-5121.	1.9	62
1550	Enantio- and Diastereoselectivities in Chiral Sulfur Ylide Promoted Asymmetric Aziridination Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 8163-8174.	1.7	42
1551	Ab Initio and DFT Studies of the Thermal Rearrangement of Trimethylsilylsilylene. <i>Organometallics</i> , 2008, 27, 2123-2127.	1.1	4
1552	DFT Study on the Diels-Alder Cycloaddition between Alkenyl-M(0) (M = Cr, W) Carbene Complexes and Neutral 1,3-Dienes. <i>Journal of Organic Chemistry</i> , 2008, 73, 2083-2089.	1.7	46
1553	Understanding the Participation of Quadricyclane as Nucleophile in Polar [2 <sub>i</sub> f + 2 <sub>i</sub> f + 2 <sub>i</sub> e] Cycloadditions toward Electrophilic $\pi$ Molecules. <i>Journal of Organic Chemistry</i> , 2008, 73, 8791-8799.	1.7	220
1554	Infrared Spectroscopic and Density Functional Theory Studies on the Reactions of Yttrium and Lanthanum Atoms with Nitrous Oxide in Excess Argon. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6289-6294.	1.1	7
1555	Allene as the Parent Substrate in Zinc-Mediated Biomimetic Hydration Reactions of Cumulenes. <i>Journal of Organic Chemistry</i> , 2008, 73, 8265-8278.	1.7	7
1556	Face-Selective Diels-Alder Reactions between Unsymmetrical Cyclohexadienes and Symmetric trans-Dienophile: An Experimental and Computational Investigation. <i>Journal of Organic Chemistry</i> , 2008, 73, 435-444.	1.7	10
1557	Combined Experimental and Computational Studies on Carbon-Carbon Reductive Elimination from Bis(hydrocarbyl) Complexes of (PCP)Ir. <i>Journal of the American Chemical Society</i> , 2008, 130, 11317-11327.	6.6	64

#	ARTICLE	IF	CITATIONS
1558	On the Catalytic Role of Ge <sup>+</sup> and Se <sup>+</sup> in the Oxygen Transport Activation of N <sub>2</sub> O by CO. Journal of Chemical Theory and Computation, 2008, 4, 316-321.	2.3	9
1559	A DFT Study on the Mechanism of Cyclopropanation via Cu(acac) <sub>2</sub> -Catalyzed Diazo Ester Decomposition. Organometallics, 2008, 27, 4600-4610.	1.1	24
1560	Base-Induced Decomposition of Alkyl Hydroperoxides in the Gas Phase. Part 3. Kinetics and Dynamics in HO <sup>•</sup> + CH <sub>3</sub> OOH, C <sub>2</sub> H <sub>5</sub> OOH, and <i>tert</i> -C <sub>4</sub> H <sub>9</sub> OOH Reactions. Journal of Physical Chemistry A, 2008, 112, 9516-9525.	1.1	17
1561	Photoisomerization Reactions of Cyclopropene and 1,3,3-Trimethylcyclopropene: A Theoretical Study. Journal of Chemical Theory and Computation, 2008, 4, 1263-1273.	2.3	6
1562	Diastereoselective Addition of Zincated Hydrazones to Alkenylboronates and Stereospecific Trapping of Boron/Zinc Bimetallic Intermediates by Carbon Electrophiles. Journal of the American Chemical Society, 2008, 130, 15688-15701.	6.6	28
1563	Intrinsic Reaction Coordinate Analysis of the Activation of CH <sub>4</sub> by Molybdenum Atoms: A Density Functional Theory Study of the Crossing Seams of the Potential Energy Surfaces. Organometallics, 2008, 27, 181-188.	1.1	25
1564	Deeper Insight into the Mechanism of the Reaction of Photogenerated Metallaketenes and Imines. Journal of the American Chemical Society, 2008, 130, 13892-13899.	6.6	30
1565	Computational Study of the Reaction of CH <sub>2</sub> (X <sup>3</sup> B <sub>1</sub> ) with CH <sub>3</sub> OH. Journal of Physical Chemistry A, 2008, 112, 12492-12497.	1.1	6
1566	Effect of Substituents on the GPx-like Activity of Ebselen: Steric versus Electronic. Journal of Physical Chemistry A, 2008, 112, 1013-1017.	1.1	41
1567	Structural Reorganization and Preorganization in Enzyme Active Sites: Comparisons of Experimental and Theoretically Ideal Active Site Geometries in the Multistep Serine Esterase Reaction Cycle. Journal of the American Chemical Society, 2008, 130, 15361-15373.	6.6	96
1568	A Quantum Chemistry Study of the Cl Atom Reaction with Formaldehyde. Journal of Physical Chemistry A, 2008, 112, 9-22.	1.1	22
1569	Computational Study on Kinetics and Mechanisms of Unimolecular Decomposition of Succinic Acid and Its Anhydride. Journal of Physical Chemistry A, 2008, 112, 6621-6629.	1.1	10
1570	Kinetics and Mechanism of the NCN + NO <sub>2</sub> Reaction Studied by Experiment and Theory. Journal of Physical Chemistry A, 2008, 112, 10185-10192.	1.1	9
1571	A Quantum Chemical Study of the Generation of a Potential Prebiotic Compound, Cyanoacetaldehyde, and Related Sulfur Containing Species. Journal of Physical Chemistry A, 2008, 112, 11009-11016.	1.1	21
1572	Influence of Ligands on the Dynamics of Hydrogen Elimination in Cationic Complexes of Co and Rh. Journal of Physical Chemistry A, 2008, 112, 13139-13148.	1.1	15
1573	Approach to the Atmospheric Chemistry of Methyl Nitrate and Methylperoxy Nitrite. Chemical Mechanisms of Their Formation and Decomposition Reactions in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 249-255.	1.1	41
1574	Theoretical Studies of the sp <sup>2</sup> versus sp <sup>3</sup> C-H Bond Activation Chemistry of 2-Picoline by (C <sub>5</sub> Me <sub>5</sub> ) <sub>2</sub> An(CH <sub>3</sub> ) <sub>2</sub> Complexes (An = Th, U). Organometallics, 2008, 27, 1384-1392.	1.1	36
1575	Theoretical Study of the Acid-Promoted Hydrolysis of Oxazolin-5-one: A Microhydration Model. Journal of Physical Chemistry B, 2008, 112, 10659-10667.	1.2	16

#	ARTICLE	IF	CITATIONS
1576	Experimental and Theoretical Study of the Reactions between Neutral Vanadium Oxide Clusters and Ethane, Ethylene, and Acetylene. <i>Journal of the American Chemical Society</i> , 2008, 130, 1932-1943.	6.6	137
1577	Reaction Mechanism and Stereoselectivity of Ruthenium <sup>II</sup> -Porphyrin-Catalyzed Intramolecular Amidation of Sulfamate Ester: A DFT Computational Study. <i>Journal of Organic Chemistry</i> , 2008, 73, 529-537.	1.7	42
1578	Substituent Effects on the Ring-Opening Mechanism of Lithium Bromocyclopropylidenoids to Allenes. <i>Journal of Organic Chemistry</i> , 2008, 73, 8182-8188.	1.7	18
1579	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. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5224-5235.	1.1	21
1580	<sup>13</sup> C, <sup>18</sup> O, and D Fractionation Effects in the Reactions of CH <sub>3</sub> OH Isotopologues with Cl and OH Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11099-11114.	1.1	15
1581	A Linear Energy Relationship between Activation Energy and Absolute Hardness: A Case Study with the O( <sup>3</sup> P) Atom-Addition Reactions to Polyaromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8205-8207.	1.1	9
1582	Theoretical Study on the Nitration of Methane by Acyl Nitrate Catalyzed by H-ZSM5 Zeolite. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8916-8919.	1.1	5
1583	Effect of Lewis Acid Catalysts on Diels-Alder and Hetero-Diels-Alder Cycloadditions Sharing a Common Transition State. <i>Journal of Organic Chemistry</i> , 2008, 73, 7472-7480.	1.7	52
1584	Theoretical Study of HCN + C <sub>2</sub> H <sub>2</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8188-8197.	1.1	2
1585	Theoretical Study of the Reaction Mechanism of HCN <sup>+</sup> and CH <sub>4</sub> of Relevance to Titan's Ion Chemistry. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2693-2701.	1.1	4
1586	Density Functional Theory Investigation into the Mechanism for $\hat{I}$ -2-Alkyne to Vinylidene Isomerization by the Addition of Phenylacetylene to [( $\hat{I}$ -3-C <sub>3</sub> H <sub>5</sub> )Rh(PiPr <sub>3</sub> ) <sub>2</sub> ]. <i>Organometallics</i> , 2008, 27, 4325-4333.	1.1	34
1587	Theoretical Analysis of the Hydrogen-Transfer Reaction to C <sup>•</sup> N, C <sup>•</sup> C, and C <sup>•</sup> C Bonds Catalyzed by Shvo <sup>TM</sup> s Ruthenium Complex. <i>Organometallics</i> , 2008, 27, 4854-4863.	1.1	44
1588	Thermal Decomposition Mechanisms of Methanol, Ethanol, and 1-Propanol on the Si(100)-2 $\times$ 1 Surface. <i>Journal of Physical Chemistry C</i> , 2008, 112, 6907-6913.	1.5	11
1589	Mechanisms for the Reactions of Hydroxyl Radicals with Acrolein: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 941-950.	2.3	19
1590	Hydrothermal Reaction of Cu(II)/Pyrazine-2,3,5-tricarboxylic acid and Characterization of the Copper(II) Complexes. <i>Inorganic Chemistry</i> , 2008, 47, 5225-5233.	1.9	47
1591	Reactions of Ruthenium Acetylide and Vinylidene Complexes Containing a 2-Pyridyl Group. <i>Organometallics</i> , 2008, 27, 5212-5220.	1.1	13
1592	Computational Modeling of Cytosine Photophysics and Photochemistry: From the Gas Phase to DNA. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 473-492.	0.6	3
1593	Halogen Bonding with Dihalogens and Interhalogens. , 2007, , 65-104.		59

#	ARTICLE	IF	CITATIONS
1594	DFT STUDY ON THE MECHANISM OF DNA DAMAGE CAUSED BY THE ISOMERIZATION OF DNA PURINE BASE. Journal of Theoretical and Computational Chemistry, 2008, 07, 457-472.	1.8	7
1595	A DFT STUDY ON THE REACTION MECHANISM OF SrO + CH <sub>4</sub> . Journal of Theoretical and Computational Chemistry, 2008, 07, 189-203.	1.8	5
1596	Theoretical Study on Reaction Mechanism of Aluminum-Water System. Chinese Journal of Chemical Physics, 2008, 21, 245-249.	0.6	15
1597	The role of the excited electronic states in the C <sup>++</sup> +H <sub>2</sub> O reaction. Journal of Chemical Physics, 2008, 128, 144310.	1.2	4
1598	Kinetic and theoretical study of the reaction of Cl atoms with a series of linear thiols. Journal of Chemical Physics, 2008, 129, 194303.	1.2	5
1599	Quantum chemical study on influence of substituents and solvents in reaction complexing ethylene with nickel dithiolene. Molecular Simulation, 2008, 34, 631-636.	0.9	3
1600	The reaction pathways of the oxygen plasma pulse in the hafnium oxide atomic layer deposition process. Applied Physics Letters, 2008, 93, 124104.	1.5	16
1601	Theoretical Studies on the Kinetics and Mechanisms of Reactions for Methyl Vinyl Ether and Ozone. Chinese Journal of Chemical Physics, 2008, 21, 324-332.	0.6	1
1602	<i>Ab initio</i> Study on Structures and Isomerization of Magnesium Fluorosilylenoid H <sub>2</sub> SiFMgF. Chinese Journal of Chemical Physics, 2008, 21, 541-546.	0.6	6
1603	The reaction path of CO and Fe<math>\times 2</math>/<math>\times 2</math>/O<math>\times 3</math>/<math>\times 3</math>/ in a chemical-looping combustion system. , 2009, , .		0
1604	AB INITIO INVESTIGATIONS OF THE RADICAL-RADICAL REACTION: N (4S) + NCO (X <sup>2</sup> ). Journal of Theoretical and Computational Chemistry, 2009, 08, 587-595.	1.8	2
1605	Density functional computations of Rh(I)-catalysed hydroacylation and hydrogenation of ethene using formic acid. Molecular Simulation, 2009, 35, 419-427.	0.9	4
1606	Insights into the Maillard reaction. The mechanism of Schiff's base formation from the reaction force perspective. Molecular Physics, 2009, 107, 1587-1596.	0.8	6
1607	SINGLET METHYLENE AND HALOCARBENES INSERTIONS INTO POLAR N-H BONDS OF AMINES. Journal of Theoretical and Computational Chemistry, 2009, 08, 1143-1153.	1.8	2
1608	Optical activity in conformationally flexible molecules: a theoretical study of large-amplitude vibrational averaging in (<math>R</math>)-3-chloro-1-butene. Molecular Physics, 2009, 107, 1041-1057.	0.8	32
1609	A quantum chemistry study of Diels-Alder dimerizations in benzene and anthracene. Journal of Chemical Physics, 2009, 131, 024313.	1.2	16
1610	[N <sub>3</sub> MN <sub>5</sub> ] <sup>q</sup> : A Type of Low-Lying Sandwich-like Isomer on [N <sub>8</sub> M] <sup>q</sup> Hypersurface with (M, q) = (Ni, 0), (Co, 1), and (Fe, 2).	1.1	11
1611	Experimental and Theoretical Study of Hydrogen Atom Abstraction from Ethylene by Stoichiometric Zirconium Oxide Clusters. Chinese Journal of Chemical Physics, 2009, 22, 635-641.	0.6	13



#	ARTICLE	IF	CITATIONS
1612	The reaction of N <sub>2</sub> O with phenylium ions C <sub>6</sub> (H,D) <sup>5+</sup> : An integrated experimental and theoretical mechanistic study. <i>Journal of Chemical Physics</i> , 2009, 131, 024304.	1.2	8
1613	Regio-, Peri-, and Torquoselectivity in Hydroxy Heptatrienyl Cation Electrocyclizations: The Iso/Homo-Nazarov Reaction. <i>Chemistry - A European Journal</i> , 2009, 15, 1944-1956.	1.7	29
1614	Regioselectivity Control in the Metal-Catalyzed Functionalization of $\beta^3$ -Allenols, Part...2: Theoretical Study. <i>Chemistry - A European Journal</i> , 2009, 15, 1909-1928.	1.7	41
1615	Reactions of Ruthenium Vinylidene and Acetylide Complexes Containing Trichloromethyl Groups: Preparation of a Cyclobutenonyl Complex by Solid-State Photolysis. <i>Chemistry - A European Journal</i> , 2009, 15, 3221-3229.	1.7	10
1616	Mechanism of Pd(OAc) <sub>2</sub> /Pyridine Catalyst Reoxidation by O <sub>2</sub> : Influence of Labile Monodentate Ligands and Identification of a Biomimetic Mechanism for O <sub>2</sub> Activation. <i>Chemistry - A European Journal</i> , 2009, 15, 2915-2922.	1.7	101
1617	Density Functional Studies on Isomerization of Prostaglandin-H <sub>2</sub> to Prostacyclin Catalyzed by Cytochrome P450. <i>Chemistry - A European Journal</i> , 2009, 15, 4464-4473.	1.7	16
1618	On the Origin of Reversible Hydrogen Activation by Phosphine-Boranes. <i>Chemistry - A European Journal</i> , 2009, 15, 12846-12855.	1.7	40
1619	Thermal Ni-H Bond Activation on Anionic and Cationic Platinum Clusters: Non-Predetermined Reaction Pathways Indicate Transitions to a Bulk Surface Reactivity. <i>Chemistry - A European Journal</i> , 2009, 15, 8465-8474.	1.7	15
1620	A Novel Multistep Mechanism for the Stereocontrolled Ring Opening of Hindered Sulfamidates: Mild, Green, and Efficient Reactivity with Alcohols. <i>Chemistry - A European Journal</i> , 2009, 15, 9810-9823.	1.7	23
1621	Propene Oxidation with the Anionic Cluster V <sub>4</sub> O <sub>11</sub> <sup>-</sup> : Selective Epoxidation. <i>Chemistry - A European Journal</i> , 2009, 15, 10747-10751.	1.7	24
1622	Metal-Catalyzed Cyclization of $\beta^2$ - and $\beta^3$ -Allenols Derived from $\langle \text{D} \rangle$ -Glyceraldehyde: Synthesis of Enantiopure Dihydropyrans and Tetrahydrooxepines: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2009, 15, 9127-9138.	1.7	47
1623	D $\pi$ -Benzannulation Reactions: Heteroatom and Substituent Effects in Chromium Fischer Carbene Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 12503-12520.	1.7	21
1624	Condensation of $\beta^2$ -Diester Titanium Enolates with Carbonyl Substrates: A Combined DFT and Experimental Investigation. <i>Chemistry - A European Journal</i> , 2009, 15, 11537-11550.	1.7	35
1625	A DFT-Based Analysis of the Grossly Varying Reactivity Pattern in Room-Temperature Activation and Dehydrogenation of CH <sub>4</sub> by Main-Group Atomic M <sup>+</sup> (M=Ga, Ge, As, and Se). <i>Chemistry - A European Journal</i> , 2009, 15, 11559-11565.	1.7	14
1626	Difluorophosphoryl Nitrene F <sub>2</sub> P(O)N: Matrix Isolation and Unexpected Rearrangement to F <sub>2</sub> PNO. <i>Chemistry - A European Journal</i> , 2009, 15, 13466-13473.	1.7	18
1627	Isotope-Sensitive Degenerate [1,3]-Hydrogen Migration versus Competitive Enol-Keto Tautomerization. <i>Chemistry - A European Journal</i> , 2009, 15, 11815-11819.	1.7	7
1628	DFT Studies on the Thermal Activation of Molecular Oxygen by Bare [Ni(H)(OH)] <sup>+</sup> . <i>Helvetica Chimica Acta</i> , 2009, 92, 151-164.	1.0	11
1629	Investigation on the Scavenging Mechanism of 1,4-Dicarbonyls by Pyridoxamine: A Density Functional Theory Study. <i>Chinese Journal of Chemistry</i> , 2009, 27, 1452-1458.	2.6	1

#	ARTICLE	IF	CITATIONS
1630	Different Catalytic Effects of a Single Water Molecule: The Gas-Phase Reaction of Formic Acid with Hydroxyl Radical in Water Vapor. <i>ChemPhysChem</i> , 2009, 10, 3034-3045.	1.0	69
1631	DFT Studies on Double Hydrogen Bond Catalysis of Reactions of Distinct Polarity. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1207-1213.	1.2	3
1632	Controlling Selectivity for Cycloadditions of Nitrones and Alkenes Tethered by Benzimidazoles: Combining Experiment and Theory. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 1578-1584.	1.2	10
1633	An Analysis of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Benzonitrile $\langle i \rangle N \langle /i \rangle$ -Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices. <i>European Journal of Organic Chemistry</i> , 2009, 2009, 3036-3044.	1.2	71
1634	The mechanism of double proton transfer in dimers of uracil and 2-thiouracil—The reaction force perspective. <i>Journal of Computational Chemistry</i> , 2009, 30, 389-398.	1.5	26
1635	Theoretical study on the gas-phase reaction mechanism between nickel monoxide and methane for syngas production. <i>Journal of Computational Chemistry</i> , 2009, 30, 847-863.	1.5	5
1636	Theoretical prediction regarding structural and thermodynamical characteristics of stable $CH_3PO_2$ isomers and unimolecular decomposition mechanisms of species $CH_3P(O)_2$ , $CH_3O_2P(O)_2$ , and $CH_2P(O)_2OH$ . <i>Journal of Computational Chemistry</i> , 2009, 30, 2334-2350.	1.5	7
1637	Effect of metal ions on radical type and proton-coupled electron transfer channel: $\dot{F}$ -Radical vs $\dot{C}$ -Radical and $\dot{F}$ -channel vs $\dot{C}$ -channel in the imide units. <i>Journal of Computational Chemistry</i> , 2009, 30, 2694-2705.	1.5	12
1638	CHARMM: The biomolecular simulation program. <i>Journal of Computational Chemistry</i> , 2009, 30, 1545-1614.	1.5	7,077
1639	A theoretical study of topomerization of imine systems: Inversion, rotation or mixed mechanisms?. <i>Journal of Computational Chemistry</i> , 2010, 31, 520-531.	1.5	31
1640	Computational determination of fundamental pathway and activation barriers for acetohydroxyacid synthase-catalyzed condensation reactions of $\alpha$ -keto acids. <i>Journal of Computational Chemistry</i> , 2010, 31, 1592-1602.	1.5	19
1641	Theoretical study on the gas-phase reaction mechanism between rhodium monoxide and methane for methanol production. <i>Journal of Computational Chemistry</i> , 2010, 31, 938-953.	1.5	8
1642	How the choice of a computational model could rule the chemical interpretation: The Ni(II) catalyzed ethylene dimerization as a case study. <i>Journal of Computational Chemistry</i> , 2010, 31, 1053-1062.	1.5	8
1643	Theoretical and kinetic study of the $H + C_2H_5CN$ reaction. <i>Journal of Computational Chemistry</i> , 2010, 31, 1126-1134.	1.5	6
1644	Ion/Molecule reactions in $SiH_4/H_2S$ and $GeH_4/H_2S$ mixtures. <i>Journal of Mass Spectrometry</i> , 2009, 44, 725-734.	0.7	5
1645	Gas-phase reactions of $XH_3^+$ ( $X = C, Si, Ge$ ) with $NF_3$ : a comparative investigation on the detailed mechanistic aspects. <i>Journal of Mass Spectrometry</i> , 2009, 44, 1348-1358.	0.7	8
1647	Difluoro- $\langle \sup \rangle 5 \langle /sup \rangle$ -Phosphinonitrile $F_2P\frac{1}{2}N$ : Matrix Isolation and Photoisomerization into $FP\frac{3}{4}NF$ . <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4828-4831.	7.2	31
1648	Puckering transitions of pseudoproline residues. <i>Biopolymers</i> , 2009, 91, 444-455.	1.2	15

#	ARTICLE	IF	CITATIONS
1649	Conformational preferences and <i>cis</i> → <i>trans</i> isomerization of <i>N</i> -3,4-dihydroproline residue. <i>Biopolymers</i> , 2009, 92, 387-398.	1.2	13
1650	Conformational preferences and prolyl <i>cis</i> → <i>trans</i> isomerization of phosphorylated Ser/Thr-Pro motifs. <i>Biopolymers</i> , 2010, 93, 330-339.	1.2	12
1651	Density functional theory investigation of electrophilic addition reaction of bromine to tricyclo[4.2.2.2,5]dodeca-1,5-diene. <i>Journal of Molecular Modeling</i> , 2009, 15, 397-403.	0.8	3
1652	The reaction force and the transition region of a reaction. <i>Journal of Molecular Modeling</i> , 2009, 15, 707-710.	0.8	101
1653	Formation of novel 1,3-thiazole- and 1,2-thiazole-fused aporphines and study on the simultaneously occurring benzothiazole→benzothiazole-type isomerization. <i>Monatshefte für Chemie</i> , 2009, 140, 387-396.	0.9	5
1654	High temperature rate constants for OH+ alkanes. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 107-114.	2.4	42
1655	<i>N</i> -Arylmethyl-7-azabicyclo[2.2.1]heptane derivatives: synthesis and reaction mechanisms. <i>Tetrahedron</i> , 2009, 65, 9224-9232.	1.0	3
1656	Carbocation rearrangements in aspernomine biosynthesis. <i>Tetrahedron Letters</i> , 2009, 50, 1578-1581.	0.7	15
1657	Theoretical investigation of mono- and bi-function alkylating agents transformed from nitrosodimethylamine derivatives. <i>Computational and Theoretical Chemistry</i> , 2009, 893, 106-110.	1.5	5
1658	Substituent effects on the tautomerism of monochalcogenocarboxylic acids XC(O)YH (X=H, F, NH <sub>2</sub> ). <i>Tj ETQq1 1 0.784314 rgBT /Ove</i> 896, 80-84.	1.5	9
1659	Ab initio studies of the thermal decomposition pathways of 1-bromo-3,3,3-trifluoropropene. <i>Computational and Theoretical Chemistry</i> , 2009, 899, 98-110.	1.5	10
1660	Theoretical study of intramolecular anion radical cycloaddition of the phenyl-substituted bis(enone). <i>Computational and Theoretical Chemistry</i> , 2009, 901, 202-209.	1.5	9
1661	Theoretical study on the reactions of CF/CCl with O <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , 2009, 905, 94-100.	1.5	0
1662	Theoretical study on the structures and dissociation processes of hexatomic sulphur. <i>Computational and Theoretical Chemistry</i> , 2009, 906, 1-5.	1.5	3
1663	Mechanism of the CH <sub>3</sub> NH <sub>2</sub> →HNO <sub>2</sub> reaction: Ab initio DFT/TST study. <i>Computational and Theoretical Chemistry</i> , 2009, 909, 57-65.	1.5	10
1664	Ab initio study of the potential energy surface and product branching ratios for the reaction of O(1D) with CH <sub>3</sub> CH <sub>2</sub> F. <i>Computational and Theoretical Chemistry</i> , 2009, 910, 126-135.	1.5	3
1665	A detailed theoretical study of the interaction of thiourea with <i>cis</i> -diaqua(ethylenediamine) platinum(II). <i>Computational and Theoretical Chemistry</i> , 2009, 913, 97-106.	1.5	12
1666	Theoretical study on the mechanism of nickel(0)-mediated coupling between carbon dioxide and epoxyethane. <i>Computational and Theoretical Chemistry</i> , 2009, 916, 125-134.	1.5	26

#	ARTICLE	IF	CITATIONS
1667	Theoretical investigation of reactions between ammonia and precursors from the ozonolysis of ethene. <i>Chemical Physics</i> , 2009, 362, 8-15.	0.9	11
1668	Shock tube measurements of high temperature rate constants for OH with cycloalkanes and methylcycloalkanes. <i>Combustion and Flame</i> , 2009, 156, 1126-1134.	2.8	56
1669	The structure and energetics of triplet [B, C, F, H <sub>2</sub> ]. <i>Journal of Fluorine Chemistry</i> , 2009, 130, 836-845.	0.9	7
1670	Exploring rearrangements along the fragmentation pathways of diuron anion: A combined experimental and computational investigation. <i>International Journal of Mass Spectrometry</i> , 2009, 288, 6-15.	0.7	13
1671	Simulation of proton migration pathways in phenolsulfonic acid-based membranes by B3LYP/6-31G** DFT calculations. <i>Russian Chemical Bulletin</i> , 2009, 58, 1581-1588.	0.4	8
1672	An ab initio and density functional theory study on the mechanism for the reaction of OH with 2-ethylfuran. <i>Structural Chemistry</i> , 2009, 20, 525-532.	1.0	15
1673	A density functional theory study of copper-catalyzed aziridination of olefins. <i>Structural Chemistry</i> , 2009, 20, 1013-1018.	1.0	5
1674	The reaction force. A scalar property to characterize reaction mechanisms. <i>Journal of Mathematical Chemistry</i> , 2009, 45, 911-927.	0.7	39
1675	AB initio quantum chemical study of the reaction mechanism of ethynide ion formation in the C <sub>2</sub> H <sub>2</sub> /MOH/DMSO system (M = Li, Na, K). <i>Journal of Structural Chemistry</i> , 2009, 50, 27-33.	0.3	5
1676	Methylation reaction for four DNA base molecules by methanediazonium ions. <i>Science in China Series B: Chemistry</i> , 2009, 52, 26-30.	0.8	2
1677	Theoretical study of the mechanism for C-H bond activation in spin-forbidden reaction between Ti <sup>+</sup> and C <sub>2</sub> H <sub>4</sub> . <i>Science in China Series B: Chemistry</i> , 2009, 52, 295-303.	0.8	0
1678	Theoretical study on the reaction of CN radicals with ClO radicals by density functional theory. <i>Science in China Series B: Chemistry</i> , 2009, 52, 1973-1979.	0.8	0
1679	Theoretical study of partial oxidation of ethylene by vanadium trioxide cluster cation. <i>Science Bulletin</i> , 2009, 54, 2814-2821.	4.3	12
1680	Theoretical mechanistic study on the radical-molecule reaction of CH <sub>2</sub> Br/CHBrCl with NO <sub>2</sub> . <i>Theoretical Chemistry Accounts</i> , 2009, 122, 207-216.	0.5	3
1681	DNA bindings of a novel anticancer drug, trans-[PtCl <sub>2</sub> (isopropylamine)(3-picoline)], and kinetic competition of purine bases with protein residues in the bifunctional substitutions: a theoretical DFT study. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 455-468.	0.5	10
1682	Reaction force analyses of nitro-aci tautomerizations of trinitromethane, the elusive trinitromethanol, picric acid and 2,4-dinitro-1H-imidazole. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 355-363.	0.5	29
1683	Phenomenological description of the transition state, and the bond breaking and bond forming processes of selected elementary chemical reactions: an information-theoretic study. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 445-460.	0.5	45
1684	Chlorination of ammonia and aliphatic amines by Cl <sub>2</sub> : DFT study of medium and substituent effects. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 59-68.	0.9	10

#	ARTICLE	IF	CITATIONS
1685	Theoretical investigation of an unusual substituent effect on the dienophilicity of $\pi$ -C <sub>18</sub> H <sub>14</sub> Pt <sub>2</sub> functionality present in $\pi$ -phosphaindolizines. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 125-129.	0.9	13
1686	Understanding the stereo- and regioselectivities of the polar Diels-Alder reactions between 2-acetyl-1,4-benzoquinone and methyl substituted 1,3-butadienes: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 578-584.	0.9	8
1687	Negative ion fragmentations of deprotonated peptides. The unusual case of <i>iso</i> -Asp: a joint experimental and theoretical study. Comparison with positive ion cleavages. <i>Rapid Communications in Mass Spectrometry</i> , 2009, 23, 1993-2002.	0.7	13
1688	Theoretical study on structures and stabilities of N <sub>4</sub> X (X = O, S, Se, Te) series. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 226-235.	1.0	12
1689	DFT study on Ru <sup>II</sup> -catalyzed cyclization of terminal alkynals to cycloalkenes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 679-687.	1.0	7
1690	Bonding and correlation analysis of various Si <sub>2</sub> CO isomers on the potential energy surface. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 907-919.	1.0	0
1691	Modern valence bond description of the electronic mechanism of a [1,3] sigmatropic rearrangement linking bicyclo[3.2.0]hept-2-ene and bicyclo[2.2.1]hept-2-ene (norbornene). <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1807-1811.	1.0	5
1692	Mechanism of rhodium-catalyzed hydroacylation of propylene using formaldehyde: A computational study. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 850-859.	1.0	0
1693	Direct dynamics study on the mechanism and the kinetics of the reaction of CH <sub>3</sub> NH <sub>2</sub> with OH. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1566-1575.	1.0	24
1694	A DFT study on the hydrolysis mechanism of NH-tautomeric antitumor of [HL]([ <i>trans</i> -RuCl <sub>4</sub> L(dmso) <sub>2</sub> ]). <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1252-1263.	1.0	1
1695	A potential energy surface bifurcation in terpene biosynthesis. <i>Nature Chemistry</i> , 2009, 1, 384-389.	6.6	109
1696	Reactions of the dications C <sub>7</sub> H <sub>6</sub> 2+, C <sub>7</sub> H <sub>7</sub> 2+, and C <sub>7</sub> H <sub>8</sub> 2+ with methane: Predominance of doubly charged intermediates. <i>International Journal of Mass Spectrometry</i> , 2009, 280, 32-37.	0.7	29
1697	Benzylic Newman-Kwart rearrangement of O-azidobenzyl thiocarbamates triggered by phosphines: pseudopericyclic [1,3] shifts via uncoupled concerted mechanisms. <i>Tetrahedron</i> , 2009, 65, 2579-2590.	1.0	19
1698	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl- $\beta$ -lactams to succinimide derivatives. <i>Tetrahedron</i> , 2009, 65, 3432-3440.	1.0	59
1699	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with $\alpha$ -methylene ketones. A DFT study. <i>Tetrahedron</i> , 2009, 65, 4644-4651.	1.0	31
1700	Microwave-assisted reactions of nitroheterocycles with dienes. Diels-Alder and tandem hetero Diels-Alder/[3,3] sigmatropic shift. <i>Tetrahedron</i> , 2009, 65, 5328-5336.	1.0	53
1701	Thermodynamic and kinetic factors in the aza-Cope rearrangement of a series of iminium cations. <i>Tetrahedron</i> , 2009, 65, 10311-10316.	1.0	11
1702	Is anthracene cofactor or spectator for the thermolysis of anthracenyl acylnitroso cycloadducts in the presence of a diene?. <i>Tetrahedron Letters</i> , 2009, 50, 2555-2558.	0.7	8

#	ARTICLE	IF	CITATIONS
1703	A theoretical study nickel-catalyzed cyclopropanation reactions. Nickel(0) versus nickel(II). Computational and Theoretical Chemistry, 2009, 893, 56-66.	1.5	13
1704	Study on the Z/E thermal isomerization of acetaldehyde N,N-dimethylhydrazone in cyclohexane by density functional theory computations. Computational and Theoretical Chemistry, 2009, 893, 84-87.	1.5	1
1705	DFT and TDDFT study of carbon trioxide. Computational and Theoretical Chemistry, 2009, 897, 32-35.	1.5	7
1706	Understanding the role of the bifunctional titanium catalyst in cyanosilylation of ketones: A computational study. Computational and Theoretical Chemistry, 2009, 899, 61-70.	1.5	6
1707	A DFT study on the hydrolysis mechanism of the potential antitumor Ru(III) complex TzNAMI. Computational and Theoretical Chemistry, 2009, 901, 137-144.	1.5	10
1708	Theoretical and experimental studies on mechanism and rate constant for the Baeyer-Villiger oxidation of cyclohexanone by H <sub>2</sub> O <sub>2</sub> in phenol. Computational and Theoretical Chemistry, 2009, 901, 117-127.	1.5	5
1709	Theoretical study on the reaction of NbS <sup>+</sup> (3 $\sigma$ *, 1 $\pi$ ) with COS in gas phase. Computational and Theoretical Chemistry, 2009, 901, 249-257.	1.5	2
1710	Understanding the influence of Lewis acids in the regioselectivity of the Diels-Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study. Computational and Theoretical Chemistry, 2009, 902, 103-108.	1.5	10
1711	A theoretical study of CH <sub>3</sub> ONO+H reaction. Computational and Theoretical Chemistry, 2009, 904, 7-13.	1.5	1
1712	Ab initio study of the reactions: Ethylene+H+vinyl, propylene+methyl+vinyl, and propylene+H+propen-2-yl. Computational and Theoretical Chemistry, 2009, 904, 43-48.	1.5	0
1713	Ion-molecule reaction mechanism of SF <sub>2</sub> +PSCl <sub>3</sub> . Computational and Theoretical Chemistry, 2009, 908, 61-68.	1.5	0
1714	Theoretical investigation of the isomerization of N <sub>2</sub> O <sub>3</sub> and the N-nitrosation of dimethylamine by asym-N <sub>2</sub> O <sub>3</sub> , sym-N <sub>2</sub> O <sub>3</sub> , and trans-cis N <sub>2</sub> O <sub>3</sub> isomers. Computational and Theoretical Chemistry, 2009, 908, 107-113.	1.5	15
1715	The effect of electron-withdrawing groups in the fragmentation of the radical anions of benzyl phenyl ethers. Computational and Theoretical Chemistry, 2009, 913, 228-235.	1.5	3
1716	Theoretical study on the detailed reaction mechanisms of carbonyl oxide with formic acid. Computational and Theoretical Chemistry, 2009, 916, 159-167.	1.5	48
1717	Molecular simulation studies on chemical reactivity of methylcyclopentadiene. Journal of Hazardous Materials, 2009, 165, 141-147.	6.5	14
1718	Replay of amide type resonance in 6-[(dimethylamino)methylene]1,3-dimethylaminouracil: A dynamic NMR and density functional theory study. Journal of Molecular Structure, 2009, 929, 134-140.	1.8	6
1719	Theoretical investigation on antioxidant activity of vitamins and phenolic acids for designing a novel antioxidant. Journal of Molecular Structure, 2009, 930, 15-20.	1.8	70
1720	Theoretical DFT studies of chromium tricarbonyl complexes with polycyclic aromatic ligands. Journal of Organometallic Chemistry, 2009, 694, 1195-1211.	0.8	26

#	ARTICLE	IF	CITATIONS
1721	Triplet-sensitized photolysis of alkoxy carbonyl azides in solution and matrices. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 201, 157-167.	2.0	15
1722	Atomic radical-molecule reaction N (4S)+NO <sub>2</sub> (2A <sub>1</sub> ): Mechanistic study. <i>Chemical Physics</i> , 2009, 358, 80-84.	0.9	3
1723	Theoretical study on kinetics of the H <sub>2</sub> CO+O <sub>2</sub> →HCO+HO <sub>2</sub> reaction. <i>Chemical Physics Letters</i> , 2009, 469, 81-84.	1.2	8
1724	Noble gas-selenium molecular species: A theoretical investigation of FNgSe <sup>+</sup> (Ng=He-Xe). <i>Chemical Physics Letters</i> , 2009, 470, 49-53.	1.2	18
1725	Cooperative activation in ring-opening hydrolysis of epoxides by Co-salen complexes: A first principle study. <i>Chemical Physics Letters</i> , 2009, 470, 259-263.	1.2	20
1726	Interaction and photobinding between 8-methoxypsoralen and thymine. <i>Chemical Physics Letters</i> , 2009, 471, 128-132.	1.2	7
1727	Computational study on decarboxylation mechanism of β-lactamases inhibitors: Clavulanate vs. sulbactam. <i>Chemical Physics Letters</i> , 2009, 472, 248-253.	1.2	3
1728	Stereoselectivity of the aza-Diels-Alder reaction between cyclopentadiene and protonated phenylethylimine derived from glyoxylates. A density functional theory study. <i>Chemical Physics Letters</i> , 2009, 477, 60-64.	1.2	14
1729	A theoretical study of the kinetics of OH radical addition to halogen substituted propenes. <i>Chemical Physics Letters</i> , 2009, 481, 29-33.	1.2	14
1730	Direct dynamic study on the hydrogen abstraction reaction of H <sub>2</sub> CO with NCO. <i>International Journal of Chemical Kinetics</i> , 2009, 41, 394-400.	1.0	1
1731	On the Relative Preference of Enamine/Iminium Pathways in an Organocatalytic Michael Addition Reaction. <i>Chemistry - an Asian Journal</i> , 2009, 4, 714-724.	1.7	27
1732	Ion-Molecule Reactions of O <sub>2</sub> , S <sub>2</sub> -Dimethyl Methylphosphonothioate: Evidence for Intramolecular Sulfur Oxidation during VX Perhydrolysis. <i>Journal of Organic Chemistry</i> , 2009, 74, 9319-9327.	1.7	24
1733	Kinetic and Thermodynamic Stability of the Group 13 Trihydrides. <i>Inorganic Chemistry</i> , 2009, 48, 7953-7961.	1.9	20
1734	Theoretical determination of the favorable mechanism of the reaction between AlX and HX (X = Br, Cl). <i>J. Phys. Chem. A</i> , 2009, 113, 10784-10791.	1.0	14
1735	An experimental and theoretical study of the interaction of n-butylmercaptan with phenylacetylene in acid medium. <i>Russian Journal of Physical Chemistry A</i> , 2009, 83, 405-411.	0.1	0
1736	Proton-Regulated Electron Transfers from Tyrosine to Tryptophan in Proteins: Through-Bond Mechanism versus Long-Range Hopping Mechanism. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16681-16688.	1.2	23
1737	Quantum Mechanical/Molecular Mechanical and Density Functional Theory Studies of a Prototypical Zinc Peptidase (Carboxypeptidase A) Suggest a General Acid-General Base Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 9780-9788.	6.6	80
1738	Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl)oxiranes: A Dual Role of the Catalyst. <i>Journal of Organic Chemistry</i> , 2009, 74, 2982-2991.	1.7	50

#	ARTICLE	IF	CITATIONS
1739	Kinetic Rates and Linear Free Energy Relationships for Water Dissociation on Transition and Noble Metal Dimers. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6971-6978.	1.1	11
1740	Gosteliâˆ™Claisen Rearrangement: DFT Study of Substituentâˆ™Rate Effects. <i>Journal of Organic Chemistry</i> , 2009, 74, 4336-4342.	1.7	30
1741	Theoretical Study of the Regioselectivity of [2 + 2] Photocycloaddition Reactions of Acrolein with Olefins. <i>Journal of Physical Chemistry A</i> , 2009, 113, 332-344.	1.1	48
1742	Mechanistic Analysis of Intramolecular Free Radical Reactions toward Synthesis of 7-Azabicyclo[2.2.1]heptane Derivatives. <i>Journal of Organic Chemistry</i> , 2009, 74, 4061-4067.	1.7	3
1743	Platinum(II)-Complexed Tetrahydroimidazo[1,2-b][1,2,4]oxadiazoles Derived from Metal-Mediated 1,3-Dipolar Cycloaddition. Novel Type of Heterocycles, Which Do Not Exist without the Metal Center. <i>Organometallics</i> , 2009, 28, 1406-1413.	1.1	34
1744	Câ•C Bond Cleavage on Neutral VO <sub>3</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>n</sub> Clusters. <i>Journal of the American Chemical Society</i> , 2009, 131, 1057-1066.	6.6	70
1745	Combined Crossed Molecular Beam and Theoretical Studies of the N( <sup>2</sup> D) + CH <sub>4</sub> Reaction and Implications for Atmospheric Models of Titan. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11138-11152.	1.1	90
1746	Reaction Mechanism of the Îµ Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. <i>Journal of the American Chemical Society</i> , 2009, 131, 1550-1556.	6.6	64
1747	Theoretical Analysis on the Transition State of the Anticancer Drug <i>cis</i> -[PtCl <sub>2</sub> (isopropylamine) <sub>2</sub> ] and Its <i>cis</i> Isomer Binding to DNA Purine Bases. <i>Journal of Physical Chemistry B</i> , 2009, 113, 2110-2127.	1.2	15
1748	On the Mechanism of Palladium(0) Catalyzed, Copper(I) Carboxylate Mediated Thioorganicâˆ™Boronic Acid Desulfative Coupling. A Noninnocent Role for the Carboxylate Ligand. <i>Organometallics</i> , 2009, 28, 4639-4642.	1.1	34
1749	Effect of N7-Protonated Purine Nucleosides on Formation of C8 Adducts in Carcinogenic Reactions of Arylnitrenium Ions with Purine Nucleosides: A Quantum Chemistry Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5645-5652.	1.2	10
1750	Ab Initio Study of the Geometry, Stability, and Aromaticity of the Cyclic S <sub>2</sub> N <sub>3</sub> <sup>+</sup> Cation Isomers and Their Isoelectronic Analogues. <i>Inorganic Chemistry</i> , 2009, 48, 6773-6780.	1.9	15
1751	Understanding the Stereoselection Induced by Chiral Anthracene Templates in Dielsâˆ™Alder Cycloaddition: A DFT Study. <i>Journal of Organic Chemistry</i> , 2009, 74, 2328-2336.	1.7	11
1752	Mechanism of the Ni(0)-Catalyzed Vinylcyclopropaneâˆ™Cyclopentene Rearrangement. <i>Journal of Organic Chemistry</i> , 2009, 74, 7822-7833.	1.7	59
1753	Theoretical Investigation of the Reaction of CF <sub>3</sub> CHOCH <sub>3</sub> with OH Radical. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5951-5957.	1.1	23
1754	Kinetics of 1,4-Hydrogen Migration in the Alkyl Radical Reaction Class. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1564-1573.	1.1	39
1755	Photoswitchable Catalysts: Correlating Structure and Conformational Dynamics with Reactivity by a Combined Experimental and Computational Approach. <i>Journal of the American Chemical Society</i> , 2009, 131, 357-367.	6.6	141
1756	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. <i>Organometallics</i> , 2009, 28, 5848-5856.	1.1	7



#	ARTICLE	IF	CITATIONS
1757	Mechanisms for Formation of Diazocinones, Pyridazines, and Pyrazolines from Tetrazinesâ€”Oxyanion-Accelerated Pericyclic Cascades?. <i>Journal of Organic Chemistry</i> , 2009, 74, 4804-4811.	1.7	18
1758	Theoretical Study on the Reaction Mechanism for the Formation of 2-Methylpyridine Cobalt(I) Complex from Cobaltacyclopentadiene and Acetonitrile. <i>Organometallics</i> , 2009, 28, 3636-3649.	1.1	46
1759	Role of Dimethyl Sulfoxide in the Hydrolytic Peeling of Boron Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15565-15568.	1.5	8
1760	Kinetics of the Gas-Phase Reaction of OH with Chlorobenzene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10452-10459.	1.1	13
1761	Microwave-Assisted Intramolecular Huisgen Cycloaddition of Azido Alkynes Derived from Î±-Amino Acids. <i>Journal of Organic Chemistry</i> , 2009, 74, 1314-1321.	1.7	33
1762	Theoretical Study of Elementary Steps in the Reactions between Aluminum and Teflon Fragments under Combustive Environments. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5933-5941.	1.1	57
1763	Kinetics and Mechanism of the CN + NCO â†’ NCN + CO Reaction Studied by Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6314-6325.	1.1	6
1764	Reactions of Neutral Vanadium Oxide Clusters with Methanol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3029-3040.	1.1	47
1765	Rate Constants for OH with Selected Large Alkanes: Shock-Tube Measurements and an Improved Group Scheme. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5047-5060.	1.1	111
1766	Computational Investigation of the Mechanism of Addition of Singlet Carbenes to Bicyclobutanes. <i>Journal of Organic Chemistry</i> , 2009, 74, 4252-4261.	1.7	14
1767	Theoretical Mechanistic Study of the Oxidative Degradation of Benzene in the Troposphere: Reaction of Benzeneâ€”HO Radical Adduct with O <sub>2</sub> . <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1607-1623.	2.3	41
1768	The molecular basis for the behaviour of niobia species in oxidation reaction probed by theoretical calculations and experimental techniques. <i>Molecular Physics</i> , 2009, 107, 171-179.	0.8	20
1769	Benign Decay vs. Photolysis in the Photophysics and Photochemistry of 5-Bromouracil. A Computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5489-5495.	1.1	19
1770	Rearrangements of [C <sub>6</sub> H <sub>7</sub> Si] <sup>+</sup> Cations. A Radiochemical and Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6028-6033.	1.1	3
1771	Theoretical Study on the Reaction of Ti <sup>+</sup> with Acetone and the Role of Intersystem Crossing. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11382-11389.	1.1	9
1772	Theoretical Studies on the Water-Assisted Hydrolysis of <i>N,N</i> -Dimethyl- <i>N</i> -(2,3-dideoxy-3-thiacytidine) Formamidine with Three Water Molecules. <i>Journal of Physical Chemistry A</i> , 2009, 113, 325-331.	1.1	12
1773	Gold(I)-Catalyzed Cycloaddition of 1-(1-Alkynyl)cyclopropyl Ketones with Nucleophiles To Yield Substituted Furans: A DFT Study. <i>Organometallics</i> , 2009, 28, 3129-3139.	1.1	55
1774	Isocyanide Complexes with Platinum and Palladium and Their Reactivity toward Cycloadditions with Nitrones to Form Aminoxy-carbenes: A Theoretical Study. <i>Organometallics</i> , 2009, 28, 6593-6602.	1.1	28

#	ARTICLE	IF	CITATIONS
1775	Heterogeneous CO <sub>2</sub> Evolution from Oxidation of Aromatic Carbon-Based Materials. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8415-8420.	1.1	34
1776	Study on the Reaction Mechanism and Kinetics of the Thermal Decomposition of Nitroethane. <i>Industrial &amp; Engineering Chemistry Research</i> , 2009, 48, 8745-8751.	1.8	39
1777	Behavior of Group 6 Fischer Aminocarbene Complexes in a Supercharged Medium: A Single Electron Transfer <sup>H</sup> Atom Transfer Process. <i>Organometallics</i> , 2009, 28, 2762-2772.	1.1	13
1778	Theoretical investigation of dehydration of aquated Al(OH) <sub>2</sub> <sup>+</sup> species in aqueous solution. <i>Dalton Transactions</i> , 2009, , 1554.	1.6	17
1779	Computational Studies on the Platinum(II)-Catalyzed Cycloisomerization of 1,6-Dienes into Bicyclopropanes: A Mechanistic Quandary Evaluated by DFT. <i>Organometallics</i> , 2009, 28, 2038-2045.	1.1	5
1780	Reaction Mechanisms of a Photo-Induced [1,3] Sigmatropic Rearrangement via a Nonadiabatic Pathway. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13892-13900.	1.1	15
1781	Computational Evaluation of Enantioselective Diels <sup>A</sup> lder Reactions Mediated by Corey <sup>T</sup> 's Cationic Oxazaborolidine Catalysts. <i>Journal of Organic Chemistry</i> , 2009, 74, 861-868.	1.7	50
1782	On the Mechanism of Cyclization of 5-Hexenylchromate Intermediates in the Reactions of Fischer Carbene Complexes with a Lithium Enolate and Allylmagnesium Bromide. <i>Journal of Organic Chemistry</i> , 2009, 74, 7059-7066.	1.7	6
1783	Pronounced Cluster-Size Effects: Gas-Phase Reactivity of Bare Vanadium Cluster Cations V <sub>n</sub> <sup>+</sup> (n = 1 <sup>7</sup> ) Toward Methanol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5625-5632.	1.1	24
1784	DFT Study on the Molecular Mechanism of the [4 + 2] Cycloaddition between Thiobenzophenone and Arylalkenes <i>via</i> Radical Cations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5718-5722.	1.1	13
1785	DFT Study on the Mechanisms of Stereoselective C(2)-Vinylolation of 1-Substituted Imidazoles with 3-Phenyl-2-propylenitrile. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11035-11041.	1.1	25
1786	Theoretical exploration of the water exchange mechanism of the polyoxocation GaO <sub>4</sub> Al <sub>12</sub> (OH) <sub>24</sub> (H <sub>2</sub> O) <sub>127</sub> <sup>+</sup> in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 1588-1596.	1.6	17
1787	Cleavage of Carbon Dioxide by an Iridium-Supported Fischer Carbene. A DFT Investigation. <i>Journal of the American Chemical Society</i> , 2009, 131, 5800-5808.	6.6	43
1788	DFT studies on a new class of cage functionalized organic superbases. <i>New Journal of Chemistry</i> , 2009, 33, 583-587.	1.4	18
1789	O <sup>6</sup> -Methylguanine Repair by O <sup>6</sup> -Alkylguanine-DNA Alkyltransferase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 16285-16290.	1.2	14
1790	Consequences of Conformational Preorganization in Sesquiterpene Biosynthesis: Theoretical Studies on the Formation of the Bisabolene, Curcumene, Acoradiene, Zizaene, Cedrene, Duprezianene, and Sesquithuriferol Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2009, 131, 7999-8015.	6.6	113
1791	Isotope Effects in the Reactions of Chloroform Isotopologues with Cl, OH, and OD. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1731-1739.	1.1	6
1792	Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst. <i>Organometallics</i> , 2009, 28, 4964-4973.	1.1	10

#	ARTICLE	IF	CITATIONS
1793	Reaction Force Analysis of Solvent Effects in the Addition of HCl to Propene. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6500-6503.	1.1	32
1794	Combined kinetic and DFT studies on the stabilization of the pyramidal form of H <sub>3</sub> PO <sub>2</sub> at the heterometal site of [Mo <sub>3</sub> µ <sub>2</sub> S <sub>4</sub> (H <sub>2</sub> O) <sub>10</sub> ] <sup>4+</sup> clusters (µ <sup>2</sup> = Pd, Ni). <i>Dalton Transactions</i> , 2009, , 1579.	1.6	5
1795	Computational Investigation of the Oxidative Deboronation of Boroglycine, H <sub>2</sub> N-CH <sub>2</sub> -B(OH) <sub>2</sub> , Using H <sub>2</sub> O and H <sub>2</sub> O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2009, 113, 11028-11034.	1.1	12
1796	A Comprehensive Theoretical Study on the Coupling Reaction Mechanism of Propylene Oxide with Carbon Dioxide Catalyzed by Copper(I) Cyanomethyl. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6710-6723.	1.1	45
1797	Ground State Structures of Fe <sub>2</sub> O <sub>4</sub> <sup>6+</sup> Clusters Probed by Reactions with N <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2009, 113, 5302-5309.	1.1	47
1798	Investigation of the Scope and Regiochemistry of Alkynylboronate Cycloadditions with Sydnone. <i>Journal of the American Chemical Society</i> , 2009, 131, 7762-7769.	6.6	92
1799	Deamidation of Asparagine Residues: Direct Hydrolysis versus Succinimide-Mediated Deamidation Mechanisms. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1111-1120.	1.1	109
1800	Modeling Protein Splicing: Reaction Pathway for C-Terminal Splice and Intein Scission. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5607-5616.	1.2	25
1801	Synthesis of Trimethylplatinum(IV) Complexes with <i>N,N</i> - and <i>N,O</i> -Heterocyclic Carbene Ligands and Their Reductive C-C Elimination Reactions. <i>Journal of the American Chemical Society</i> , 2009, 131, 8861-8874.	6.6	41
1802	Quantum Mechanical Study of the Gas-Phase Reactions between a Series of Substituted Singlet Carbenes and Water. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6517-6523.	1.1	12
1803	Quantum Mechanical/Effective Fragment Potential (QM/EFP) Study of Phosphate Monoester Aminolysis in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14831-14836.	1.2	15
1804	Human Insulin-Degrading Enzyme Working Mechanism. <i>Journal of the American Chemical Society</i> , 2009, 131, 14804-14811.	6.6	56
1805	OH Radical Gas Phase Reactions with Aliphatic Ethers: A Variational Transition State Theory Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13913-13920.	1.1	103
1806	A matrix isolation and computational study of the [C, N, F, S] isomers. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9458.	1.3	18
1807	Mechanistic Study of the Manganese-Catalyzed [2 + 2 + 2] Annulation of 1,3-Dicarbonyl Compounds and Terminal Alkynes. <i>Journal of the American Chemical Society</i> , 2009, 131, 4099-4109.	6.6	53
1808	Dehydrocoupling Reactions of Borane-Secondary and -Primary Amine Adducts Catalyzed by Group-6 Carbonyl Complexes: Formation of Aminoboranes and Borazines. <i>Journal of the American Chemical Society</i> , 2009, 131, 14946-14957.	6.6	142
1809	Mechanistic Insights on the Magnesium(II) Ion-Activated Reduction of Methyl Benzoylformate with Chelated NADH Peptide <sup>12</sup> -Lactam Models. <i>Journal of Organic Chemistry</i> , 2009, 74, 6691-6702.	1.7	22
1810	Theoretical Investigation of the Reaction between Carbonyl Oxides and Ammonia. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10284-10290.	1.1	47

#	ARTICLE	IF	CITATIONS
1811	Kinetic Study of the 2-Naphthyl (C <sub>10</sub> H <sub>7</sub> ) Radical Reaction with C <sub>2</sub> H <sub>2</sub> . Journal of Physical Chemistry A, 2009, 113, 12199-12206.	1.1	10
1812	An Experimental and Theoretical Study on the Interaction of N-Heterocyclic Carbene-Derived 1,3-Dipoles with Methoxycarbonylallenes: Highly Regio- and Stereoselective [3+2]-Cycloadditions Controlled by the Structures of N-Heterocycles of 1,3-Dipoles. Journal of Organic Chemistry, 2009, 74, 2357-2367.	1.7	22
1813	CBS-QB3 + VTST Study of Methyl N-Methylcarbamate + OH Gas-Phase Reaction: Mechanism, Kinetics, and Branching Ratios. Journal of Chemical Theory and Computation, 2009, 5, 1295-1303.	2.3	12
1814	Electrocyclic Ring Opening of Charged cis-Bicyclo[3.2.0]heptadiene and Heterocyclic Derivatives. The Anti-Woodward-Hoffmann Quest (II). Journal of Organic Chemistry, 2009, 74, 2396-2402.	1.7	15
1815	Energetics and Vibrational Analysis of Methyl Salicylate Isomers. Journal of Physical Chemistry A, 2009, 113, 10385-10390.	1.1	23
1816	Mechanism and Selectivity of Cinchona Alkaloid Catalyzed [1,3]-Shifts of Allylic Trichloroacetimidates. Journal of Organic Chemistry, 2009, 74, 6944-6952.	1.7	28
1817	Mechanisms of Cascade Reactions in the Syntheses of Camptothecin-Family Alkaloids: Intramolecular [4+2] Reactions of N-Arylimidates and Alkynes. Organic Letters, 2009, 11, 5302-5305.	2.4	23
1818	Reaction of [60]fullerene with trans-epoxides: a theoretical study. Organic and Biomolecular Chemistry, 2009, 7, 1851.	1.5	5
1819	Multichannel RRKM-TST and Direct-Dynamics VTST Study of the Reaction of Hydroxyl Radical with Furan. Journal of Physical Chemistry A, 2009, 113, 2838-2846.	1.1	43
1820	A Theoretical Investigation on the Kinetics and Mechanism of the Reaction of Amidogen with Hydroxyl Radical. Journal of Physical Chemistry A, 2009, 113, 12961-12971.	1.1	28
1821	Autocatalytic degradation of white phosphorus with silylenes. Physical Chemistry Chemical Physics, 2009, 11, 5273.	1.3	25
1822	Modes of inactivation of trichodiene synthase by a cyclopropane-containing farnesyldiphosphate analog. Organic and Biomolecular Chemistry, 2009, 7, 4101.	1.5	26
1823	Ligand effect on the NMR, vibrational and structural properties of tetra- and hexanuclear ruthenium hydrido clusters: a theoretical investigation. Dalton Transactions, 2009, , 2142.	1.6	20
1824	Mechanistic Studies on the Formation of Linear Polyethylene Chain Catalyzed by Palladium Phosphine-Sulfonate Complexes: Experiment and Theoretical Studies. Journal of the American Chemical Society, 2009, 131, 14088-14100.	6.6	146
1825	Computational Modeling Study on Formation of Acyclic Clavulanate Intermediates in Inhibition of Class A $\beta$ -Lactamase: Water-Assisted Proton Transfer. Journal of Physical Chemistry A, 2009, 113, 1608-1613.	1.1	2
1826	Unimolecular Decomposition of 5-Aminotetrazole and its Tautomer 5-Iminotetrazole: New Insight from Isopotential Searching. Journal of Physical Chemistry A, 2009, 113, 2483-2490.	1.1	34
1827	Adiabatic and Nonadiabatic Reaction Pathways of the O( <sup>3</sup> P) with Propyne. Journal of Physical Chemistry A, 2009, 113, 23-34.	1.1	19
1828	Thermal C-H Bond Activation of Benzene with Cationic [Pt(CX <sub>3</sub> )(L)] <sup>+</sup> Complexes in the Gas Phase: A Combined Experimental/Theoretical Study (X = H, D; L = 1,10-Phenanthroline, 2,2'-Bipyrimidine.) Tj ETQq1 1 0.784314 rgBT2/Overlo		

#	ARTICLE	IF	CITATIONS
1829	Analyzing Kullback-Leibler information profiles: an indication of their chemical relevance. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 476-482.	1.3	31
1830	A theoretical study on the hydrolysis process of two Keppler-type antitumor complexes [TzH][trans-RuCl <sub>4</sub> (Tz) <sub>2</sub> ] and [2-NH <sub>2</sub> TzH][trans-RuCl <sub>4</sub> (2-NH <sub>2</sub> Tz) <sub>2</sub> ]. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3401.	1.3	11
1831	Theoretical study of the gas-phase ozonolysis of Î²-pinene (C <sub>10</sub> H <sub>16</sub> ). <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5643.	1.3	83
1832	The unusual reactivity of benzene and monosubstituted benzenes towards tetracyanoethylene oxide: a theoretical study. <i>New Journal of Chemistry</i> , 2009, 33, 471-478.	1.4	2
1833	Metal-ligand cooperation in the trans addition of dihydrogen to a pincer Ir(i) complex: a DFT study. <i>Dalton Transactions</i> , 2009, , 9433.	1.6	111
1834	Epoxidation of olefins catalysed by vanadium-salan complexes: a theoretical mechanistic study. <i>Dalton Transactions</i> , 2009, , 5460.	1.6	49
1835	A theoretical model study on the cyclic reaction of 4-hydroxybutanal catalyzed by Brønsted acid. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1610-1619.	0.6	7
1836	Computational study of khellin excited states and photobinding to DNA. <i>Photochemical and Photobiological Sciences</i> , 2009, 8, 1179-1186.	1.6	3
1837	The gas-phase ozonolysis of Î²-caryophyllene (C <sub>15</sub> H <sub>24</sub> ). Part II: A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4173.	1.3	66
1838	Reactivity of CO <sub>2</sub> towards Mo[N(R)Ph] <sub>3</sub> . <i>Dalton Transactions</i> , 2009, , 9266.	1.6	13
1839	Acceleration of the Z to E photoisomerization of penta-2,4-dieniminium by hydrogen out-of-plane motion: theoretical study on a model system of retinal protonated Schiff base. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6406.	1.3	21
1840	A theoretical study on the mechanism of the base-promoted decomposition of N-chloro,N-methylethanolamine. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1807.	1.5	6
1841	Insight into Mechanism of Formation of C <sub>8</sub> Adducts in Carcinogenic Reactions of Arylnitrenium Ions with Purine Nucleosides. <i>Journal of Physical Chemistry B</i> , 2009, 113, 254-259.	1.2	16
1842	A Combined Experimental and Theoretical Study of the Polar [3 + 2] Cycloaddition of Electrophilically Activated Carbonyl Ylides with Aldehydes and Imines. <i>Journal of Organic Chemistry</i> , 2009, 74, 2120-2133.	1.7	49
1843	Crossed-Beam Dynamics, Low-Temperature Kinetics, and Theoretical Studies of the Reaction S( <sup>1</sup> D) + C <sub>2</sub> H <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , 2009, 113, 15328-15345.	1.1	38
1844	Ab Initio and DFT Study of the Conformational Energy Hypersurface of Cyclic Gly-Gly-Gly. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10818-10825.	1.1	16
1845	Energy barrier of structure transition from icosahedral B <sub>12</sub> H <sub>6</sub> <sup>+</sup> to planar B <sub>12</sub> H <sub>5</sub> <sup>+</sup> and B <sub>12</sub> H <sub>4</sub> <sup>+</sup> clusters. <i>Journal of Physics: Conference Series</i> , 2009, 176, 012030.	0.3	8
1846	Cyclopropanation Reactions of Halomethylithium Carbenoids: A Computational Study of the Effects of Aggregation and Solvation. <i>Bulletin of the Chemical Society of Japan</i> , 2009, 82, 1107-1125.	2.0	13

#	ARTICLE	IF	CITATIONS
1848	Experimental and Theoretical Evidence for HS <sub>4</sub> . Journal of Physical Chemistry A, 2009, 113, 14420-14423.	1.1	2
1849	Steepest descent reaction path integration using a first-order predictor-corrector method. Journal of Chemical Physics, 2010, 133, 224101.	1.2	63
1850	The reaction between NH <sub>3</sub> <sup>+</sup> and CH <sub>3</sub> COOH: a possible process for the formation of glycine precursors in the interstellar medium. Astronomy and Astrophysics, 2010, 516, A79.	2.1	26
1852	Density Functional Theory Study of Gas Phase Hydrolysis of Titanium Tetrachloride. Bulletin of the Chemical Society of Japan, 2010, 83, 1030-1036.	2.0	12
1853	Theoretical Study of Bond-Switching in 1,6-Dihydro-6a-thia-1,6-diazapentalene (10-S-3) Systems Compared with Corresponding Oxygen Analogues. Bulletin of the Chemical Society of Japan, 2010, 83, 520-529.	2.0	7
1854	Strained iminium ylides. Russian Journal of General Chemistry, 2010, 80, 1652-1666.	0.3	10
1855	DFT investigation on mechanism of dirhodium tetracarboxylate-catalyzed O-H insertion of diazo compounds with H <sub>2</sub> O. Open Chemistry, 2010, 8, 223-228.	1.0	4
1856	Theoretical Investigation of the Selective Oxidation of Methanol to Formaldehyde on Vanadium Oxide Species Supported on Silica: Umbrella Model. Journal of Physical Chemistry C, 2010, 114, 3161-3169.	1.5	29
1857	The activation strain model of chemical reactivity. Organic and Biomolecular Chemistry, 2010, 8, 3118.	1.5	599
1858	Gold(III) six-membered NâCâN pincer complexes: synthesis, structure, reactivity and theoretical calculations. Dalton Transactions, 2010, 39, 10293.	1.6	24
1859	Selective C-H versus O-H Bond Activation of CH <sub>3</sub> OH upon Electrospraying Methanolic Solutions of MX <sub>2</sub> (M=Fe, Co, Ni; X=Br, I): A DFT Study. ChemCatChem, 2010, 2, 799-802.	1.8	19
1860	A Theoretical Study of the Mechanism of the Desymmetrization of Cyclic <i>meso</i> -Anhydrides by Chiral Amino Alcohols. ChemCatChem, 2010, 2, 1122-1129.	1.8	20
1861	A New Insight into Gold(I)-Catalyzed Hydration of Alkynes: Proton Transfer. ChemCatChem, 2010, 2, 1226-1230.	1.8	186
1862	Thermal Activation of Methane by Diatomic Metal Oxide Radical Cations: PbO <sup>+</sup> as One of the Missing Pieces. ChemCatChem, 2010, 2, 1391-1394.	1.8	30
1863	Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate. Macromolecules, 2010, 43, 5602-5610.	2.2	38
1864	Mechanism of the Organocatalyzed Decarboxylative Knoevenagel-Doebner Reaction. A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 13086-13092.	1.1	15
1865	Theoretical study on the structures, isomerization and stability of SiC <sub>4</sub> isomers. Theoretical Chemistry Accounts, 2010, 126, 15-25.	0.5	3
1866	Theoretical investigation on mechanism for OH-initiated oxidation of CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> OH. Theoretical Chemistry Accounts, 2010, 125, 45-55.	0.5	8



#	ARTICLE	IF	CITATIONS
1885	Hydrolysis and binding mechanism of AMD473 (cis-[PtCl <sub>2</sub> (NH <sub>3</sub> )(2-picoline)]) with guanine: A quantum mechanical study. <i>Computational and Theoretical Chemistry</i> , 2010, 955, 53-60.	1.5	16
1886	Computational study on the doublet [H,S,Si,O] isomers: Structure, stability and dissociation. <i>Computational and Theoretical Chemistry</i> , 2010, 955, 78-83.	1.5	0
1887	Reaction of enamines with trifluoromethyl containing carbonyl reagents. <i>Journal of Fluorine Chemistry</i> , 2010, 131, 190-199.	0.9	2
1888	Ab initio studies on the reactivity of the CF <sub>3</sub> OCH <sub>2</sub> O radical: Thermal decomposition vs. reaction with O <sub>2</sub> . <i>Journal of Molecular Modeling</i> , 2010, 16, 1473-1480.	0.8	21
1889	Theoretical studies on identity S <sub>N</sub> 2 reactions of lithium halide and methyl halide: A microhydration model. <i>Journal of Molecular Modeling</i> , 2010, 16, 1931-1937.	0.8	11
1890	DFT study of a model system for the dealkylation step catalyzed by AlkB. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 70-77.	2.2	14
1891	Isomerization of B <sub>6</sub> , B <sub>6</sub> <sup>+</sup> and B <sub>6</sub> + clusters. <i>Science China Chemistry</i> , 2010, 53, 202-209.	4.2	4
1892	A theoretical study of the carbenoids LiCH <sub>2</sub> X (X = Cl, Br, I) cyclopropanation reaction with ketene. <i>Journal of Chemical Sciences</i> , 2010, 122, 363-369.	0.7	3
1893	Theoretical study of nucleophilic halogenalkylation of propylene oxide with halogenmethane and dihalogenmethane anion. <i>Journal of Chemical Sciences</i> , 2010, 122, 901-909.	0.7	1
1894	Reactions of chlorine atoms and hydroxyl radicals with trichloroethanol: a mechanistic and kinetic study. <i>Journal of Atmospheric Chemistry</i> , 2010, 65, 73-87.	1.4	2
1895	An ab initio quantum chemical study of reaction mechanisms in the C <sub>2</sub> H <sub>2</sub> /CH <sub>3</sub> OH/KOH/DMSO system. <i>Journal of Structural Chemistry</i> , 2010, 51, 428-436.	0.3	3
1896	Liposome Damage and Modeling of Fragments of Human Islet Amyloid Polypeptide (IAPP) Support a Two-Step Model of Membrane Destruction. <i>International Journal of Peptide Research and Therapeutics</i> , 2010, 16, 43-54.	0.9	8
1897	Binding of ansa- and non-ansa-titanocene anticancer drugs to DNA: a DFT study. <i>Structural Chemistry</i> , 2010, 21, 735-744.	1.0	6
1898	Theoretical study of reaction mechanism for Se <sup>+</sup> + O <sub>3</sub> . <i>Structural Chemistry</i> , 2010, 21, 915-922.	1.0	4
1899	Different coordination modes of the dimethyldisulfide ligand in trimethylplatinum(IV) complexes. <i>Transition Metal Chemistry</i> , 2010, 35, 19-25.	0.7	1
1900	The Role of Oxazolidinones in L-Proline-Assisted Aldol-Type Reactions. <i>Topics in Catalysis</i> , 2010, 53, 1031-1038.	1.3	4
1901	High-resolution spectroscopy (XPS, <sup>1</sup> H MAS solid-state NMR) and DFT investigations into Ti-modified Phillips CrOx/SiO <sub>2</sub> catalysts. <i>Journal of Catalysis</i> , 2010, 273, 103-115.	3.1	37
1902	Structure and Stability of Interstellar Molecule C <sub>3</sub> S. <i>Chinese Journal of Chemistry</i> , 2002, 20, 1487-1493.	2.6	4



#	ARTICLE	IF	CITATIONS
1903	The Structures and Stability of HNOS Isomers. Chinese Journal of Chemistry, 2003, 21, 30-35.	2.6	5
1904	Theoretical Study on the Structures and Stability of Isomers and Complex of [Si, C, O, O] System. Chinese Journal of Chemistry, 2003, 21, 121-125.	2.6	1
1905	Theoretical Study on Gas-phase Pyrolytic Reactions of N-Ethyl, N-Isopropyl and N-t-Butyl Substituted 2-Aminopyrazine. Chinese Journal of Chemistry, 2010, 21, 126-129.	2.6	0
1906	<i>Ab initio</i> Mechanism Study on the Reaction of Chlorine Atom with Formic Acid. Chinese Journal of Chemistry, 2003, 21, 244-248.	2.6	1
1907	Density functional study on the mechanism of collision reaction among protons, N <sub>2</sub> and water vapor. Chinese Journal of Chemistry, 2004, 22, 594-598.	2.6	0
1908	Theoretical Study on the Mechanism of the Petasis-type Boronic Mannich Reaction of Organoboronic Acids, Amines, and $\alpha$ -Hydroxy Aldehydes. Chinese Journal of Chemistry, 2010, 28, 41-49.	2.6	22
1909	A Theoretical Investigation on N7(H) $\leftrightarrow$ N9(H) Tautomerization of Isolated and Monohydrated 2,6-Dithiopurine Combined with IPCM Solvent Model. Chinese Journal of Chemistry, 2010, 28, 1027-1033.	2.6	1
1910	Interface Water Catalysis of the Epoxide Opening. ChemPhysChem, 2010, 11, 65-69.	1.0	19
1911	A Theoretical Study on the Mechanism of C <sub>2</sub> H <sub>4</sub> Oxidation over a Neutral V <sub>3</sub> O <sub>8</sub> Cluster. ChemPhysChem, 2010, 11, 1718-1725.	1.0	24
1912	Ab initio and DFT studies of the thermal rearrangement of trimethylsilyl(methyl)silylene: Remarkable rearrangements of silicon intermediates. Journal of Computational Chemistry, 2010, 31, 154-163.	1.5	3
1913	Density functional investigation and bonding analysis of pentacoordinated iron complexes with mixed cyano and carbonyl ligands. Journal of Computational Chemistry, 2010, 31, 1969-1978.	1.5	1
1914	Theoretical studies on the formation mechanism and explosive performance of nitro-substituted 1,3,5-triazines. Journal of Computational Chemistry, 2010, 31, 2483-2492.	1.5	15
1915	Reactivity Pattern in the Room-Temperature Activation of NH <sub>3</sub> by the Main-Group Atomic Ions Ga <sup>+</sup> , Ge <sup>+</sup> , As <sup>+</sup> and Se <sup>+</sup> . European Journal of Inorganic Chemistry, 2010, 2010, 1516-1521.	1.0	18
1916	Anionic d <sub>8</sub> Alkyl Hydrides – Selective Formation and Reactivity of Anionic <i>cis</i> -Pt <sup>+</sup> Methyl Hydride. European Journal of Inorganic Chemistry, 2010, 2010, 1991-1999.	1.0	7
1917	Experimental and Theoretical Studies of a One-Flask Synthesis of 3H-1-Benzazepines from 2-Haloanilines and $\alpha,\beta$ -Unsaturated Ketones. European Journal of Organic Chemistry, 2010, 2010, 2363-2371.	1.2	6
1918	Theoretical Investigations towards the Staudinger Reaction Catalyzed by $\alpha$ -Heterocyclic Carbene: Mechanism and Stereoselectivity. European Journal of Organic Chemistry, 2010, 2010, 6249-6255.	1.2	23
1919	The Origin of the High Enantioselectivity in Asymmetric Cyclopropanation of Unfunctionalized Olefins. Advanced Synthesis and Catalysis, 2010, 352, 1810-1817.	2.1	5
1920	Ring Expansion versus Cyclization in $\alpha$ -Oxoazetidines-carbaldehydes Catalyzed by Molecular Iodine: Experimental and Theoretical Study in Concert. Advanced Synthesis and Catalysis, 2010, 352, 1688-1700.	2.1	39

#	ARTICLE	IF	CITATIONS
1921	Acid-Free Nickel Catalyst for Stereo- and Regioselective Hydrophosphorylation of Alkynes: Synthetic Procedure and Combined Experimental and Theoretical Mechanistic Study. <i>Advanced Synthesis and Catalysis</i> , 2010, 352, 2979-2992.	2.1	71
1923	Effect of CO on the Oxidative Addition of Arene C-H Bonds by Cationic Rhodium Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 328-353.	1.7	49
1924	Antithyroid Drugs and their Analogues Protect Against Peroxynitrite-Mediated Protein Tyrosine Nitration: A Mechanistic Study. <i>Chemistry - A European Journal</i> , 2010, 16, 1175-1185.	1.7	47
1925	The Role of Solvent on the Mechanism of Proton Transfer to Hydride Complexes: The Case of the $[W^{III}Pd^{IV}H^3(dmpe)_3(CO)]^+$ Cubane Cluster. <i>Chemistry - A European Journal</i> , 2010, 16, 1613-1623.	1.7	15
1926	Ion-Molecule Reactions of $\sigma$ -Cyclometalated $[Pt(bipy^H)]^+$ ( $bipy=2,2'$ -bipyridine) with Dimethyl Ether in Comparison with Dimethyl Sulfide: An Experimental/Computational Study. <i>Chemistry - A European Journal</i> , 2010, 16, 3962-3969.	1.7	29
1927	A Computational Study of the Olefin Epoxidation Mechanism Catalyzed by Cyclopentadienyloxidomolybdenum(VI) Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 2147-2158.	1.7	84
1928	Room-Temperature, Ligand- and Base-Free Heck Reactions of Aryl Diazonium Salts at Low Palladium Loading: Sustainable Preparation of Substituted Stilbene Derivatives. <i>Chemistry - A European Journal</i> , 2010, 16, 5191-5204.	1.7	94
1929	Stabilization of HHeF by Complexation: Is it a Really Viable Strategy?. <i>Chemistry - A European Journal</i> , 2010, 16, 6257-6264.	1.7	7
1930	Scission of Carbon Monoxide Using $TaR_3$ , $R=(N^tBu)Ph$ or $OSi^tBu_3$ : A DFT Investigation. <i>Chemistry - A European Journal</i> , 2010, 16, 8117-8132.	1.7	7
1931	Boron-Based Dipolar Multicomponent Reactions: Simple Generation of Substituted Aziridines, Oxazolidines and Pyrrolidines. <i>Chemistry - A European Journal</i> , 2010, 16, 7904-7915.	1.7	27
1932	Effect of the Nature of the Substituent in $N$ -Alkylimidazole Ligands on the Outcome of Deprotonation: Ring Opening versus the Formation of $N$ -Heterocyclic Carbene Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 8495-8507.	1.7	43
1933	Conversion of Methane to Methanol: Nickel, Palladium, and Platinum ( $d^9$ ) Cations as Catalysts for the Oxidation of Methane by Ozone at Room Temperature. <i>Chemistry - A European Journal</i> , 2010, 16, 11605-11610.	1.7	89
1934	Reactions of Alkynes with $[RuCl(cyclopentadienyl)]$ Complexes: The Important First Steps. <i>Chemistry - A European Journal</i> , 2010, 16, 8400-8409.	1.7	50
1935	Concerted and Stepwise Mechanisms in Metal-Free and Metal-Assisted [4+3] Cycloadditions Involving Allyl Cations. <i>Chemistry - A European Journal</i> , 2010, 16, 12147-12157.	1.7	53
1936	Synthesis and crystal structure of 3,5-diacetyl-4-methylpyrazole. <i>Journal of Heterocyclic Chemistry</i> , 2010, 47, 1025-1030.	1.4	3
1937	A DFT study on the reaction mechanisms of ketene-ketone [2+2+2] cycloaddition to form 3-arylgutaric anhydrides under a Lewis acid catalysis: What is the role of $BF_3$ ?. <i>Journal of Molecular Catalysis A</i> , 2010, 326, 41-47.	4.8	21
1938	Structure and decomposition of $[HFe(CO)_4(B_2H_5)]$ , a revised behavior of an old uncharacterized complex. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 1715-1721.	0.8	3
1939	DFT study of the mechanism of Cu(I)-catalyzed and uncatalyzed intramolecular cyclopropanation of iodonium ylides. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2030-2038.	0.8	7

#	ARTICLE	IF	CITATIONS
1940	Theoretical study of formation of pyridines by interaction of a cobaltacyclopentadiene with model nitriles (hydrogen cyanide or trifluoroacetonitrile): Electronic effects of nitriles on the reaction mechanism. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2240-2250.	0.8	31
1941	Computational study of reaction pathways in the course of interaction of deactivated silylenes with buta-1,3-diene. <i>Journal of Organometallic Chemistry</i> , 2010, 695, 2345-2353.	0.8	7
1942	Binding to DNA purine bases and amino acid residues of a ruthenium(II) antitumor complex: A density functional study. <i>Inorganica Chimica Acta</i> , 2010, 363, 3274-3281.	1.2	3
1943	Theoretical investigation of the dissociative interchange (I <sub>d</sub> ) mechanism for water exchange on magnesium(II) in aqueous solution. <i>Inorganica Chimica Acta</i> , 2010, 363, 3627-3631.	1.2	5
1944	Coordination chemistry of nickel(II) nitrate with superbasic guanidines as studied by electrospray mass spectrometry. <i>International Journal of Mass Spectrometry</i> , 2010, 290, 22-31.	0.7	9
1945	Could the reactions of formic acid with CH <sub>3</sub> NH <sub>2</sub> + / CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup> produce protonated glycine?. <i>International Journal of Mass Spectrometry</i> , 2010, 295, 21-25.	0.7	6
1946	DFT and PIO study of the influences of Mo valence state and surface hydroxyl on supported-MoO <sub>x</sub> catalysts for ethylene polymerization. <i>Journal of Molecular Catalysis A</i> , 2010, 321, 50-60.	4.8	18
1947	Theoretical study on the mechanisms of the conversion of methyl lactate over sodium polyphosphate catalyst. <i>Journal of Molecular Catalysis A</i> , 2010, 323, 91-100.	4.8	19
1948	Experimental and theoretical studies on ethylene polymerization using SiO <sub>2</sub> -supported silyl chromate type catalysts prepared by a green method. <i>Journal of Molecular Catalysis A</i> , 2010, 330, 56-65.	4.8	8
1949	Brønsted acid-catalyzed tert-butylation of phenol, o-cresol and catechol: A comparative computational study. <i>Journal of Molecular Catalysis A</i> , 2010, 332, 145-151.	4.8	13
1950	Study of selected benzyl azides by UV photoelectron spectroscopy and mass spectrometry. <i>Journal of Molecular Structure</i> , 2010, 980, 163-171.	1.8	11
1951	Theoretical study on the mechanism for the reaction of OH with CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> OH. <i>Chemical Physics</i> , 2010, 367, 52-61.	0.9	6
1952	Experimental and computational investigation of the unexpected formation of 2-substituted polyoxygenated furans from conveniently functionalized carbohydrates. <i>Tetrahedron</i> , 2010, 66, 736-742.	1.0	15
1953	Stereomodulating effect of remote groups on the NADH-mimetic reduction of alkyl acryloylformates with 1,4-dihydronicotinamide-2-lactam amides. <i>Tetrahedron</i> , 2010, 66, 3187-3194.	1.0	10
1954	The hydrolysis chemistry of anticancer drug titanocene dichloride: An insight from theoretical study. <i>Computational and Theoretical Chemistry</i> , 2010, 940, 45-49.	1.5	25
1955	A mechanistic investigation on the CC bond cleavage of RCN by cationic Rh(III) and Ir(III). <i>Computational and Theoretical Chemistry</i> , 2010, 941, 66-70.	1.5	3
1956	The reaction electronic flux: A new descriptor of the electronic activity taking place during a chemical reaction. Application to the characterization of the mechanism of the Schiff's base formation in the Maillard reaction. <i>Computational and Theoretical Chemistry</i> , 2010, 943, 121-126.	1.5	46
1957	OH bond cleavage step of the Wacker process: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2010, 941, 138-143.	1.5	17

#	ARTICLE	IF	CITATIONS
1958	A DFT study of the role of the Mg complex formation on the mechanism of the 1,3-dipolar cycloadditions of benzonitrile oxides with acryloylpyrazolidinone. Computational and Theoretical Chemistry, 2010, 942, 26-31.	1.5	11
1959	Mechanism of atmospheric ozonolysis of sabinene: A DFT study. Computational and Theoretical Chemistry, 2010, 942, 32-37.	1.5	15
1960	An ab initio study of the mechanisms of the di- and tri-merization of thiocarbonyl compounds resulting in cyclic oligomers. Computational and Theoretical Chemistry, 2010, 944, 83-88.	1.5	6
1961	Mechanism for the gas-phase of sulfur vapor with ozone reaction: A theoretical study. Computational and Theoretical Chemistry, 2010, 944, 110-115.	1.5	3
1962	Theoretical investigation on the reaction mechanism of N <sub>2</sub> O+CO catalyzed by Ir <sup>+</sup> and Co <sup>+</sup> . Computational and Theoretical Chemistry, 2010, 945, 53-56.	1.5	2
1963	A theoretical study of ground and excited state proton transfer and rotamerism in salicylanilide and its 1:1 complex with methanol. Computational and Theoretical Chemistry, 2010, 945, 110-115.	1.5	1
1964	On the origin of decomposition of triphenyl phosphite ozonide accelerated by ammonia or pyridine water solution. Computational and Theoretical Chemistry, 2010, 948, 71-77.	1.5	2
1965	A computational study on the reaction mechanisms of N-formylation of amines under a Lewis acid catalysis. Computational and Theoretical Chemistry, 2010, 951, 89-92.	1.5	11
1966	Theoretical study on the reaction of Nb <sup>+</sup> with COS in the gas phase. Computational and Theoretical Chemistry, 2010, 953, 39-46.	1.5	0
1967	A theoretical study of the 2NCO+2N <sub>2</sub> H reaction. Computational and Theoretical Chemistry, 2010, 958, 10-14.	1.5	3
1968	Theoretical investigation of the reaction mechanism of atomic oxygen radical anion with pyridine. Computational and Theoretical Chemistry, 2010, 958, 82-91.	1.5	0
1969	HDA cycloadditions of 1-diethoxyphosphonyl-1,3-butadiene with nitroso heterodienophiles: A computational investigation. Computational and Theoretical Chemistry, 2010, 959, 49-54.	1.5	8
1970	Density functional theory study of relevant properties of lanthanum species and 1-butene activation over lanthanum modified zeolite. Computational and Theoretical Chemistry, 2010, 962, 1-6.	1.5	6
1971	Experimental and theoretical study of pyrazole N-alkylation catalyzed by basic modified molecular sieves. Chemical Engineering Journal, 2010, 161, 377-383.	6.6	15
1972	A detailed theoretical DFT study of the hydrolysis mechanism of orally active anticancer drug ZD0473. Chemical Physics Letters, 2010, 487, 108-115.	1.2	30
1973	Theoretical study of the gas phase reaction of methyl acetate with the hydroxyl radical: Structures, mechanisms, rates and temperature dependencies. Chemical Physics Letters, 2010, 490, 116-122.	1.2	26
1974	Theoretical study on the atmospheric formation of cis and trans-OSSO complexes. Chemical Physics Letters, 2010, 494, 315-322.	1.2	12
1975	Decarboxylation of pyrrole-2-carboxylic acid: A DFT investigation. Chemical Physics Letters, 2010, 496, 36-41.	1.2	10

#	ARTICLE	IF	CITATIONS
1976	Theoretical study on the mechanism of S <sub>2</sub> + O <sub>2</sub> reaction. Chemical Physics Letters, 2010, 497, 1-6.	1.2	9
1977	trans-Platinum anticancer drug AMD443: A detailed theoretical study by DFTâ€‘TST method on the hydrolysis mechanism. Chemical Physics Letters, 2010, 497, 142-148.	1.2	13
1978	Theoretical investigation for the reaction of N <sub>2</sub> O with CO catalyzed by MO <sup>+</sup> (M=Ru, Os). Chemical Physics Letters, 2010, 498, 245-252.	1.2	5
1979	Theoretical study on the formation of tetraoxygen conformational isomerism in the CO <sub>2</sub> with O <sub>3</sub> reaction. Chemical Physics Letters, 2010, 499, 51-55.	1.2	5
1980	Quantum Chemical Study on the Interactions of NO <sub>3</sub> with RDX and Four Decomposition Intermediates. Propellants, Explosives, Pyrotechnics, 2010, 35, 315-320.	1.0	12
1981	A DFTâ€‘based exploration augmented by Xâ€‘ray and NMR of the stereoselectivity in the 1,3â€‘dipolar cycloaddition of 1â€‘pyrrolineâ€‘1â€‘oxide to methyl cinnamate and benzylidene acetophenone. Journal of Physical Organic Chemistry, 2010, 23, 1187-1195.	0.9	11
1982	Singlet methylene insertion into polar Oâ€‘H and Nâ€‘H bonds of water and ammoniaâ€‘Ab initio and DFT study. International Journal of Quantum Chemistry, 2010, 110, 1310-1316.	1.0	1
1983	A comparative theoretical study of the reactivities of the Al <sup>+</sup> and Cu <sup>+</sup> ions toward methylamine and dimethylamine. International Journal of Quantum Chemistry, 2010, 110, 1583-1593.	1.0	2
1984	Reaction mechanism of cysteine proteases model compound HSH with diketone inhibitor PhCOCOCH <sub>3</sub> â€‘X <sub>2</sub> , (X = F, Cl, n = 0, 1, 2). International Journal of Quantum Chemistry, 2010, 110, 1660-1674.	1.0	12
1985	Gasâ€‘phase intramolecular anion rearrangements of some trimethylsilylâ€‘containing systems revisited. A theoretical approach. Rapid Communications in Mass Spectrometry, 2010, 24, 57-62.	0.7	1
1986	Exploring rearrangements along the fragmentation of glutaric acid negative ion: a combined experimental and theoretical study. Rapid Communications in Mass Spectrometry, 2010, 24, 1198-1206.	0.7	16
1987	Are the anions MeO(CO) (n = 1 and 2) methoxide anion donors in the gas phase? A theoretical investigation. Rapid Communications in Mass Spectrometry, 2010, 24, 1895-1901.	0.7	2
1988	Thermodynamics and Dynamic Kinetics of the Oxidation of Selenomethionine to Methionine Selenoxide: A Dft Study. Progress in Reaction Kinetics and Mechanism, 2010, 35, 417-422.	1.1	4
1990	Competition Between Azido Cleavage and Triplet Nitrene Formation in Azidomethylacetophenones. Australian Journal of Chemistry, 2010, 63, 1645.	0.5	9
1991	The catalytic effect of water on the keto-enol tautomerisation reaction of thioformic acid. Molecular Physics, 2010, 108, 1375-1384.	0.8	19
1992	Theoretical study for the reaction of CH <sub>3</sub> CN with O(P <sub>3</sub> ). Journal of Chemical Physics, 2010, 132, 064301.	1.2	17
1993	Experimental and theoretical studies of reactions of neutral vanadium and tantalum oxide clusters with NO and NH <sub>3</sub> . Journal of Chemical Physics, 2010, 133, 174314.	1.2	28
1994	Theoretical Study of the HOCH <sub>2</sub> OOâ€‘ + HO <sub>2</sub> â€‘ Reaction: Detailed Molecular Mechanisms of the Three Reaction Channels. Zeitschrift Fur Physikalische Chemie, 2010, 224, 1081-1093.	1.4	8

#	ARTICLE	IF	CITATIONS
1995	Experimental and Theoretical Study of Hydrogen Atom Abstraction from C <sub>2</sub> H <sub>6</sub> and C <sub>4</sub> H <sub>10</sub> by Zirconium Oxide Clusters Anions. Chinese Journal of Chemical Physics, 2010, 23, 133-137.	0.6	20
1996	Theoretical Study of Interaction Between S <sub>2</sub> and SiH <sub>x</sub> (x = 1, 2, 3) in Porous Silicon. Chinese Journal of Chemical Physics, 2010, 23, 281-286.	0.6	1
1997	Structure, Stability, and Generation of CH <sub>3</sub> CNS. Australian Journal of Chemistry, 2010, 63, 1686.	0.5	17
1998	Mechanistic Investigation on the Reaction of O <sup>+</sup> with CH <sub>3</sub> CN Using Density Functional Theory. Chinese Journal of Chemical Physics, 2010, 23, 643-648.	0.6	1
1999	Understanding Regioselective Cleavage in Peptide Hydrolysis by a Palladium(II) Aqua Complex: A Theoretical Point of View. Journal of Physical Chemistry B, 2010, 114, 8525-8535.	1.2	11
2000	Mechanism of Acid-Catalyzed Hydrolysis of Formamide from Cluster-Continuum Model Calculations: Concerted versus Stepwise Pathway. Journal of Physical Chemistry A, 2010, 114, 12918-12927.	1.1	71
2001	Identification of pseudodiatom behavior in polyatomic bond dissociation: Reaction force analysis. Journal of Chemical Physics, 2010, 132, 154308.	1.2	9
2002	Dimerization of Indanedione ketene to Spiro-oxetanone: A Theoretical Study. Journal of Organic Chemistry, 2010, 75, 5499-5504.	1.7	5
2003	Modulating Reactivity and Diverting Selectivity in Palladium-Catalyzed Heteroaromatic Direct Arylation Through the Use of a Chloride Activating/Blocking Group. Journal of Organic Chemistry, 2010, 75, 1047-1060.	1.7	299
2004	Regioselective Synthesis of Heterocycles Containing Nitrogen Neighboring an Aromatic Ring by Reductive Ring Expansion Using Diisobutylaluminum Hydride and Studies on the Reaction Mechanism. Journal of Organic Chemistry, 2010, 75, 627-636.	1.7	77
2005	Quantum chemical dissection of the classic terpinyl/pinyl/bornyl/camphyl cation conundrum—the role of pyrophosphate in manipulating pathways to monoterpenes. Organic and Biomolecular Chemistry, 2010, 8, 4589.	1.5	73
2006	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	1.1	16
2007	Kinetics of thermoneutral intermolecular hydrogen migration in alkyl radicals. Physical Chemistry Chemical Physics, 2010, 12, 10988.	1.3	29
2008	Mechanism and Branching Ratios of Hydroxy Ethers + <sup>•</sup> OH Gas phase Reactions: Relevance of H Bond Interactions. Journal of Physical Chemistry A, 2010, 114, 7525-7536.	1.1	17
2009	Reaction Force and Its Link to Diabatic Analysis: A Unifying Approach to Analyzing Chemical Reactions. Journal of Physical Chemistry Letters, 2010, 1, 2858-2862.	2.1	46
2010	Ab Initio Study of the Pathways and Barriers of Tricyclo[4.1.0.0 <sup>2,7</sup> ]heptene Isomerization. Journal of Physical Chemistry A, 2010, 114, 11798-11806.	1.1	5
2011	Compelling Computational Evidence for the Concerted Cyclization of the ABC Rings of Hopene from Protonated Squalene. Journal of the American Chemical Society, 2010, 132, 17111-17117.	6.6	44
2012	Catalysis of Carboxypeptidase A: Promoted-Water versus Nucleophilic Pathways. Journal of Physical Chemistry B, 2010, 114, 9259-9267.	1.2	33

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2013	Ab Initio Chemical Kinetic Study for Reactions of H Atoms with SiH <sub>4</sub> and Si <sub>2</sub> H <sub>6</sub> : Comparison of Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 2010, 114, 633-639.	1.1	21
2014	Mechanism of the Aminolysis of Fischer Alkoxy and Thiocarbene Complexes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 5821-5836.	1.7	19
2015	Diffusion of Atomic Oxygen on the Si(100) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12649-12658.	1.5	18
2016	Effect of Alkyl Substituents on Photorelease from Butyrophenone Derivatives. <i>Journal of Organic Chemistry</i> , 2010, 75, 1393-1401.	1.7	21
2017	Synthesis and Reactivity of an Iridium(I) Acetylonyl PNP Complex. Experimental and Computational Study of Metal <sup>+</sup> Ligand Cooperation in H <sup>+</sup> H and C <sup>+</sup> H Bond Activation via Reversible Ligand Dearomatization. <i>Organometallics</i> , 2010, 29, 3817-3827.	1.1	97
2018	Comparative Theoretical Study of 1,3-Dipolar Cycloadditions of Allyl-Anion Type Dipoles to Free and Pt-Bound Nitriles. <i>Journal of Organic Chemistry</i> , 2010, 75, 1474-1490.	1.7	34
2019	Structures and Energetics of Unimolecular Thermal Degradation of Isopropyl Butanoate as a Model Biofuel: Density Functional Theory and Ab Initio Studies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7996-8002.	1.1	14
2020	Catalysis in the Oil Droplet/Water Interface for Aromatic Claisen Rearrangement. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4325-4333.	1.1	23
2021	Conformational Preferences of X-Pro Sequences: Ala-Pro and Aib-Pro Motifs. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14077-14086.	1.2	10
2022	Propene Oxidation on V <sub>4</sub> O <sub>11</sub> Cluster: Reaction Dynamics to Acrolein. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6542-6549.	1.1	10
2023	Thermal Decomposition Pathways of Hydroxylamine: Theoretical Investigation on the Initial Steps. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9262-9269.	1.1	52
2024	Experimental and Theoretical Study of the Reactions between Vanadium <sup>+</sup> Silicon Heteronuclear Oxide Cluster Anions with <i>n</i> -Butane. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12271-12279.	1.5	83
2025	Facile Activation of Dihydrogen by a Phosphinito-Bridged Pt(I) <sup>+</sup> Pt(I) Complex. <i>Journal of the American Chemical Society</i> , 2010, 132, 4752-4765.	6.6	23
2026	Ab Initio Chemical Kinetics for SiH <sub>3</sub> Reactions with Si <sub>x</sub> H <sub>2x+2</sub> (x = 1-4). <i>Journal of Physical Chemistry A</i> , 2010, 114, 13353-13361.	1.1	8
2027	Computational Study on the Reactivity of Tetrazines toward Organometallic Reagents. <i>Journal of Organic Chemistry</i> , 2010, 75, 6196-6200.	1.7	13
2028	Mechanistic Study on the Gold-Catalyzed C <sup>+</sup> S Bond Formation of $\pm$ -Thioallenes To Form 2,5-Dihydrothiophenes. <i>Journal of Organic Chemistry</i> , 2010, 75, 8516-8521.	1.7	35
2029	Nonadiabatic ab Initio Dynamics of a Model Protonated Schiff Base of 9-cis Retinal. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8190-8201.	1.1	30
2030	Transition Metal Intervention for a Classic Reaction: Assessing the Feasibility of Nickel(0)-Promoted [1,3] Sigmatropic Shifts of Bicyclo[3.2.0]hept-2-enes. <i>Organometallics</i> , 2010, 29, 3541-3545.	1.1	18

#	ARTICLE	IF	CITATIONS
2031	Mechanism Insight into the Cyanide-Catalyzed Benzoin Condensation: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9222-9230.	1.1	24
2032	Comparative DFT Analysis of Ligand and Solvent Effects on the Mechanism of H <sub>2</sub> Activation in Water Mediated by Half-Sandwich Complexes [Cp <sup>2</sup> Ru(PTA) <sub>2</sub> Cl] (Cp <sup>2</sup> = ) <i>Journal of Organometallics</i> , 2010, 29, 5121-5131.	1.1	32
2033	Differentiating Mechanistic Possibilities for the Thermal, Intramolecular [2 + 2] Cycloaddition of Allene. <i>Journal of the American Chemical Society</i> , 2010, 132, 11952-11966.	6.6	94
2034	A DFT Study on the Mechanism of the Coupling Reaction between Chloromethyloxirane and Carbon Dioxide Catalyzed by Re(CO) <sub>5</sub> Br. <i>Organometallics</i> , 2010, 29, 2069-2079.	1.1	30
2035	Ab Initio Chemical Kinetics for the Reaction of an H Atom with Si <sub>3</sub> H <sub>8</sub> . <i>Journal of Physical Chemistry A</i> , 2010, 114, 3642-3648.	1.1	15
2036	An Ab Initio Study of the Ground and Excited State Chemistry of Phenyldiazirine and Phenyldiazomethane. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5902-5912.	1.1	23
2037	Valence Isomerization of Phosphepines. <i>Organometallics</i> , 2010, 29, 6653-6659.	1.1	15
2038	Formation of Beyerene, Kaurene, Trachylobane, and Atiserene Diterpenes by Rearrangements That Avoid Secondary Carbocations. <i>Journal of the American Chemical Society</i> , 2010, 132, 5375-5386.	6.6	77
2039	The Reactivity of Phosphagermaallene Mes <sup>*</sup> P=C=Ge( <i>i</i> -Bu)Tip toward Aldehydes and Ketones: an Experimental and Theoretical Study. <i>Organometallics</i> , 2010, 29, 2566-2578.	1.1	26
2040	Cationic Noble Gas Hydrides: A Theoretical Investigation of Dinuclear HNgFNg <sup>+</sup> (Ng = ) <i>Journal of Organometallics</i> , 2010, 29, 2566-2578.	1.1	29
2041	Theoretical Study of Initial Adsorptions and Subsequent Surface Rearrangements of H <sub>2</sub> O <sub>2</sub> on Si(100)-2 × 1 Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14187-14192.	1.5	4
2042	Mechanistic Insight into the Gas-Phase Reactions of Methylamine with Ground State Co <sup>3+</sup> ( <sup>3</sup> F) and Ni <sup>2+</sup> ( <sup>2</sup> D). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12490-12497.	1.1	4
2043	Computational Study on the Growth of Gallium Nitride and a Possible Source of Oxygen Impurity. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5016-5025.	1.1	10
2044	Density functional studies on copper-catalysed asymmetric aziridination of diazoacetate with imines. <i>Molecular Simulation</i> , 2010, 36, 15-25.	0.9	3
2045	On the Dissociation of Ground State trans-HOOO Radical: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2743-2750.	2.3	42
2046	Theoretical Investigations on the Reaction of Monosubstituted Tertiary-Benzylamine Selenols with Hydrogen Peroxide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10706-10711.	1.1	16
2047	Theoretical Investigation of the Oxidation of Propane by FeO <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2010, 114, 2701-2709.	1.1	9
2048	Dynamics of Formation of Products D <sub>2</sub> CN <sup>+</sup> , DCN <sup>+</sup> , and CD <sub>3</sub> <sup>+</sup> in the Reaction of N <sup>+</sup> with CD <sub>4</sub> : A Crossed-Beam and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1384-1391.	1.1	6



#	ARTICLE	IF	CITATIONS
2049	Phenomenological Description of a Three-Center Insertion Reaction: An Information-Theoretic Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1906-1916.	1.1	17
2050	Detailed Modeling of Low-Temperature Propane Oxidation: 1. The Role of the Propyl + O <sub>2</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6594-6607.	1.1	70
2051	Structural Elucidation of Cisoid and Transoid Cyclization Pathways of a Sesquiterpene Synthase Using 2-Fluorofarnesyl Diphosphates. <i>ACS Chemical Biology</i> , 2010, 5, 377-392.	1.6	60
2052	Hydrogen Generation from Alcohols Catalyzed by Ruthenium <sup>II</sup> -Triphenylphosphine Complexes: Multiple Reaction Pathways. <i>Journal of the American Chemical Society</i> , 2010, 132, 8056-8070.	6.6	215
2053	Intramolecular Double Proton Transfer from 2-Hydroxy-2-iminoacetic Acid to 2-Amino-2-oxoacetic Acid. <i>Journal of Organic Chemistry</i> , 2010, 75, 1419-1426.	1.7	11
2054	How an Enzyme Might Accelerate an Intramolecular Diels-Alder Reaction: Theozymes for the Formation of Salvileucalin B. <i>Organic Letters</i> , 2010, 12, 1164-1167.	2.4	19
2055	Reaction Pathway of Methylenation of Carbonyl Compounds with Bis(iodozincio)methane. <i>Journal of the American Chemical Society</i> , 2010, 132, 17452-17458.	6.6	34
2056	A Theoretical Study of the Reaction of $\dot{\text{I}}^2$ -Carotene with the Nitrogen Dioxide Radical in Solution. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4366-4372.	1.2	41
2057	Isomerization and Decomposition of a Model Nerve Agent: A Computational Analysis of the Reaction Energetics and Kinetics of Dimethyl Ethylphosphonate. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10717-10725.	1.1	17
2058	Reactions of Germenes with Some <i>para</i> -Quinones: Formation of a Tricyclic Compound from 1,4-Benzoquinone Undergoing an Unexpected Rearrangement. <i>Organometallics</i> , 2010, 29, 4849-4857.	1.1	10
2059	Effect of Hydration on the Hydrogen Abstraction Reaction by HO in DMS and its Oxidation Products. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4857-4863.	1.1	56
2060	The capture of $\dot{\text{E}}^{\text{TM}}\text{H}$ and $\dot{\text{E}}^{\text{TM}}\text{OH}$ radicals by vitamin C and implications for the new source for the formation of the anion free radical. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5256.	1.3	18
2061	Electronic Structural Comparison of the Reactions of Dioxygen and Alkenes with Nitrogen-Chelated Palladium(0). <i>Inorganic Chemistry</i> , 2010, 49, 8200-8207.	1.9	23
2062	Photophysics and Photodeprotection Reactions of <i>p</i> -Methoxyphenacyl Phototriggers: An Ultrafast and Nanosecond Time-Resolved Spectroscopic and Density Functional Theory Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 5837-5851.	1.7	9
2063	Favored Reaction Mechanism of Calcium-Dependent Phospholipase A <sub>2</sub> . Insights from Density Functional Exploration. <i>Journal of Physical Chemistry B</i> , 2010, 114, 11584-11593.	1.2	5
2064	On the OH initiated oxidation of C <sub>2</sub> -C <sub>5</sub> aliphatic aldehydes in the presence of mineral aerosols. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 3587-3597.	1.6	38
2065	Theoretical Analysis of Factors Controlling Pd-Catalyzed Decarboxylative Coupling of Carboxylic Acids with Olefins. <i>Journal of the American Chemical Society</i> , 2010, 132, 638-646.	6.6	211
2066	Theoretical Study of the Gas-Phase Reactions of Iodine Atoms (I <sup>2</sup> P <sub>3/2</sub> ) with H <sub>2</sub> , H <sub>2</sub> O, HI, and OH. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9270-9288.	1.1	32

#	ARTICLE	IF	CITATIONS
2067	Theoretical Study of Acid-Catalyzed Hydrolysis of Epoxides. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5187-5194.	1.1	27
2068	Understanding the mechanism of non-polar Diels-Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 5495.	1.5	85
2069	Radical formation of amino acid precursors in interstellar regions? Ser, Cys and Asp. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4934.	1.5	11
2070	Radical routes to interstellar glycolaldehyde. The possibility of stereoselectivity in gas-phase polymerization reactions involving CH <sub>2</sub> O and $\dot{E}^{\text{TM}}\text{CH}_2\text{OH}$ . <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4757.	1.5	15
2071	Ni-, Pd-, or Pt-catalyzed ethylene dimerization: a mechanistic description of the catalytic cycle and the active species. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1040.	1.5	20
2072	Dissecting a Dyotropic Rearrangement. <i>Journal of Organic Chemistry</i> , 2010, 75, 1693-1700.	1.7	23
2073	Fundamental Reaction Pathways for Cytochrome P450-Catalyzed 5 $\alpha$ -Hydroxylation and <i>N</i> -Demethylation of Nicotine. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9023-9030.	1.2	21
2074	Adsorption and dehydrogenation of methanol on alkali-cation-exchanged zeolite: A first-principles density functional study. <i>Microporous and Mesoporous Materials</i> , 2010, 127, 90-95.	2.2	19
2075	Mechanistic Study on the Gas-Phase Generation of $\alpha$ -Cyclometalated [M(bipy- $\pi$ )] <sup>+</sup> ETQqO O O rgBT /Overlock 10 Tf 50 42	1.1	57
2076	Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4884.	1.5	56
2077	Mechanistic and Kinetic Study of CH <sub>2</sub> O+O <sub>3</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3516-3522.	1.1	28
2078	Ring-Opening Mechanism of Lithium Bromosilacyclopropylidenoids to Silaallenes. <i>Organometallics</i> , 2010, 29, 6739-6743.	1.1	15
2079	Direct Observation of the Gas Phase Reaction of the Cyclohexyl Radical with Dioxygen Using a Distonic Radical Ion Approach. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1446-1456.	1.1	41
2080	Gas-Phase Nucleophilic and Elimination Reactions in Simple Alkyl Nitrates. <i>Journal of Physical Chemistry A</i> , 2010, 114, 11910-11919.	1.1	17
2081	Ping-Pong at Gold: Proton Jump Between Coordinated Phenyl and $\eta^1$ -Benzene Ligands, A Computational Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 8135-8141.	1.1	11
2082	The mechanism of the Stevens and Sommelet-Hauser Rearrangements. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 3608-3617.	1.7	73
2083	Mechanisms of the Au- and Pt-Catalyzed Intramolecular Acetylenic Schmidt Reactions: A DFT Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 7842-7854.	1.7	57
2084	Is an elementary reaction step really elementary? Theoretical decomposition of asynchronous concerted mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4142.	1.3	30

#	ARTICLE	IF	CITATIONS
2085	Stereoselectivity in oxyallyl-furan (4 + 3) cycloadditions: control of intermediate conformations and dispersive stabilisation in cycloadditions involving oxazolidinone auxiliaries. <i>Chemical Science</i> , 2010, 1, 387.	3.7	62
2086	Origins of Stereoselectivity in the $\alpha$ -Alkylation of Chiral Hydrazones. <i>Journal of Organic Chemistry</i> , 2010, 75, 8578-8584.	1.7	30
2087	Tandem 1,5-Hydride Shift/1,5-S,N-Cyclization with Ethylene Extrusion of 1,3-Oxathiolane-Substituted Ketenimines and Carbodiimides. An Experimental and Computational Study. <i>Journal of Organic Chemistry</i> , 2010, 75, 3737-3750.	1.7	44
2088	Effect of the Zeolite Nanocavity on the Reaction Mechanism of <i>n</i> -Hexane Cracking: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7850-7856.	1.5	80
2089	Theoretical Study of the Catalytic Mechanism of DNA-(N4-Cytosine)-Methyltransferase from the Bacterium <i>Proteus vulgaris</i> . <i>Journal of Physical Chemistry B</i> , 2010, 114, 8467-8473.	1.2	10
2090	Importance of the Nature of $\alpha$ -Substituents in Pyrrolidine Organocatalysts in Asymmetric Michael Additions. <i>Journal of Organic Chemistry</i> , 2010, 75, 7310-7321.	1.7	31
2091	On the Existence of an N-Metalated N-Heterocyclic Carbene: A Theoretical Study. <i>Organometallics</i> , 2010, 29, 4639-4642.	1.1	19
2092	Reduction of Hydrogen Peroxide by Glutathione Peroxidase Mimics: Reaction Mechanism and Energetics. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1996-2000.	1.1	29
2093	Computational Study of Alkynes Insertion into Metal-Hydride Bonds Catalyzed by Bimetallic Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 9875-9883.	1.9	18
2094	3,4-Ethylenedioxythiophene and 3,4-Ethylenedioxysephenophene: Synthesis and Reactivity of C-Si Bond. <i>Journal of Organic Chemistry</i> , 2010, 75, 4868-4871.	1.7	29
2095	Bisoxazoline-copper(I)-catalyzed aziridination of diazoacetate with imines: A DFT study. <i>Canadian Journal of Chemistry</i> , 2010, 88, 981-990.	0.6	4
2096	Isomers of OCS and their reaction with H <sub>2</sub> O on singlet potential energy surface. <i>Molecular Physics</i> , 2010, 108, 3353-3364.	0.8	3
2097	Computational calculations in microwave-assisted organic synthesis (MAOS). Application to cycloaddition reactions. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1000.	1.5	37
2098	A tangled web-interconnecting pathways to amorphadiene and the amorphene sesquiterpenes. <i>Chemical Science</i> , 2010, 1, 609.	3.7	32
2099	Reactivity of a rhenium hydroxo-carbonyl complex toward carbon disulfide: insights from theory. <i>Dalton Transactions</i> , 2010, 39, 874-882.	1.6	6
2100	Is the planar hexacoordinate nitrogen molecule NB <sup>-</sup> viable?. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 13153.	1.3	13
2101	Computational study of oxygen atom (3P and 1D) reactions with CF <sub>3</sub> CN. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10846.	1.3	4
2102	Towards understanding a mechanism for reversible hydrogen storage: theoretical study of transition metal catalysed dehydrogenation of sodium alanate. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4012.	1.3	20

#	ARTICLE	IF	CITATIONS
2103	Theoretical study of electronic structures of $[(\text{H}_2\text{O})_3(\text{O}^-)\text{Mn}(\frac{1}{4}\text{-oxo})_2\text{Mn}(\text{OH}_2)_4]^{q+}$ ( $q = 2$ or $3$ ) with Mn $\hat{\text{a}}$ “O bond. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2730.	1.3	7
2104	Active sites of stoichiometric cerium oxide cations ( $\text{Ce}_m\text{O}_{2m+}$ ) probed by reactions with carbon monoxide and small hydrocarbon molecules. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3984.	1.3	141
2105	Methane activation by $\text{V}_3\text{PO}_{10}\ddot{\text{E}}^{\text{TM}+}$ and $\text{V}_4\text{O}_{10}\ddot{\text{E}}^{\text{TM}+}$ clusters: A comparative study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12223.	1.3	89
2106	The reactions of $\text{SO}_3$ with $\text{HO}_2$ radical and $\text{H}_2\text{O}\hat{\text{a}}$ “ $\text{HO}_2$ radical complex. Theoretical study on the atmospheric formation of $\text{HSO}_5$ and $\text{H}_2\text{SO}_4$ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2116.	1.3	106
2107	Formation of nitriles and imines in the atmosphere of Titan: combined crossed-beam and theoretical studies on the reaction dynamics of excited nitrogen atoms $\text{N}(2\text{D})$ with ethane. <i>Faraday Discussions</i> , 2010, 147, 189.	1.6	79
2108	Rate Constants and Kinetic Isotope Effects on the Reaction of $\text{C}_2(\text{X})\hat{\text{I}}\xi\text{g}^+$ with $\text{CH}_4$ and $\text{CD}_4$ . <i>Journal of Physical Chemistry A</i> , 2010, 114, 4580-4585.	1.1	5
2109	DFT Study of the Structure and Reactivity of the Terminal Pt(IV)-Oxo Complex Bearing No Electron-Withdrawing Ligands. <i>Journal of the American Chemical Society</i> , 2010, 132, 14886-14900.	6.6	49
2110	$\text{SO}_3\text{H}$ -Functionalized Ionic Liquid Catalyzed Alkylation of Catechol with <i>tert</i> -Butyl Alcohol. <i>Industrial &amp; Engineering Chemistry Research</i> , 2010, 49, 8157-8163.	1.8	22
2111	Gas Phase Reaction of Nitric Acid with Hydroxyl Radical without and with Water. A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9151-9162.	1.1	74
2112	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory: Ozone Addition on Benzene. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12900-12906.	1.1	19
2113	Energetics of the Lighter Chalcogen Analogues of Carboxylic Acid Esters. <i>Journal of Physical Chemistry B</i> , 2010, 114, 16253-16262.	1.2	15
2114	Photodissociation and photoisomerization dynamics of $\text{CH}_2\hat{\text{I}}\rightarrow\text{CHCHO}$ in solution. <i>Journal of Chemical Physics</i> , 2010, 132, 124510.	1.2	8
2115	Theoretical analysis of <i>trans</i> - $[\text{PtCl}_2(\text{NH}_3)_2(\text{thiazole})]$ and <i>trans</i> - $[\text{PtCl}_2(\text{thiazole})_2]$ binding to biological targets $\hat{\text{a}}$ “ Factors influence binding kinetics and adduct stability. <i>Canadian Journal of Chemistry</i> , 2010, 88, 1240-1246.	0.6	6
2116	Theoretical study on the mechanism of $\text{H}_2$ activation mediated by two transition metal thiolate complexes: Homolytic for Ir, heterolytic for Rh. <i>Dalton Transactions</i> , 2010, 39, 857-863.	1.6	21
2117	Radon hydrides: structure and bonding. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2222-2227.	1.3	40
2118	Chemo-, regio-, and diastereoselectivity preferences in the reaction of a sulfur ylide with a dienal and an enone. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 1642.	1.5	7
2119	Mechanistic Insight into Protonolysis and <i>Cis</i> $\hat{\text{a}}$ “ <i>Trans</i> Isomerization of Benzylplatinum(II) Complexes Assisted by Weak Ligand-to-Metal Interactions. A Combined Kinetic and DFT Study. <i>Inorganic Chemistry</i> , 2011, 50, 2224-2239.	1.9	14
2120	The Taxadiene-Forming Carbocation Cascade. <i>Journal of the American Chemical Society</i> , 2011, 133, 18249-18256.	6.6	49

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2121	The association reaction between C <sub>2</sub> H and 1-butyne: a computational chemical kinetics study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4583.	1.3	7
2122	Thermal C-H Bond Activation of Benzene, Toluene, and Methane with Cationic [M(X)(bipy)] <sup>+</sup> (M = Ni, Pd). <i>Journal of Physical Chemistry A</i> , 2011, 115, 10743-10751.	1.1	46
2123	Aromaticity and Activation Strain Analysis of [3 + 2] Cycloaddition Reactions between Group 14 Heteroallenes and Triple Bonds. <i>Journal of Organic Chemistry</i> , 2011, 76, 2310-2314.	1.7	86
2124	Étude DFT (À« density functional theory À») des réactions d'addition de l'ozone sur les doubles liaisons des terpènes : limonène, Î <sup>2</sup> -phellandrène et terpinolène. <i>Canadian Journal of Chemistry</i> , 2011, 89, 703-708.	0.6	3
2125	Comparison of photoenolization and alcohol release from alkyl-substituted benzoyl benzoic esters. <i>Canadian Journal of Chemistry</i> , 2011, 89, 331-338.	0.6	6
2126	Tuning the Laplaza-Cummins 3-coordinate M[N(R)Ph] <sub>3</sub> catalyst to activate and cleave CO <sub>2</sub> . <i>Dalton Transactions</i> , 2011, 40, 5569.	1.6	12
2127	Double ionization of cycloheptatriene and the reactions of the resulting C <sub>7</sub> Hn <sup>2+</sup> dications (n = 6, 8) with xenon. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18330.	1.3	20
2128	Kinetics of the C-C bond beta scission reactions in alkyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15037.	1.3	25
2129	Theoretical investigation of the photochemical reaction mechanism of cyclopropenone decarbonylation. <i>Molecular Physics</i> , 2011, 109, 1785-1795.	0.8	5
2130	Theoretical study on the reaction of CH <sub>3</sub> CHCl + NO <sub>2</sub> . <i>Molecular Physics</i> , 2011, 109, 2525-2532.	0.8	0
2131	Thermal Stability of Endohedral First-Row Transition-Metal TM@ZnSi Structures, i = 12, 16. <i>Journal of Physical Chemistry C</i> , 2011, 115, 7829-7835.	1.5	7
2132	Pyrolysis of tert-Butyl tert-Butanethiosulfinate, t-BuS(O)St-Bu: A Computational Perspective of the Decomposition Pathways. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3068-3078.	1.1	7
2133	Impact of Water on the OH + HOCl Reaction. <i>Journal of the American Chemical Society</i> , 2011, 133, 3345-3353.	6.6	92
2134	Mechanistic Studies on the Reversible Hydrogenation of Carbon Dioxide Catalyzed by an Ir-PNP Complex. <i>Organometallics</i> , 2011, 30, 6742-6750.	1.1	288
2135	How Racemic Secondary Alkyl Electrophiles Proceed to Enantioselective Products in Negishi Cross-Coupling Reactions. <i>Organometallics</i> , 2011, 30, 3284-3292.	1.1	60
2136	A Theoretical Study of the H-Abstraction Reactions from HOI by Moist Air Radiolytic Products (H, OH). <i>Journal of Physical Chemistry A</i> , 2011, 115, 6664-6674.	1.1	15
2137	Substituent Effect on the Acid-Promoted Hydrolysis of 2-Aryloxazolin-5-one: Normal vs Reverse. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4995-5004.	1.1	6
2138	The Mechanism of H <sub>2</sub> Activation by (Amino)Carbenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3050-3059.	1.1	38

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2139	Comprehensive DFT Study of the Mechanism of Vanadium-Catalyzed Amination of Benzene with Hydroxylamine. <i>Organometallics</i> , 2011, 30, 5675-5686.	1.1	7
2140	Physical Constraints on Sesquiterpene Diversity Arising from Cyclization of the Eudesm-5-yl Carbocation. <i>Journal of the American Chemical Society</i> , 2011, 133, 12632-12641.	6.6	35
2141	Quantum Chemical and Theoretical Kinetics Study of the O( <sup>3</sup> P) + CS <sub>2</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4263-4269.	1.1	10
2142	Zwitterionic Ladder Stilbenes with Phosphonium and Borate Bridges: Intramolecular Cascade Cyclization and Structure-Photophysical Properties Relationship. <i>Organometallics</i> , 2011, 30, 3870-3879.	1.1	63
2143	Mechanisms of the Thermal Cyclotrimerizations of Fluoro- and Chloroacetylenes: Density Functional Theory Investigation and Intermediate Trapping Experiments. <i>Journal of the American Chemical Society</i> , 2011, 133, 10864-10877.	6.6	45
2144	From Inert to Explosive, The Hydrolytic Reactivity of R <sup>+</sup> NSO Compounds Understood: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3095-3105.	1.1	9
2145	Pd-Catalyzed Copolymerization of Methyl Acrylate with Carbon Monoxide: Structures, Properties and Mechanistic Aspects toward Ligand Design. <i>Journal of the American Chemical Society</i> , 2011, 133, 6761-6779.	6.6	63
2146	Collision-Induced Dissociation and Density Functional Theory Studies of CO Adsorption over Zirconium Oxide Cluster Ions: Oxidative and Nonoxidative Adsorption. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5238-5246.	1.1	51
2147	On the Memory of Chirality in Gold(I)-Catalyzed Intramolecular Carboalkoxylation of Alkynes. <i>Journal of Organic Chemistry</i> , 2011, 76, 3791-3796.	1.7	41
2148	Stereoselectivities and Regioselectivities of (4 + 3) Cycloadditions Between Allenamide-Derived Chiral Oxazolidinone-Stabilized Oxyallyls and Furans: Experiment and Theory. <i>Journal of the American Chemical Society</i> , 2011, 133, 14443-14451.	6.6	55
2149	Coordination of Ethylene to a Zwitterionic Rh(III) Half-Sandwich Complex: Influence of Ambiphilic Ligands on Reactivity. <i>Organometallics</i> , 2011, 30, 511-519.	1.1	39
2150	[2 + 2] Photocycloaddition Reaction Dynamics of Triplet Pyrimidines. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5335-5345.	1.1	13
2151	Theoretical Investigation for the Cycle Reaction of N <sub>2</sub> O (x <sup>1</sup> + <sup>+</sup> ) with CO (x <sup>1</sup> + <sup>+</sup> ) Catalyzed by IrO <sub>2</sub> (x <sup>1</sup> + <sup>+</sup> ) (x <sup>1</sup> = 1). <i>Journal of Physical Chemistry A</i> , 2011, 115, 11023-11032.	1.1	13
2152	Gas-Phase Reactions of the Bare Th <sup>2+</sup> and U <sup>2+</sup> Ions with Small Alkanes, CH <sub>4</sub> , C <sub>2</sub> H <sub>6</sub> , and C <sub>3</sub> H <sub>8</sub> : Experimental and Theoretical Study of Elementary Organoactinide Chemistry. <i>Journal of the American Chemical Society</i> , 2011, 133, 1955-1970.	6.6	49
2153	Pyrolysis Mechanisms of Thiophene and Methylthiophene in Asphaltenes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2882-2891.	1.1	27
2154	Mechanical and Kinetic Studies of the Formation of Polyhalogenated Dibenzo-p-dioxins from Hydroxylated Polybrominated Diphenyl Ethers and Chlorinated Derivatives. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13489-13497.	1.1	15
2155	Theoretical Investigation on Reaction of Sulbactam with Wild-Type SHV-1 β-Lactamase: Acylation, Tautomerization, and Deacylation. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10298-10310.	1.2	4
2156	Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2837-2846.	1.1	36

#	ARTICLE	IF	CITATIONS
2157	Theoretical Study on the Gas Phase Reaction of Sulfuric Acid with Hydroxyl Radical in the Presence of Water. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1350-1357.	1.1	40
2158	Theoretical Investigations on the Mechanism of Benzoin Condensation Catalyzed by Pyrido[1,2- <i>a</i> ]-2-ethyl[1,2,4]triazol-3-ylidene. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1408-1417.	1.1	36
2159	Facile Direct Insertion of Nitrosonium Ion (NO <sup>+</sup> ) into a Ruthenium <sup>II</sup> Aryl Bond. <i>Organometallics</i> , 2011, 30, 1311-1314.	1.1	28
2160	Analysis of the Reaction between O <sub>2</sub> and Nitrogen-Containing Char Using the Density Functional Theory. <i>Energy &amp; Fuels</i> , 2011, 25, 670-675.	2.5	25
2161	How Many Secondary Carbocations Are Involved in the Biosynthesis of Avermitilol?. <i>Organic Letters</i> , 2011, 13, 1294-1297.	2.4	37
2162	DFT Study on the Cycloreversion of Thietane Radical Cations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5443-5448.	1.1	4
2163	Cross-Linking Mechanisms of Arginine and Lysine with $\alpha,\beta$ -Dicarbonyl Compounds in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13542-13555.	1.1	19
2164	Organoactinides Promote the Dimerization of Aldehydes: Scope, Kinetics, Thermodynamics, and Calculation Studies. <i>Journal of the American Chemical Society</i> , 2011, 133, 1341-1356.	6.6	66
2165	On the Mechanism of Cyclopropanation Reactions Catalyzed by a Rhodium(I) Catalyst Bearing a Chelating Imine-Functionalized NHC Ligand: A Computational Study. <i>Organometallics</i> , 2011, 30, 6562-6571.	1.1	13
2166	Ligand Exchange Reaction Involving Ru(III) Compounds in Aqueous Solution: A Hybrid Quantum Mechanical/Effective Fragment Potential Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2030-2037.	1.2	7
2167	Integrating steepest-descent reaction pathways for large molecules. <i>Journal of Chemical Physics</i> , 2011, 134, 204103.	1.2	31
2168	Transition States and Energetics of Nucleophilic Additions of Thiols to Substituted $\alpha,\beta$ -Unsaturated Ketones: Substituent Effects Involve Enone Stabilization, Product Branching, and Solvation. <i>Journal of Organic Chemistry</i> , 2011, 76, 5074-5081.	1.7	84
2170	Unusual Properties of Usual Molecules. Conformational Analysis of Cyclohexene, Its Derivatives and Heterocyclic Analogues. , 2011, , 557-578.		2
2171	DFT Study of Thermal 1,3-Dipolar Cycloaddition Reactions between Alkynyl Metal(0) Fischer Carbene Complexes and 3- <i>H</i> -1,2-Dithiole-3-thione Derivatives. <i>Organometallics</i> , 2011, 30, 466-476.	1.1	38
2172	An Aza Cyclopropylcarbinyl-Homoallyl Radical Rearrangement <sup>†</sup> Radical Cyclization Cascade. Synthesis of Dibenzoimidazoazepine and Oxazepine Derivatives. <i>Journal of Organic Chemistry</i> , 2011, 76, 5384-5391.	1.7	19
2173	Mechanistic Insights on N-Heterocyclic Carbene-Catalyzed Annulations: The Role of Base-Assisted Proton Transfers. <i>Journal of Organic Chemistry</i> , 2011, 76, 5606-5613.	1.7	86
2174	Single Strand Break in DNA Coupled to the O <sup>+</sup> P Bond Cleavage. A Computational Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1911-1917.	1.2	23
2175	Effects of the substituents on the reactivity of carbonyl oxides. A theoretical study on the reaction of substituted carbonyl oxides with water. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13034.	1.3	173

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2176	Insights on the mechanism of proton transfer reactions in amino acids. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7773.	1.3	31
2177	Theoretical Analysis of the Mechanism of Palladium(II) Acetate-Catalyzed Oxidative Heck Coupling of Electron-Deficient Arenes with Alkenes: Effects of the Pyridine-Type Ancillary Ligand and Origins of the meta-Regioselectivity. <i>Journal of the American Chemical Society</i> , 2011, 133, 20218-20229.	6.6	154
2178	Electronic structure and reactivity of a biradical cluster: Sc <sub>3</sub> O <sub>6</sub> <sup>3+</sup> . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10084.	1.3	32
2179	Mechanistic Study on the Fluorination of K <sub>4</sub> [B(CN) <sub>4</sub> ] with ClF Enabling the High Yield and Large Scale Synthesis of K <sub>4</sub> [B(CF <sub>3</sub> ) <sub>3</sub> ] and K <sub>3</sub> [B(CF <sub>3</sub> ) <sub>3</sub> BCN]. <i>Inorganic Chemistry</i> , 2011, 50, 10268-10273.	1.9	34
2180	Density functional studies on diimine chelated palladium complex catalyzed Suzuki–Miyaura cross-coupling reaction: the impact of Lewis base employed in transmetalation process. <i>Dalton Transactions</i> , 2011, 40, 6458.	1.6	24
2181	Structure of the Oxygen-Rich Cluster Cation Al <sub>2</sub> O <sub>7</sub> <sup>+</sup> and its Reactivity toward Methane and Water. <i>Journal of the American Chemical Society</i> , 2011, 133, 16930-16937.	6.6	73
2182	Multichannel RRKM-TST and CVT Rate Constant Calculations for Reactions of CH <sub>2</sub> OH or CH <sub>3</sub> O with HO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2011, 115, 3291-3300.	1.1	18
2183	Theoretical Study of Mechanism and Selectivity of Copper-Catalyzed C–H Bond Amidation of Indoles. <i>Journal of Organic Chemistry</i> , 2011, 76, 9246-9252.	1.7	44
2184	Kinetic, DFT and TD-DFT studies on the mechanism of stabilization of pyramidal H <sub>3</sub> PO <sub>3</sub> at the [Mo <sub>3</sub> S <sub>4</sub> (H <sub>2</sub> O) <sub>10</sub> ] <sup>4+</sup> clusters (M <sup>2+</sup> = Pd, Ni). <i>Dalton Transactions</i> , 2011, 40, 8589.	1.6	3
2185	Which One among the Pt-Containing Anticancer Drugs More Easily Forms Monoadducts with G and A DNA Bases? A Comparative Study among Oxaliplatin, Nedaplatin, and Carboplatin. <i>Inorganic Chemistry</i> , 2011, 50, 6965-6971.	1.9	54
2186	Dinuclear Zn(II) Complex Catalyzed Phosphodiester Cleavage Proceeds via a Concerted Mechanism: A Density Functional Theory Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 2904-2915.	6.6	55
2187	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11239.	1.3	18
2188	Theoretical Studies on Reactions of the Stabilized H <sub>2</sub> COO with HO <sub>2</sub> and the HO <sub>2</sub> ··H <sub>2</sub> O Complex. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6559-6567.	1.1	71
2189	Understanding the Electronic Reorganization along the Nonpolar [3 + 2] Cycloaddition Reactions of Carbonyl Ylides. <i>Journal of Organic Chemistry</i> , 2011, 76, 373-379.	1.7	89
2190	Syntheses and Crystal Structures of the closo-Borates M <sub>2</sub> [B <sub>7</sub> H <sub>7</sub> ] and M[B <sub>7</sub> H <sub>8</sub> ] (M =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1 [B <sub>n</sub> H <sub>n</sub> ] <sup>2-</sup> (n = 6–12). <i>Inorganic Chemistry</i> , 2011, 50, 2580-2589.	1.9	25
2191	Ab Initio and RRKM Study of the HCN/HNC Elimination Channels from Vinyl Cyanide. <i>Journal of Physical Chemistry A</i> , 2011, 115, 979-985.	1.1	26
2192	Mechanisms of Hydrolysis–Oligomerization of Aluminum Alkoxide Al(OC <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> . <i>Journal of Physical Chemistry A</i> , 2011, 115, 4719-4728.	1.1	25
2193	A DFT Study of the Ambiphilic Nature of Arylpalladium Species in Intramolecular Cyclization Reactions. <i>Journal of Organic Chemistry</i> , 2011, 76, 1592-1598.	1.7	21



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2194	A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 4295.	1.5	33
2195	A New Class of Antimalarial Dioxanes Obtained through a Simple Two-Step Synthetic Approach: Rational Design and Structure-Activity Relationship Studies. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8526-8540.	2.9	17
2196	Stereocontrolled Ring-Opening of a Hindered Sulfamidate with Nitrogen-Containing Aromatic Heterocycles: Synthesis of Chiral Quaternary Imidazole Derivatives. <i>Journal of Organic Chemistry</i> , 2011, 76, 4034-4042.	1.7	25
2197	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6616.	1.5	45
2198	Experimental and Theoretical Study of the Reactions between Cerium Oxide Cluster Anions and Carbon Monoxide: Size-Dependent Reactivity of $Ce_nO_{2n+1}^+$ ( $n = 1-21$ ). <i>Journal of Physical Chemistry C</i> , 2011, 115, 13329-13337.	1.5	76
2199	A DFT study on the thermal reaction mechanisms of fluorobutanesulfonyl azide with pyrazine under solvent free condition. <i>Computational and Theoretical Chemistry</i> , 2011, 968, 39-43.	1.1	5
2200	Theoretical studies on the reactions of thymine with six methylating agents. <i>Computational and Theoretical Chemistry</i> , 2011, 972, 25-31.	1.1	1
2201	Theoretical views on the cycle reaction of $N_2O(1^1\Sigma^+) + NH_3(1A_1) + O_2$ catalyzed by $Fe^+$ and utilizing the energy span model to study its kinetic information. <i>Computational and Theoretical Chemistry</i> , 2011, 974, 143-150.	1.1	3
2202	Increasing complexity models for describing the generation of substrate radicals at the active site of ethanolamine ammonia-lyase/B12. <i>Computational and Theoretical Chemistry</i> , 2011, 975, 52-60.	1.1	3
2203	Theoretical mechanistic study of OH-initiated atmospheric oxidation reaction of allyl alcohol in the presence of $O_2$ and $NO$ . <i>Computational and Theoretical Chemistry</i> , 2011, 977, 111-122.	1.1	2
2204	A MP2(full) and CCSD(T) theoretical investigation on the dihydrogen-bonded interactions between $HNa$ and $RBBH$ ( $R = F, Cl, H, CN, NC$ and $CO$ ). <i>Computational and Theoretical Chemistry</i> , 2011, 977, 201-208.	1.1	6
2205	Thermodynamic and kinetic stability of magnesium dication solvated by tetramethylethylenediamine. <i>Computational and Theoretical Chemistry</i> , 2011, 978, 104-109.	1.1	4
2206	Oxidation of Zinc-Thiolate Complexes of Biological Interest by Hydrogen Peroxide: A Theoretical Study. <i>Inorganic Chemistry</i> , 2011, 50, 5407-5416.	1.9	25
2207	The Ultrafast Photoisomerizations of Rhodopsin and Bathorhodopsin Are Modulated by Bond Length Alternation and HOOP Driven Electronic Effects. <i>Journal of the American Chemical Society</i> , 2011, 133, 3354-3364.	6.6	157
2208	Products and Mechanism of Acene Dimerization. A Computational Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 10803-10816.	6.6	110
2209	Mechanistic Studies of Wacker-Type Intramolecular Aerobic Oxidative Amination of Alkenes Catalyzed by $Pd(OAc)_2/Pyridine$ . <i>Journal of Organic Chemistry</i> , 2011, 76, 1031-1044.	1.7	78
2210	Can Human Prolidase Enzyme Use Different Metals for Full Catalytic Activity?. <i>Inorganic Chemistry</i> , 2011, 50, 3394-3403.	1.9	37
2211	Approaching and Bond Breaking Energies in the $C-H$ Activation and Their Application in Catalyst Design. <i>Journal of Physical Chemistry A</i> , 2011, 115, 904-910.	1.1	14

#	ARTICLE	IF	CITATIONS
2212	A Mechanistic Study of the 2-Thienylmethyl + HO <sub>2</sub> Radical Recombination Reaction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 14546-14557.	1.1	6
2213	DFT Studies on the Reaction of CpCo(PPh <sub>3</sub> ) <sub>2</sub> with Diphenylphosphinoalkynes: Formation of Cobaltacycles and Cyclobutadiene-Substituted CpCoCb Diphosphines. <i>Organometallics</i> , 2011, 30, 3740-3748.	1.1	13
2214	Origins of the diastereoselectivity in hydrogen bonding directed Diels-Alder reactions of chiral dienes with achiral dienophiles: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 8079.	1.5	18
2215	Theoretical investigation on mechanism of asymmetric Michael addition of malononitrile to chalcones catalyzed by Cinchona alkaloid aluminium(III) complex. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6402.	1.5	21
2216	Theoretical insights into the metal-free and formal [2 + 2 + 2] cycloaddition strategy via intramolecular cascade propargylic ene/Diels-Alder reactions with tautomerization. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 5997.	1.5	8
2217	Mechanism of intramolecular catalysis in the hydrolysis of alkyl monoesters of 1,8-naphthalic acid. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6163.	1.5	8
2218	Mechanism and electronic effects in nitrogen ylide-promoted asymmetric aziridination reaction. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 2123.	1.5	8
2219	Quantum chemical study of interactions of carbenes and their analogs of the EH <sub>2</sub> and EH <sub>X</sub> types (E =) Tj ETQq1 1 0.784314 rgBT /Over Russian Chemical Bulletin, 2011, 60, 2147-2160.	0.4	4
2220	Novel [4 + 2] cycloaddition reactions of alkyne and enyne key-units: Direct access to bicyclic aromatic and heteroaromatic products. A theoretical mechanistic study. <i>Chemical Science</i> , 2011, 2, 2332-2341.	3.7	15
2221	An efficient approach to azirino and pyrrolo-fused dibenzazepines. Conformations of substituted dibenzo[c,f]pyrrolo[1,2-a]azepines. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 3886.	1.5	28
2222	Theoretical Study on Mechanism of Copper(I)-Catalyzed Cross-Coupling between Aryl Halides and Alkylamines. <i>Organometallics</i> , 2011, 30, 633-641.	1.1	76
2223	Organocatalytic, Enantioselective Intramolecular [6 + 2] Cycloaddition Reaction for the Formation of Tricyclopentanoids and Insight on Its Mechanism from a Computational Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 20175-20185.	6.6	66
2224	DFT Study on the Mechanism of DNA Damage Caused by the Isomerization of DNA Purine Base. <i>International Journal of Chemistry</i> , 2011, 3, .	0.3	0
2225	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. <i>Current Organic Chemistry</i> , 2011, 15, 3566-3575.	0.9	79
2226	Theoretical Insights into the Enantioselectivity and Mechanism of Diels-Alder Reactions Involving Chiral Cationic Oxazaborolidinium Catalyst. <i>Bulletin of the Chemical Society of Japan</i> , 2011, 84, 196-204.	2.0	6
2227	Positive Ion Chemistry of SiH <sub>4</sub> /GeF <sub>4</sub> Gaseous Mixtures Studied by Ion Trap Mass Spectrometry and <i>Ab Initio</i> Calculations. <i>European Journal of Mass Spectrometry</i> , 2011, 17, 197-206.	0.5	2
2228	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. <i>Tetrahedron</i> , 2011, 67, 8383-8391.	1.0	9
2229	Infrared photoreaction of 2-chloroethyltrifluorosilane. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011, 222, 77-80.	2.0	2

#	ARTICLE	IF	CITATIONS
2230	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. <i>Polymer</i> , 2011, 52, 5503-5512.	1.8	20
2231	Energetics and rearrangements of the isomeric picoline dications. <i>International Journal of Mass Spectrometry</i> , 2011, 308, 81-88.	0.7	3
2232	A theoretical study of the kinetics of the forward and reverse reactions $\text{HI} + \text{CH}_3 = \text{I} + \text{CH}_4$ . <i>Chemical Physics Letters</i> , 2011, 517, 149-154.	1.2	22
2233	Theoretical study of the reactivity of $(\text{CH}_3)_2\text{AlCH}_2\text{I}$ promoted cyclopropanation reactions. <i>Arabian Journal of Chemistry</i> , 2011, 4, 379-382.	2.3	1
2234	Computational study on the mechanisms of action of the potential anticancer drug trans-isopropylaminodimethylaminodichloroplatinum (trans-IPADMADP) and its cis isomer with DNA purine bases. <i>Inorganica Chimica Acta</i> , 2011, 376, 44-56.	1.2	9
2235	Theoretical study on the mechanism and kinetics of the reaction of 2,2,4,4-tetrabrominated diphenyl ether (BDE-47) with OH radicals. <i>Atmospheric Environment</i> , 2011, 45, 1525-1531.	1.9	26
2236	A theoretical investigation of gas phase $\text{NO}_3$ initiated nitration of p-cresol. <i>Chemical Physics</i> , 2011, 389, 39-46.	0.9	11
2237	Regioselectivity in the Nitration of Dialkoxybenzenes. <i>Journal of Organic Chemistry</i> , 2011, 76, 1285-1294.	1.7	24
2238	Alkyne Insertion into the $\text{M}\xi\text{P}$ and $\text{M}\xi\text{H}$ Bonds (M=Pd, Ni, Pt, and Rh): A Theoretical Mechanistic Study of the $\text{C}\xi\text{P}$ and $\text{C}\xi\text{H}$ Bond Formation Steps. <i>Chemistry - an Asian Journal</i> , 2011, 6, 1423-1430.	1.7	47
2239	Theoretical studies on the electron capture properties of the $\text{H}_2\text{SO}_4\text{HOO}\ddot{\text{O}}^{\text{TM}}$ complex and its implications as an alternative source of HOOH. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 5931.	1.3	8
2240	$\text{In silico}$ mechanistic studies as predictive tools in microwave-assisted organic synthesis. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 2371.	1.5	19
2241	Computational study on decomposition kinetics of $\text{CH}_3\text{CFCIO}$ radical. <i>Journal of Chemical Sciences</i> , 2011, 123, 733-741.	0.7	7
2242	Quantum-chemical simulation of the allyl isomerization of allylbenzene in the presence of gold atom. <i>Russian Journal of Physical Chemistry A</i> , 2011, 85, 646-653.	0.1	3
2243	Reaction Mechanism and Chemoselectivity of Intermolecular Cycloaddition Reactions between Phenyl-Substituted Cyclopropenone Ketal and Methyl Vinyl Ketone. <i>Journal of Organic Chemistry</i> , 2011, 76, 3086-3095.	1.7	11
2244	Photolysis of (3-Methyl-2-azirin-2-yl)-phenylmethanone: Direct Detection of a Triplet Vinylnitrene Intermediate. <i>Journal of Organic Chemistry</i> , 2011, 76, 9934-9945.	1.7	32
2245	Triplet-Sensitized Photoreactivity of a Geminal Diazidoalkane. <i>Journal of Organic Chemistry</i> , 2011, 76, 8177-8188.	1.7	15
2246	Intermolecular $\text{C}\xi\text{H}$ Activations of Hydrocarbons Initiated by $\text{Cp}^*\text{M}(\text{NO})(\text{CH}_2)_2\text{CMe}_3(\text{I}^{\text{sup}3}\text{-CH}_2)_2\text{CHCHPh}$ Complexes (M =) Tj ETIQ0 0 0 28 BT /Overl	1.0	28
2247	Geometry optimization. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 790-809.	6.2	250

#	ARTICLE	IF	CITATIONS
2248	Finding minimum energy reaction paths on ab initio potential energy surfaces using the fast marching method. <i>Journal of Mathematical Chemistry</i> , 2011, 49, 1291-1301.	0.7	3
2249	Theoretical study on the reaction mechanism of the OH-initiated oxidation of CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> OH. <i>Structural Chemistry</i> , 2011, 22, 589-604.	1.0	7
2250	Theoretical study on the atmospheric formation of sulfur trioxide as the primary agent for acid rain. <i>Structural Chemistry</i> , 2011, 22, 817-822.	1.0	10
2251	Theoretical study on the gas-phase reaction mechanism between rhodium monoxide cation and methane. <i>Structural Chemistry</i> , 2011, 22, 983-997.	1.0	6
2252	Mechanistic study on the atmospheric formation of acid rain base on the sulfur dioxide. <i>Structural Chemistry</i> , 2011, 22, 1331-1338.	1.0	16
2253	Theoretical study of anticancer drug trans-[Pd(dmnp) <sub>2</sub> Cl <sub>2</sub> ] binding to DNA purine bases, phosphate group and amino acid residues. <i>Structural Chemistry</i> , 2011, 22, 1353-1364.	1.0	7
2254	Theoretical investigation of Ni(PMe <sub>3</sub> ) <sub>4</sub> -catalyzed intermolecular hydroacylation of alkynes with benzaldehydes. <i>Transition Metal Chemistry</i> , 2011, 36, 793-799.	0.7	7
2255	Theoretical investigation of the first-shell mechanism of acetylene hydration catalyzed by a biomimetic tungsten complex. <i>Journal of Biological Inorganic Chemistry</i> , 2011, 16, 745-752.	1.1	27
2256	A computational study of the mechanism of the unimolecular elimination of $\alpha,\beta$ -unsaturated aldehydes in the gas phase. <i>Journal of Molecular Modeling</i> , 2011, 17, 21-26.	0.8	11
2257	Ab initio studies on the decomposition kinetics of CF <sub>3</sub> OCF <sub>2</sub> O radical. <i>Journal of Molecular Modeling</i> , 2011, 17, 415-422.	0.8	26
2258	Nitrosation of malononitrile by HONO, ClNO and N <sub>2</sub> O <sub>3</sub> : A theoretical study. <i>Journal of Molecular Modeling</i> , 2011, 17, 1017-1027.	0.8	2
2259	Topological description of the bond-breaking and bond-forming processes of the alkene protonation reaction in zeolite chemistry: an AIM study. <i>Journal of Molecular Modeling</i> , 2011, 17, 2501-2511.	0.8	11
2260	Theoretical studies on model reaction pathways of prostaglandin H <sub>2</sub> isomerization to prostaglandin D <sub>2</sub> /E <sub>2</sub> . <i>Theoretical Chemistry Accounts</i> , 2011, 128, 191-206.	0.5	3
2261	Direct ab initio MD study on the hydrogen abstraction reaction of triplet state acetone from methanol molecule. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 207-213.	0.5	0
2262	The reaction between HO and (H <sub>2</sub> O) <sub>n</sub> (n=1, 3) clusters: reaction mechanisms and tunneling effects. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 579-592.	0.5	37
2263	Thermolysis of 2-methyloxetane: a computational study. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 327-339.	0.5	1
2264	Theoretical study of the C-F bond activation in methyl fluoride by alkaline-earth metal monocations. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 609-618.	0.5	6
2265	The geometric, energetic, and electronic properties of charged phosphorus-doped silicon clusters, P <sub>n</sub> <sup>+</sup> /P <sub>n</sub> <sup>-</sup> (n=1-8). <i>Theoretical Chemistry Accounts</i> , 2011, 130, 1009-1022.	0.5	7

#	ARTICLE	IF	CITATIONS
2266	DFT and ONIOM study on the alkylation of the lithium enolate in solution: microsolvation cluster models for CH <sub>2</sub> =CHOLi <sup>+</sup> ·nCH <sub>3</sub> Cl·m(THF)O <sup>-</sup> . <i>Theoretical Chemistry Accounts</i> , 2011, 130, 323-331.	0.5	13
2267	Potential energy surfaces and mechanisms for activation of ethane by gas-phase Pt <sup>+</sup> : A density functional study. <i>Chemical Physics Letters</i> , 2011, 501, 554-561.	1.2	11
2268	The formation and decomposition of firefly dioxetanone. <i>Chemical Physics Letters</i> , 2011, 506, 269-275.	1.2	25
2269	Atmospheric reactivity of CH <sub>3</sub> I and CH <sub>2</sub> I <sub>2</sub> with OH radicals: A comparative study of the H- versus I-abstraction. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 275-284.	1.1	22
2270	Density Functional Theory and Mass Spectrometry of Phthalate Fragmentations Mechanisms: Modeling Hyperconjugated Carbocation and Radical Cation Complexes with Neutral Molecules. <i>Journal of the American Society for Mass Spectrometry</i> , 2011, 22, 1999-2010.	1.2	21
2271	DFT studies on the cascade rearrangement reactions of the cubylcarbanyl radical. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 147-154.	0.9	2
2272	Hydrolysis and retroaldol cleavage of ethyl (1 <i>R</i> ,2 <i>S</i> )-adamantyl-3-hydroxybutyrate: competing reactions. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 578-587.	0.9	5
2273	Understanding the kinetic solvent effects on the 1,3-dipolar cycloaddition of benzonitrile N-oxide: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 611-618.	0.9	79
2274	Mass spectrometric stereoisomeric differentiation between 1 <i>R</i> - and 1 <i>S</i> -ascorbic acid 2-O-glucosides. Experimental and density functional theory study. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 806-814.	0.7	9
2275	Computational study on the mechanism for the gas-phase reaction of dimethyl disulfide with OH. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 644-651.	1.0	13
2276	A DFT study of a novel oxime anticancer <i>trans</i> platinum complex: Monofunctional and bifunctional binding to purine bases. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1907-1920.	1.0	11
2277	Gas-phase reaction mechanism of Pd <sup>+</sup> with CH <sub>3</sub> CHO: A density functional theoretical study. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2359-2365.	1.0	0
2278	A mechanism of the 1,3-dipolar cycloaddition between the hydrogen nitril HNO <sub>2</sub> and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2378-2389.	1.0	9
2279	On the contribution of intramolecular kinetics properties of an important rotamer of vinylpyranoanthocyanin phenol pigment (portisin). <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1355-1360.	1.0	1
2280	The DFT study on mechanisms for NCO with C <sub>2</sub> H <sub>5</sub> reaction. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2922-2930.	1.0	1
2281	Methanol vinylation mechanism in the KOH/DMSO/CH <sub>3</sub> OH/C <sub>2</sub> H <sub>2</sub> system. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2519-2524.	1.0	20
2282	Theoretical study on the mechanisms of the nucleophilic substitution reactions of hydrosulfide ion and halomethanes. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3643-3653.	1.0	1
2283	A theoretical study on decomposition and rearrangement reaction mechanism of trichloroacetyl chloride (CCl <sub>3</sub> COCl). <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3482-3496.	1.0	5

#	ARTICLE	IF	CITATIONS
2284	Steric and electronic effects on the heterolytic H <sub>2</sub> splitting by phosphineboranes R <sub>3</sub> B/PR <sub>3</sub> (R = C <sub>6</sub> F <sub>5</sub> , Ph; R <sup>2</sup> =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50,742 Td (C computational study. International Journal of Quantum Chemistry, 2011, 111, 3761-3775.	1.0	10
2285	A density functional theory study on the Diels-Alder reactions with vinylallenes as dienes. International Journal of Quantum Chemistry, 2011, 111, 3805-3815.	1.0	4
2286	Direct MP2 molecular dynamics studies of H atom reaction with CD <sub>4</sub> and CH <sub>4</sub> . International Journal of Quantum Chemistry, 2011, 111, 4433-4442.	1.0	1
2287	Gas-phase chemistry of ionized and protonated GeF <sub>4</sub> : a joint experimental and theoretical study. Journal of Mass Spectrometry, 2011, 46, 465-477.	0.7	10
2288	Structure and Conformational Properties of Azido(difluoro)phosphane, F <sub>2</sub> PN <sub>3</sub> . European Journal of Inorganic Chemistry, 2011, 2011, 895-905.	1.0	7
2289	The Effect of Strain on the Rh <sup>I</sup> -Catalyzed Rearrangement of Allylamines. European Journal of Organic Chemistry, 2011, 2011, 553-561.	1.2	3
2290	Comprehensive DFT Study on Site-, Regio-, and Stereoselectivity of Diels-Alder Reactions Leading to 5-Hydroxybenzofurans. European Journal of Organic Chemistry, 2011, 2011, 721-729.	1.2	5
2291	Tandem 1,5-Hydride Shift/6-Electrocyclization of Ketenimines and Carbodiimides Substituted with Cyclic Acetal and Dithioacetal Functions: Experiments and Computations. European Journal of Organic Chemistry, 2011, 2011, 1896-1913.	1.2	46
2292	The Mechanism of the Acid-Catalyzed Benzidine Rearrangement of Hydrazobenzene: A Theoretical Study. European Journal of Organic Chemistry, 2011, 2011, 2326-2333.	1.2	27
2293	Computational Insights into the Roles of Steric and Electrostatic Interactions in Arsenic Ylide Mediated Aziridination Reactions. European Journal of Organic Chemistry, 2011, 2011, 3458-3466.	1.2	5
2294	Insight into the Mechanism of Quinoline Formation by the Chromium(0) Fischer Carbene Catalytic Transmetalation to Palladium and Rhodium: Application to the Synthesis of the Alkaloids of <i>Ruta chalepensis</i> . European Journal of Organic Chemistry, 2011, 2011, 3293-3300.	1.2	12
2295	Concerning the Electronic Control of Torsion Angles in Biphenyls. European Journal of Organic Chemistry, 2011, 2011, 6502-6506.	1.2	19
2296	Kinetic Study and NBO Analysis of the Dehydrogenation Mechanism of Five-membered Ring Heterocyclic 2,5-Dihydro-[furan, thiophene, selenophene. Chinese Journal of Chemistry, 2011, 29, 2249-2256.	2.6	1
2297	Double-Oxygen-Atom Transfer in Reactions of Ce <sup>III</sup> O <sub>2</sub> (m = 2) (m = 2) with C <sub>2</sub> H <sub>2</sub> . ChemPhysChem, 2011, 12, 2110-2117.	1.0	26
2298	A theoretical survey on the structures, energetics, and isomerization pathways of the B <sub>5</sub> O radical. Journal of Computational Chemistry, 2011, 32, 771-777.	1.5	11
2299	A free-energy perturbation method based on Monte Carlo simulations using quantum mechanical calculations (QM/MC/FEP method): Application to highly solvent-dependent reactions. Journal of Computational Chemistry, 2011, 32, 778-786.	1.5	15
2300	Theoretical mechanistic study on the reaction of CN radical with HNCN. Journal of Computational Chemistry, 2011, 32, 1449-1455.	1.5	3
2301	Electronic and chelation effects on the unusual C2-methylation of <i>N</i> -substituted phenylaziridines with lithium organocuprates. Journal of Computational Chemistry, 2011, 32, 1859-1868.	1.5	0

#	ARTICLE	IF	CITATIONS
2302	Role of stereoelectronic features of imine and enamine in ( <i>S</i> )-proline catalyzed mannich reaction of acetaldehyde: An <i>in silico</i> study. <i>Journal of Computational Chemistry</i> , 2011, 32, 1962-1970.	1.5	11
2303	Alkaline hydrolysis of ethylene phosphate: An <i>ab initio</i> study by supermolecule model and polarizable continuum approach. <i>Journal of Computational Chemistry</i> , 2011, 32, 2545-2554.	1.5	11
2304	C-H bond activation of methane in aqueous solution: A hybrid quantum mechanical/effective fragment potential study. <i>Journal of Computational Chemistry</i> , 2011, 32, 3383-3392.	1.5	9
2305	Theoretical study on the gas-phase reaction mechanism between palladium monoxide and methane. <i>Journal of Computational Chemistry</i> , 2011, 32, 3440-3455.	1.5	6
2309	Efficient and Selective Gas-Phase Monomethylation versus N-H Bond Activation of Ammonia by $\text{Zn}(\text{CH}_3)_3$ : Atomic Zinc as a Leaving Group in an $\text{S}_\text{N}2$ Reaction. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 5387-5391.	7.2	25
2310	Diatomic $[\text{CuO}]$ and Its Role in the Spin-Selective Hydrogen- and Oxygen-Atom Transfers in the Thermal Activation of Methane. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4966-4969.	7.2	156
2311	Catalytic Redox Reactions in the $\text{CO}/\text{N}_2/\text{O}$ System Mediated by the Bimetallic Oxide-Cluster Couple $\text{AlVO}_3/\text{AlVO}_4$ . <i>Angewandte Chemie - International Edition</i> , 2011, 50, 12351-12354.	7.2	66
2312	Conformational preference and <i>cis</i> - <i>trans</i> isomerization of $\alpha$ -methylproline residues. <i>Biopolymers</i> , 2011, 95, 51-61.	1.2	25
2313	Can Enantioselectivity be Computed in Enthalpic Barrierless Reactions? The Case of $\text{CuI}$ -Catalyzed Cyclopropanation of Alkenes. <i>Chemistry - A European Journal</i> , 2011, 17, 529-539.	1.7	14
2314	Mechanism of the Dehydrogenative Silylation of Alcohols Catalyzed by Cationic Gold Complexes: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2011, 17, 2256-2265.	1.7	36
2315	1,2-Diphosphaacenaphthene 1,2-Dications: Synthetic, Stereochemical and Computational Study of the Stabilising Role of Naphthalene-1,8-diyl Backbone. <i>Chemistry - A European Journal</i> , 2011, 17, 2666-2677.	1.7	22
2316	C-H Activation on Aluminum-Vanadium Bimetallic Oxide Cluster Anions. <i>Chemistry - A European Journal</i> , 2011, 17, 3449-3457.	1.7	54
2317	Formation of Organoxenon Dications in the Reactions of Xenon with Dications Derived from Toluene. <i>Chemistry - A European Journal</i> , 2011, 17, 4012-4020.	1.7	22
2318	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. <i>Chemistry - A European Journal</i> , 2011, 17, 5076-5085.	1.7	14
2319	Versatile Stereoselective Cycloadditions between Heterocumulenes and Phosphagermaallene $\text{Tip}(\text{t-Bu})\text{Ge}(\text{PMe}_2)_3$ : Experimental and Theoretical Investigations. <i>Chemistry - A European Journal</i> , 2011, 17, 12763-12772.	1.7	14
2320	The $\text{Pt}(\text{CH})_2$ The Gas-Phase Generation of Platinum-Methylidyne Clusters $\text{Pt}(\text{CH})_n$ ( $n=1, 2$ ) and Their Reactions with Hydrocarbons and Ammonia. <i>Chemistry - A European Journal</i> , 2011, 17, 11761-11772.	1.7	18
2321	Controlled Rearrangement of Lactam-Tethered Allenols with Brominating Reagents: A Combined Experimental and Theoretical Study on $\text{I}^+$ - versus $\text{I}^2$ -Keto Lactam Formation. <i>Chemistry - A European Journal</i> , 2011, 17, 11559-11566.	1.7	30
2322	Acid-Catalyzed Reactions of Twisted Amides in Water Solution: Competition between Hydration and Hydrolysis. <i>Chemistry - A European Journal</i> , 2011, 17, 11919-11929.	1.7	36

#	ARTICLE	IF	CITATIONS
2323	Imidazole to NHC Rearrangements at Molybdenum Centers: An Experimental and Theoretical Study. Chemistry - A European Journal, 2011, 17, 8584-8595.	1.7	38
2324	Enantioselective and Diastereoselective Tsuji-Trost Allylic Alkylation of Lactones: An Experimental and Computational Study. Chemistry - A European Journal, 2011, 17, 11243-11249.	1.7	32
2325	Theoretical and Experimental Studies on the Carbon Nanotube Surface Oxidation by Nitric Acid: Interplay between Functionalization and Vacancy Enlargement. Chemistry - A European Journal, 2011, 17, 11467-11477.	1.7	93
2326	CO <sub>2</sub> Insertion into Metal-Carbon Bonds: A Computational Study of Rh <sup>I</sup> Pincer Complexes. Chemistry - A European Journal, 2011, 17, 10329-10338.	1.7	46
2327	Thermal Activation of Methane and Ethene by Bare MO <sub>n</sub> (M=Ge, Sn, and Pb): A Combined Theoretical/Experimental Study. Chemistry - A European Journal, 2011, 17, 9619-9625.	1.7	45
2328	Mechanistic Origin of Ligand-Controlled Regioselectivity in Pd-Catalyzed C-H Activation/Arylation of Thiophenes. Chemistry - A European Journal, 2011, 17, 13866-13876.	1.7	118
2329	Catalytic Hydrofunctionalization of Alkynes through Pt-H Bond Addition: The Unique Role of Orientation and Properties of the Phosphorus Group in the Insertion Step. Chemistry - A European Journal, 2011, 17, 12623-12630.	1.7	32
2330	Quantum chemical and RRKM/master equation studies of cyclopropene ozonolysis. Computational and Theoretical Chemistry, 2011, 965, 305-312.	1.1	13
2331	Computational interpretation of the stereoselectivity for a dirhodium tetracarboxylate-catalyzed amidation reaction. Computational and Theoretical Chemistry, 2011, 963, 284-289.	1.1	11
2332	Products and mechanism of the Cl-initiated atmospheric oxidation of furan: A theoretical study. Computational and Theoretical Chemistry, 2011, 963, 348-356.	1.1	2
2333	Theoretical approach of the mechanism of the reactions of chlorine atoms with aliphatic aldehydes. Computational and Theoretical Chemistry, 2011, 965, 321-327.	1.1	9
2334	On the kinetic mechanism of the hydrogen and oxygen abstraction reactions of CH <sub>3</sub> S with HOO: A dual-level direct dynamics study. Computational and Theoretical Chemistry, 2011, 964, 169-175.	1.1	7
2335	Theoretical studies on the gas phase reaction mechanisms and kinetics of glyoxal with HO <sub>2</sub> with water and without water. Computational and Theoretical Chemistry, 2011, 964, 248-256.	1.1	14
2336	Cationic noble gas hydrides-2: A theoretical investigation on HNgHNgH <sup>+</sup> (Ng=Ar, Kr, Xe). Computational and Theoretical Chemistry, 2011, 964, 318-323.	1.1	19
2337	Theoretical study of anticancer drug cis-dichloro(pyridin-2-ylcarboxaldimine)-palladium(II) compounds containing bulky fluorinated aryl groups binding to purine bases: The activity of three isomers. Computational and Theoretical Chemistry, 2011, 965, 28-40.	1.1	1
2338	Theoretical study on the mechanism for the reaction of OH with CH <sub>2</sub> CHCH(OH)CH <sub>3</sub> . Computational and Theoretical Chemistry, 2011, 965, 68-83.	1.1	3
2339	Density functional study for the C-F bond activation of the reaction of [Pt(PCy <sub>3</sub> ) <sub>2</sub> ] with C <sub>6</sub> F <sub>6</sub> . Computational and Theoretical Chemistry, 2011, 965, 92-100.	1.1	12
2340	Theoretical study on the structures, isomerization, and stability of [Si, C, N, S] isomers. Computational and Theoretical Chemistry, 2011, 965, 123-130.	1.1	0



#	ARTICLE	IF	CITATIONS
2341	The gaseous addition-diketone mechanism of aniline and phenylacetylene: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 186-195.	1.1	2
2342	A DFT study on the mechanisms of tungsten-catalyzed Baeyer-Villiger reaction using hydrogen peroxide as oxidant. <i>Computational and Theoretical Chemistry</i> , 2011, 966, 207-212.	1.1	15
2343	Theoretical studies on the isomers and tautomers of 22-membered macrocyclic ligand. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 75-80.	1.1	1
2344	Theoretical insight into [Pd(en)(H <sub>2</sub> O) <sub>2</sub> ] <sup>2+</sup> binding to Guanine form [Pd(en)(guanine)] <sub>4</sub> <sup>4+</sup> : Kinetic control and thermodynamic control. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 102-112.	1.1	1
2345	A DFT study on enantioselective synthesis of aza-β-lactams via NHC-catalyzed [2+2] cycloaddition of ketenes with diazenedicarboxylates. <i>Journal of Molecular Catalysis A</i> , 2011, 334, 108-115.	4.8	46
2346	Influence of diosgenin structure on the polymerization kinetics of acrylamide: An experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2011, 985, 34-47.	1.8	2
2347	Probing the reactivation process of sarin-inhibited acetylcholinesterase with β-nucleophiles: Hydroxylamine anion is predicted to be a better antidote with DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 1039-1046.	1.3	22
2348	DFT calculation and AIM-analysis of the substituent influence on the structure of (1-azabuta-1,3-diene)tetracarbonyliron(0) complexes. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 622-631.	0.8	1
2349	Kinetics and molecular orbital calculations of desulfonation of strong acid cation-exchange resin. <i>Polymer Degradation and Stability</i> , 2011, 96, 1516-1521.	2.7	5
2350	A quantum chemical study on the polycondensation reaction of polyesters: The mechanism of catalysis in the polycondensation reaction. <i>Polymer</i> , 2011, 52, 3443-3450.	1.8	25
2351	A theoretical approach to the formation mechanism of diphenyldithieno[3,2-b:2',3'-d]thiophene from 1,8-diketone, 4,5-bis(benzoylmethylthio)thiophene: a DFT study. <i>Tetrahedron</i> , 2011, 67, 6275-6280.	1.0	6
2352	Computational predictions on the stereoselectivity of N-heterocyclic carbene catalyzed β-lactam synthesis. <i>Tetrahedron: Asymmetry</i> , 2011, 22, 942-947.	1.8	19
2353	Trajectory calculations of OH radical- and Cl atom-initiated reaction of glyoxal: atmospheric chemistry of the HC(O)CO radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6296.	1.3	16
2354	Hydrolysis Mechanism of the NAMI-A-type Antitumor Complex (HL)[ <i>trans</i> -RuCl <sub>4</sub> L(dmso- <i>S</i> )] (L=1-methyl-1,2,4-triazole). <i>Chinese Journal of Chemical Physics</i> , 2011, 24, 383-390.	0.6	0
2355	Heterocyclization of Allenes Catalyzed by Late Transition Metals: Mechanisms and Regioselectivity. <i>Topics in Current Chemistry</i> , 2011, 302, 183-224.	4.0	19
2356	Proposal of an Amide-Directed Carbocupration Mechanism for Copper-Catalyzed meta-Selective C-H Arylation of Acetanilides by Diaryliodonium Salts. <i>Chinese Journal of Chemical Physics</i> , 2011, 24, 711-723.	0.6	1
2357	Theoretical Study of the Mechanism of the CBr <sub>2</sub> + C <sub>3</sub> O <sub>2</sub> Reaction. <i>Advanced Materials Research</i> , 2011, 356-360, 31-34.	0.3	0
2358	Biosynthesis via carbocations: Theoretical studies on terpene formation. <i>Natural Product Reports</i> , 2011, 28, 1035.	5.2	312

#	ARTICLE	IF	CITATIONS
2359	Do the mercaptocarbene (Hâ€“Câ€“Sâ€“H) and selenocarbene (Hâ€“Câ€“Seâ€“H) congeners of hydroxycarbene (Hâ€“Câ€“Oâ€“H) undergo 1,2-H-tunneling?. Collection of Czechoslovak Chemical Communications, 2011, 76, 645-667.	1.0	14
2360	A Dft Study of Solvent Effects on the Cycloaddition of Norbornadiene and 3,4â€“Dihydroisoquinoline-N-Oxide. Progress in Reaction Kinetics and Mechanism, 2011, 36, 252-258.	1.1	12
2361	Dependence of dispersion coefficients on atomic environment. Journal of Chemical Physics, 2011, 135, 234109.	1.2	31
2362	PHYSISORPTION TO CHEMISORPTION TRANSFORMATION OF A H2 MOLECULE ON B-DOPED FULLERENE C59B. Journal of Theoretical and Computational Chemistry, 2011, 10, 839-847.	1.8	5
2363	A THEORETICAL STUDY ON THE TWO REACTIONS OF CH3OH WITH NH(3Î£-) AND NH2(2B1). Journal of Theoretical and Computational Chemistry, 2011, 10, 679-690.	1.8	1
2364	A DFT STUDY ON THE HYDROLYSIS MECHANISM OF THE NAMI-A-TYPE ANTITUMOR COMPLEX (HL)[<i>trans</i>-<font>RUCl<sub>4</sub>L</font>(dmsO-S)](L=4-amino-1,2,4-triazole). Journal of Theoretical and Computational Chemistry, 2011, 10, 581-604.	1.8	13
2365	Unusual mechanism for H3+ formation from ethane as obtained by femtosecond laser pulse ionization and quantum chemical calculations. Journal of Chemical Physics, 2011, 134, 114302.	1.2	51
2366	Condensed phase molecular dynamics using interpolated potential energy surfaces with application to the resolution process of coumarin 153. Journal of Chemical Physics, 2011, 135, 014107.	1.2	26
2367	Silylene Reaction with Acetylene: Elucidating the Mechanism by Theoretical Identification of a New Intermediate. Progress in Reaction Kinetics and Mechanism, 2011, 36, 323-328.	1.1	0
2368	Ab Initio Study and Nbo Analysis of the Unimolecular Decomposition Kinetics of 2,2-Dimethyloxetane. Progress in Reaction Kinetics and Mechanism, 2012, 37, 277-290.	1.1	3
2369	Activation of Propane C-H and C-C Bonds by Gas-Phase Pt Atom: A Theoretical Study. International Journal of Molecular Sciences, 2012, 13, 9278-9297.	1.8	15
2370	Experimental and Theoretical Study on Pyrolysis of Isopsoralen. Chinese Journal of Chemical Physics, 2012, 25, 249-253.	0.6	1
2371	Density Functional Study of NO Desorption from Oxidation of Nitrogen Containing Char by O<sub>2</sub>. Combustion Science and Technology, 2012, 184, 445-455.	1.2	24
2372	THEORETICAL INVESTIGATIONS ON THE MECHANISM OF ACTIVATION OF AMMONIA BY A p-DIMETHYLAMINOPYRIDINE COORDINATED <font>SI=O</font> DOUBLE BOND. Journal of Theoretical and Computational Chemistry, 2012, 11, 437-481.	1.8	1
2373	DFT Calculations of the Elimination Kinetics of Silacyclobutanes and its Methyl Derivatives in the Gas-Phase. Phosphorus, Sulfur and Silicon and the Related Elements, 2012, 187, 619-631.	0.8	3
2374	Theoretical Studies on the Mechanistic Insertions of Singlet Methylene and Halomethylene into Polar Sâ€“H Bonds of Methanethiol, Ethanethiol, 1-Propanethiol and 2-Propanethiol. Phosphorus, Sulfur and Silicon and the Related Elements, 2012, 187, 1347-1366.	0.8	2
2375	Mechanism and Regioselectivity of the 1,3-Dipolar Cycloaddition of Methyleneamine N-Oxide with Cyclopent-3-Ene-1,2-Dione and its Aza, Oxa and Thia Analogues: A Dft Approach. Progress in Reaction Kinetics and Mechanism, 2012, 37, 90-102.	1.1	3
2376	A Density Functional Theory Study of Cyclization of Citronellal. Progress in Reaction Kinetics and Mechanism, 2012, 37, 173-182.	1.1	6

#	ARTICLE	IF	CITATIONS
2377	Synthesis of Ethylenediamine in a Tubular Reactor: Experimental and Theoretical Kinetics. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 411-422.	1.1	1
2378	A DFT Study on the Cycloaddition of Dimethyl Acetylenedicarboxylate and 3,4-dihydroisoquinoline-N-oxide. <i>Progress in Reaction Kinetics and Mechanism</i> , 2012, 37, 436-441.	1.1	1
2379	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. <i>Current Organic Chemistry</i> , 2012, 16, 1711-1722.	0.9	7
2380	Understanding the Bond Formation in Hetero-Diels-Alder Reactions. An ELF Analysis of the Reaction of Nitroethylene with Dimethylvinylamine. <i>Current Organic Chemistry</i> , 2012, 16, 2343-2351.	0.9	19
2381	Understanding the Mechanism of the Intramolecular Stetter Reaction. A DFT Study. <i>Molecules</i> , 2012, 17, 1335-1353.	1.7	34
2382	Side-chain degradation of perfluorosulfonic acid membranes: An ab initio study. <i>Journal of Materials Research</i> , 2012, 27, 1982-1991.	1.2	25
2383	Applications of Normal Coordinates of Internal Vibrations to Generate Perturbed Structures: Dynamic Behavior of Weak to Strong Interactions Elucidated by Atoms-in-Molecules Dual Functional Analysis. <i>Bulletin of the Chemical Society of Japan</i> , 2012, 85, 1293-1305.	2.0	39
2384	Germyl Cations with Ge <sup>+</sup> S Bonds: An Experimental and Theoretical Study on the Gaseous F <sub>n</sub> Ge(SH) <sup>+</sup> (n = 0-2). <i>European Journal of Mass Spectrometry</i> , 2012, 18, 447-456.	0.5	1
2385	Mechanisms and Kinetics for the Thermal Decomposition of 2-Azido-N,N-Dimethylethanamine (DMAZ). <i>Journal of Physical Chemistry A</i> , 2012, 116, 3561-3576.	1.1	16
2386	Efficacy of carbenes for CO <sub>2</sub> chemical fixation and activation by their superbasicity/alcohol: a DFT study. <i>New Journal of Chemistry</i> , 2012, 36, 2549.	1.4	27
2387	Gold-catalyzed bis-cyclization of 1,2-diol- or acetonide-tethered alkynes. Synthesis of $\beta$ -lactam-bridged acetals: a combined experimental and theoretical study. <i>Tetrahedron</i> , 2012, 68, 10748-10760.	1.0	19
2388	Carbenoid Alkene Insertion Reactions of Oxiranyllithiums. <i>Journal of Organic Chemistry</i> , 2012, 77, 8605-8614.	1.7	7
2389	Mechanism Study of the Intramolecular Anti-Michael Addition of N-Alkylfurylacrylamides. <i>Journal of Organic Chemistry</i> , 2012, 77, 8744-8749.	1.7	15
2390	Refined Transition-State Models for Proline-Catalyzed Asymmetric Michael Reactions under Basic and Base-Free Conditions. <i>Journal of Organic Chemistry</i> , 2012, 77, 10516-10524.	1.7	21
2391	Theoretical Study on the Mechanism and Kinetics for the Self-Reaction of C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> Radicals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4610-4620.	1.1	36
2392	Theoretical assessment of the viability of thermal [2+2] processes for formation of plumisclerin A. <i>Tetrahedron Letters</i> , 2012, 53, 6919-6922.	0.7	12
2393	Intramolecular Pd(0)-Catalyzed Reactions of (2-Iodoanilino)-aldehydes: A Joint Experimental-Computational Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 10272-10284.	1.7	36
2394	Coupling of Azomethine Ylides with Nitrilium Derivatives of Closo-Decaborate Clusters: A Synthetic and Theoretical Study. <i>ChemPlusChem</i> , 2012, 77, 1075-1086.	1.3	25

#	ARTICLE	IF	CITATIONS
2395	An exploration of the mechanisms for the formation of 3,4-bis(4-aminofurazan-3-yl)-furoxan by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2012, 997, 88-93.	1.1	5
2396	Monomer- and polymer radicals of vinyl compounds: EPR and DFT studies of geometric and electronic structures in the adsorbed state. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 98, 367-377.	2.0	3
2397	Comparison of Three Chain-of-States Methods: Nudged Elastic Band and Replica Path with Restraints or Constraints. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5035-5051.	2.3	23
2398	Using Efficient Predictor-Corrector Reaction Path Integrators for Studies Involving Projected Frequencies. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5013-5019.	2.3	6
2399	Can cytosine, thymine and uracil be formed in interstellar regions? A theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 652-662.	1.5	28
2400	Revisiting sesquiterpene biosynthetic pathways leading to santalene and its analogues: a comprehensive mechanistic study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7996.	1.5	14
2401	Perspectives on the Reaction Force. <i>Advances in Quantum Chemistry</i> , 2012, 64, 189-209.	0.4	36
2402	o-Benzenedisulfonimide and its chiral derivative as Brønsted acids catalysts for one-pot three-component Strecker reaction. Synthetic and mechanistic aspects. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4058.	1.5	26
2403	Origin of the synchronicity in bond formation in polar Diels-Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 3841.	1.5	51
2404	Why Is the Oxidation State of Iron Crucial for the Activity of Heme-Dependent Aldoxime Dehydratase? A QM/MM Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9396-9408.	1.2	21
2405	Changes in Charge Distribution, Molecular Volume, Accessible Surface Area and Electronic Structure along the Reaction Coordinate for a Carbocationic Triple Shift Rearrangement of Relevance to Diterpene Biosynthesis. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8902-8909.	1.1	21
2406	Sulfuric Acid as Autocatalyst in the Formation of Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2012, 134, 20632-20644.	6.6	126
2407	Computational Assessment of 1,3-Dipolar Cycloaddition of Nitrile Oxides with Ethene and [60]Fullerene. <i>Heterocycles</i> , 2012, 84, 719.	0.4	7
2408	Iron-Catalyzed Direct Suzuki-Miyaura Reaction: Theoretical and Experimental Studies on the Mechanism and the Regioselectivity. <i>ACS Catalysis</i> , 2012, 2, 1829-1837.	5.5	28
2409	A Frontier Molecular Orbital Theory Approach to Understanding the Mayr Equation and to Quantifying Nucleophilicity and Electrophilicity by Using HOMO and LUMO Energies. <i>Asian Journal of Organic Chemistry</i> , 2012, 1, 336-345.	1.3	127
2410	Re-examining the Mechanisms of Competing Pericyclic Reactions of 1,3,7-Octatriene. <i>Chemistry - A European Journal</i> , 2012, 18, 11029-11035.	1.7	6
2411	Enantiomerization Mechanism of Thalidomide and the Role of Water and Hydroxide Ions. <i>Chemistry - A European Journal</i> , 2012, 18, 14305-14313.	1.7	30
2412	Facile Oxidative Rearrangements Using Hypervalent Iodine Reagents. <i>ChemistryOpen</i> , 2012, 1, 245-250.	0.9	66

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2413	Remarkable influence of mild Lewis acid catalysts on cycloadditions leading to tetrasubstituted isoxazolidines: DFT analysis augmented by X-ray and NMR studies. <i>Monatshefte für Chemie</i> , 2012, 143, 1687-1703.	0.9	6
2414	Theoretical studies on the Mo-catalyzed asymmetric intramolecular Pauson-Khand-type [2+2+1] cycloadditions of 3-allyloxy-1-propynylphosphonates. <i>Journal of Molecular Modeling</i> , 2012, 18, 3489-3499.	0.8	2
2415	The degradation mechanism of phenol induced by ozone in wastes system. <i>Journal of Molecular Modeling</i> , 2012, 18, 3821-3830.	0.8	11
2416	Ruthenium hydride-catalyzed regioselective addition of benzaldehyde to dienes leading to $\beta,\gamma$ -unsaturated ketones: a DFT study. <i>Journal of Molecular Modeling</i> , 2012, 18, 4955-4963.	0.8	8
2417	An accurate theoretical study of energy barriers of alkaline hydrolysis of carboxylic esters. <i>Research on Chemical Intermediates</i> , 2012, 38, 2175-2190.	1.3	13
2418	Quantum chemical study of the mechanism for OH-initiated atmospheric oxidation reaction of (Z)-CF <sub>3</sub> CFCHF. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 22-31.	1.1	9
2419	Quasi-classical trajectory and direct-dynamics CVT study on the initiation steps of methanol combustion. <i>Journal of the Iranian Chemical Society</i> , 2012, 9, 957-969.	1.2	2
2420	Superacid-Promoted Ionization of Alkanes Without Carbonium Ion Formation: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9979-9984.	1.1	14
2421	Interaction of vanadium oxide cluster anions with water: an experimental and theoretical study on reactivity and mechanism. <i>Dalton Transactions</i> , 2012, 41, 5562.	1.6	23
2422	Neutral noble gas compounds exhibiting a Xe-Xe bond: structure, stability and bonding situation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14869.	1.3	43
2423	Synthetic studies towards the mulberry Diels-Alder adducts: H-bond accelerated cycloadditions of chalcones. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 6010.	1.5	22
2424	Aquation and dimerization of osmium(ii) anticancer complexes: a density functional theory study. <i>RSC Advances</i> , 2012, 2, 436-446.	1.7	13
2425	The effects of H-bonding and sterics on the photoreactivity of a trimethyl butyrophenone derivative. <i>Photochemical and Photobiological Sciences</i> , 2012, 11, 744-751.	1.6	5
2426	Synthetic and computational studies of the palladium(iv) system Pd(alkyl)(aryl)(alkynyl)(bidentate)(triflate) exhibiting selectivity in C-C reductive elimination. <i>Dalton Transactions</i> , 2012, 41, 11820.	1.6	19
2427	Simplification through complexity: the role of Ni-complexes in catalysed diyne-cyclobutanone [4+2+2] cycloadditions, a comparative DFT study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6937.	1.3	10
2428	Mechanistic insights on platinum- and palladium-pincer catalyzed coupling and cyclopropanation reactions between olefins. <i>Dalton Transactions</i> , 2012, 41, 8430.	1.6	18
2429	DFT Study on the Mechanism of PtCl <sub>2</sub> -Catalyzed Rearrangement of Cyclopropenes to Allenes. <i>Organometallics</i> , 2012, 31, 4020-4030.	1.1	13
2430	Computational study on the thermal decomposition and isomerization of the CH <sub>3</sub> OCF <sub>2</sub> O radical. <i>Canadian Journal of Chemistry</i> , 2012, 90, 403-409.	0.6	14

#	ARTICLE	IF	CITATIONS
2431	Irreversible phototautomerization of o-phthalaldehyde through electronic relocation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 6561.	1.3	19
2432	Fusing cubanes to 1,5-hexadiene. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14756.	1.3	0
2433	An ELF analysis of the C=C bond formation step in the N-heterocyclic carbene-catalyzed hydroacylation of unactivated C=C double bonds. <i>RSC Advances</i> , 2012, 2, 7127.	1.7	21
2434	Predicting the interactions of organometallic ruthenium ethylenediamine complexes with mononucleotides: insights from density functional theory. <i>RSC Advances</i> , 2012, 2, 7849.	1.7	2
2435	Attack of radicals and protons on ladderane lipids: quantum chemical calculations and biological implications. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5514.	1.5	16
2436	Theoretical investigation on copper hydrides catalyzed hydrosilylation reaction of 3-methylcyclohex-2-enone: mechanism and ligands' effect. <i>Catalysis Science and Technology</i> , 2012, 2, 564-569.	2.1	8
2437	Origins of reversing diastereoselectivity of $\alpha,\beta$ -dichloro- $\beta$ -butenolides and $\beta$ -butyrolactams in direct vinylogous aldol addition: a computational study. <i>RSC Advances</i> , 2012, 2, 8460.	1.7	8
2438	On the Origins of Faster Oxo Exchange for Uranyl(V) versus Plutonyl(V). <i>Journal of the American Chemical Society</i> , 2012, 134, 15488-15496.	6.6	45
2439	Atmospheric Fate of Methacrolein. 2. Formation of Lactone and Implications for Organic Aerosol Production. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5763-5768.	1.1	58
2440	Mechanistic and Kinetic Study of $CF_3CH_2CH_2 + OH$ Reaction. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3172-3181.	1.1	28
2441	Gas-Phase Chemical Dynamics Simulations on the Bifurcating Pathway of the Pimaradienyl Cation Rearrangement: Role of Enzymatic Steering in Abietic Acid Biosynthesis. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1212-1222.	2.3	46
2442	Comparative DFT Study To Determine if $\alpha$ -Oxoaldehydes are Precursors for Pentosidine Formation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2986-2996.	1.1	14
2443	Theoretical Investigation on the Chiral Diamine-Catalyzed Epoxidation of Cyclic Enones: Mechanism and Effects of Cocatalyst. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1251-1260.	1.1	14
2444	Theoretical Investigation of Water Gas Shift Reaction Catalyzed by Iron Group Carbonyl Complexes $M(CO)_5$ (M = Fe, Ru, Os). <i>Journal of Physical Chemistry A</i> , 2012, 116, 2529-2535.	1.1	31
2445	Reaction paths of $BCl_3 + CH_4 + H_2$ in the chemical vapor deposition process. <i>Structural Chemistry</i> , 2012, 23, 1677-1692.	1.0	5
2446	Consecutive Reaction Mechanism for the Formation of Spore Photoproduct in DNA Photolesion. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11117-11123.	1.2	11
2447	Computational Design of Effective, Bioinspired HOCl Antioxidants: The Role of Intramolecular Cl <sup>+</sup> and H <sup>+</sup> Shifts. <i>Journal of the American Chemical Society</i> , 2012, 134, 19240-19245.	6.6	21
2448	A Relation Between the Eikonal Equation Associated to a Potential Energy Surface and a Hyperbolic Wave Equation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4856-4862.	2.3	3

#	ARTICLE	IF	CITATIONS
2449	Role of Perferrylâ€“Oxo Oxidant in Alkane Hydroxylation Catalyzed by Cytochrome P450: A Hybrid Density Functional Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4713-4730.	1.2	22
2450	Atmospheric Fate of Methacrolein. 1. Peroxy Radical Isomerization Following Addition of OH and O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2012, 116, 5756-5762.	1.1	166
2451	Mechanistic and Stereochemical Insights on the Pt-Catalyzed Rearrangement of Oxiranylpropargylic Esters to Cyclopentenones. <i>Journal of Organic Chemistry</i> , 2012, 77, 8733-8743.	1.7	17
2452	Mechanistic Insights into the Stepwise Dielsâ€“Alder Reaction of 4,6-Dinitrobenzofuroxan. <i>Organic Letters</i> , 2012, 14, 118-121.	2.4	26
2453	DFT Study of Internal Alkyne-to-Disubstituted Vinylidene Isomerization in [CpRu(PhCâ‰“iCar)(dppe)] <sup>+</sup> . <i>Journal of the American Chemical Society</i> , 2012, 134, 17746-17756.	6.6	55
2454	On the Origin of Regio- and Stereoselectivity in Singlet Oxygen Addition to Enecarbamates. <i>Journal of Organic Chemistry</i> , 2012, 77, 2474-2485.	1.7	14
2455	Surface Pseudorotation in Lewis-Base-Catalyzed Atomic Layer Deposition of SiO <sub>2</sub> : Static Transition State Search and Bornâ€“Oppenheimer Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26436-26448.	1.5	22
2456	Reductions of Phosphine Oxides and Sulfides by Perchlorosilanes: Evidence for the Involvement of Donor-Stabilized Dichlorosilylene. <i>Journal of Organic Chemistry</i> , 2012, 77, 1-4.	1.7	47
2457	Theoretical Investigation of the Reaction of Mn <sup>+</sup> with Ethylene Oxide. <i>Journal of Physical Chemistry A</i> , 2012, 116, 512-519.	1.1	2
2458	Effects of a Single Water Molecule on the OH + H <sub>2</sub> O <sub>2</sub> Reaction. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5821-5829.	1.1	91
2459	Computational Elucidation of the Internal Oxidant-Controlled Reaction Pathways in Rh(III)-Catalyzed Aromatic Câ€“H Functionalization. <i>Journal of Organic Chemistry</i> , 2012, 77, 3017-3024.	1.7	206
2460	Theoretical and structural studies on mechanism of the Stec reaction. <i>Tetrahedron</i> , 2012, 68, 5554-5563.	1.0	1
2461	Mechanism of the Reduction of an Oxidized Glutathione Peroxidase Mimic with Thiols. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5052-5057.	2.3	14
2462	Role of Explicit Solvents in Palladium(II)-Catalyzed Alkoxylation of Arenes: An Interesting Paradigm for Preferred Outer-Sphere Reductive Elimination over Inner-Sphere Pathway. <i>Organometallics</i> , 2012, 31, 6466-6481.	1.1	42
2463	Tuning the Regioselectivity of Palladium-Catalyzed Direct Arylation of Azoles by Metal Coordination. <i>Organometallics</i> , 2012, 31, 794-797.	1.1	61
2464	Aminolysis of a Model Nerve Agent: A Computational Reaction Mechanism Study of O,S-Dimethyl Methylphosphonothiolate. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8382-8396.	1.1	18
2465	Accurate prediction of rate constants of Dielsâ€“Alder reactions and application to design of Dielsâ€“Alder ligation. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2673.	1.5	45
2466	Elucidating active species and mechanism of the direct oxidation of benzene to phenol with hydrogen peroxide catalyzed by vanadium-based catalysts using DFT calculations. <i>RSC Advances</i> , 2012, 2, 2329.	1.7	8

#	ARTICLE	IF	CITATIONS
2467	Analysis of the Palladium-Catalyzed (Aromatic) C-H Bond Metalation-Deprotonation Mechanism Spanning the Entire Spectrum of Arenes. <i>Journal of Organic Chemistry</i> , 2012, 77, 658-668.	1.7	380
2468	Theoretical Investigation of the Mechanisms and Stereoselectivities of Reductions of Acyclic Phosphine Oxides and Sulfides by Chlorosilanes. <i>Journal of Organic Chemistry</i> , 2012, 77, 3969-3977.	1.7	43
2469	NMR and Computational Studies of the Configurational Properties of Spirodioxyselenuranes. Are Dynamic Exchange Processes or Temperature-Dependent Chemical Shifts Involved?. <i>Journal of Organic Chemistry</i> , 2012, 77, 9268-9276.	1.7	13
2470	DFT and Experimental Exploration of the Mechanism of InCl <sub>3</sub> -Catalyzed Type II Cycloisomerization of 1,6-Enynes: Identifying InCl <sub>2</sub> <sup>+</sup> as the Catalytic Species and Answering Why Nonconjugated Dienes Are Generated. <i>Journal of Organic Chemistry</i> , 2012, 77, 8527-8540.	1.7	64
2471	Rock n-™ Roll With Gold: Synthesis, Structure, and Dynamics of a (bipyridine)AuCl <sub>3</sub> Complex. <i>Organometallics</i> , 2012, 31, 7093-7100.	1.1	18
2472	Theoretical investigation of rare gas hydride cations: HRgN <sub>2</sub> <sup>+</sup> (Rg=He, Ar, Kr, and Xe). <i>Journal of Chemical Physics</i> , 2012, 136, 164312.	1.2	21
2473	Mechanism of the N-protecting group dependent annulations of 3-aryloxy alkynyl indoles under gold catalysis: a computational study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 4417.	1.5	23
2474	Reactivity of [Ba(H <sub>2</sub> O) <sub>1/2</sub> ] <sub>2</sub> <sup>2+</sup> with neutral molecules in the gas-phase: An experimental and DFT study. <i>Journal of Molecular Structure</i> , 2012, 1021, 138-146.	1.8	0
2475	Mechanism of alkene isomerization by bifunctional ruthenium catalyst: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2012, 698, 1-6.	0.8	24
2476	A DFT study on geometric preference of non-bridging form to bridging form in molybdenum complexes with phosphonium ligand. <i>Journal of Organometallic Chemistry</i> , 2012, 697, 41-50.	0.8	3
2477	A dash of protons: A theoretical study on the hydrolysis mechanism of 1-substituted silatranes and their protonated analogs. <i>Computational and Theoretical Chemistry</i> , 2012, 987, 2-15.	1.1	25
2478	A theoretical study on transition state of the antitumor drug: Gold(III) dithiocarbamate derivative interaction with cysteine and DNA purine bases. <i>Computational and Theoretical Chemistry</i> , 2012, 979, 22-32.	1.1	9
2479	Theoretical study on the mechanism for the reaction of F with CH <sub>2</sub> CHCH <sub>2</sub> Cl. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 7-13.	1.1	1
2480	Computational study on mechanism of hydrogen abstraction and selenium insertion in the reaction of triplet and singlet selenium atom with hydrogen selenide. <i>Computational and Theoretical Chemistry</i> , 2012, 980, 101-107.	1.1	4
2481	On the catalytic role of Co <sup>+</sup> in the oxygen transport activation of N <sub>2</sub> O by CO. <i>Computational and Theoretical Chemistry</i> , 2012, 982, 2-7.	1.1	4
2482	Reaction of group 16 analogues of ethoxyquin with hydrogen peroxide: A computational study. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 68-72.	1.1	5
2483	Effect of sulfur substitution for methanolysis of paraoxon: CO vs. PO bond cleavage from density-functional theory. <i>Computational and Theoretical Chemistry</i> , 2012, 982, 8-16.	1.1	5
2484	Mechanistic and kinetic study on the reaction of 2,4-dibrominated diphenyl ether (BDE-7) with OH radicals. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 31-37.	1.1	18



#	ARTICLE	IF	CITATIONS
2485	A DFT study of the role of Lewis acid catalysts in the mechanism of the 1,3-dipolar cycloaddition of nitrile imines towards electron-deficient acryloyl derivatives. <i>Computational and Theoretical Chemistry</i> , 2012, 986, 6-13.	1.1	9
2486	Theoretical study on the mechanism of the HO <sub>2</sub> plus NH <sub>2</sub> reaction. <i>Computational and Theoretical Chemistry</i> , 2012, 985, 67-71.	1.1	10
2487	Theoretical study on the formation of a pentacyclo-undecane cage lactam. <i>Computational and Theoretical Chemistry</i> , 2012, 986, 63-70.	1.1	8
2488	Ab initio calculations and iodine kinetic modeling in the reactor coolant system of a pressurized water reactor in case of severe nuclear accident. <i>Computational and Theoretical Chemistry</i> , 2012, 990, 194-208.	1.1	25
2489	New insights into the two catalyst cycles of the Pt <sup>+</sup> -catalyzed oxidation of methane by oxygen: Spin-orbit coupling, spin-inversion probabilities, and kinetic information. <i>Computational and Theoretical Chemistry</i> , 2012, 989, 75-85.	1.1	9
2490	Mechanism for the formation of benzene in the Titan™s atmosphere: A theoretical study on the mechanism of reaction. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 66-73.	1.1	8
2491	A detailed quantum chemical study of the interactions of [Pt(dien)Cl] <sup>+</sup> with a series of S-donor ligands: A computational approach. <i>Computational and Theoretical Chemistry</i> , 2012, 991, 116-123.	1.1	14
2492	Computational study of fluxional hydride bridged binuclear transition metal complexes: Effect of secondary bridging ligands. <i>Computational and Theoretical Chemistry</i> , 2012, 994, 1-5.	1.1	3
2493	Gaseous germyl cations: A theoretical investigation on the structure, properties, and mechanism of formation of and (n=0-2). <i>Computational and Theoretical Chemistry</i> , 2012, 993, 131-139.	1.1	6
2494	Quantum chemical and theoretical kinetics studies on the reaction of carbonyl sulfide with H, OH and O(3P). <i>Computational and Theoretical Chemistry</i> , 2012, 994, 25-33.	1.1	20
2495	A computational study on the reaction mechanism of C <sub>2</sub> H <sub>5</sub> S with HO <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , 2012, 994, 65-72.	1.1	8
2496	Activation of C-H and C-C bonds of ethane by gas-phase Pt atom: Potential energy surface and reaction mechanism. <i>Computational and Theoretical Chemistry</i> , 2012, 994, 112-120.	1.1	16
2497	The OH-initiated atmospheric oxidation of divinyl sulfoxide: A theoretical investigation on the reaction mechanism. <i>Chemical Physics Letters</i> , 2012, 543, 61-67.	1.2	2
2498	Theoretical investigation into the likely reaction mechanisms of benzyl alcohol with dimethyl carbonate over a faujasite zeolite catalyst. <i>Computational Materials Science</i> , 2012, 55, 217-227.	1.4	4
2499	Insights into the Dual Activation Mechanism Involving Bifunctional Cinchona Alkaloid Thiourea Organocatalysts: An NMR and DFT Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 9813-9825.	1.7	136
2500	Revisiting the Molecular Roots of a Ubiquitously Successful Synthesis: Nickel(0) Nanoparticles by Reduction of [Ni(acetylacetonate) <sub>2</sub> ]. <i>Chemistry - A European Journal</i> , 2012, 18, 14165-14173.	1.7	43
2501	Mechanistic Studies on the Gas-Phase Dehydrogenation of Alkanes at Cyclometalated Platinum Complexes. <i>Chemistry - A European Journal</i> , 2012, 18, 14055-14062.	1.7	11
2502	A Theoretical Investigation on the Oxidation of Carbon Monoxide by an Aqueous Molybdocene. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 4445-4453.	1.0	6

#	ARTICLE	IF	CITATIONS
2503	Theoretical prediction of the reaction of s-triazine with nitrate radical: A new possible route to generate oxy-s-triazine. <i>Journal of Chemical Physics</i> , 2012, 137, 214317.	1.2	3
2504	Mechanisms of Formation of Hemiacetals: Intrinsic Reactivity Analysis. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8250-8259.	1.1	30
2505	Investigation of the formation of acid rain based on the sulfur tetroxide (SO <sub>4</sub> (C <sub>2v</sub> )) and OH radical reaction. <i>Structural Chemistry</i> , 2012, 23, 1609-1615.	1.0	6
2506	Conjugate addition of isocyanides to chromone 3-carboxylic acid: an efficient one-pot synthesis of chroman-4-one 2-carboxamides. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 3406.	1.5	26
2507	Rapid Access to Substituted Piperazines via Ti(NMe <sub>2</sub> ) <sub>4</sub> -Mediated C-C Bond-Making Reactions. <i>Organometallics</i> , 2012, 31, 6005-6013.	1.1	22
2508	Why Are S <sub>N</sub> 4 (<math>S_{N4}</math>) Species Missing? Answers in a Broader Theoretical Context of Binary S-N Compounds. <i>Inorganic Chemistry</i> , 2012, 51, 13321-13327.	1.9	18
2509	Intramolecular cycloaddition of azomethine ylides, from imines of O-acylsalicylic aldehyde and ethyl diazoacetate, to ester carbonyl: experimental and DFT computational study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5582.	1.5	17
2510	Iron-catalysed transformation of molecular dinitrogen into silylamine under ambient conditions. <i>Nature Communications</i> , 2012, 3, 1254.	5.8	118
2511	An Osmium(III)/Osmium(V) Redox Couple Generating Os <sup>V</sup> (O)(OH) Center for <i>cis</i> -1,2-Dihydroxylation of Alkenes with H <sub>2</sub> O <sub>2</sub> : Os Complex with a Nitrogen-Based Tetradentate Ligand. <i>Journal of the American Chemical Society</i> , 2012, 134, 19270-19280.	6.6	44
2512	Density Functional Theory Study of N≡CN and O≡CN Bond Cleavage by an Iron Silyl Complex. <i>Organometallics</i> , 2012, 31, 3995-4005.	1.1	19
2513	Metal-assisted Lossen Rearrangement. <i>Journal of Organic Chemistry</i> , 2012, 77, 2829-2836.	1.7	33
2514	Causation in a Cascade: The Origins of Selectivities in Intramolecular Nitrene Cycloadditions. <i>Journal of the American Chemical Society</i> , 2012, 134, 12010-12015.	6.6	19
2515	Nucleophilic Degradation of Fenitrothion Insecticide and Performance of Nucleophiles: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2536-2546.	1.1	23
2516	Proposal for halogen atom transfer mechanism for Ullmann O-arylation of phenols with aryl halides. <i>Dalton Transactions</i> , 2012, 41, 13832.	1.6	32
2517	Stepwise Diels-Alder: More than Just an Oddity? A Computational Mechanistic Study. <i>Journal of Organic Chemistry</i> , 2012, 77, 6563-6573.	1.7	52
2518	High-Yield Thermolytic Conversion of Imidazolium Salts into Arduengo Carbene Adducts with BF <sub>3</sub> and PF <sub>5</sub> . <i>Organometallics</i> , 2012, 31, 1751-1760.	1.1	32
2519	Exclusive C-C Oxidative Addition in a Rhodium Thiophosphoryl Pincer Complex and Computational Evidence for an $\eta^3$ -C-H Agostic Intermediate. <i>Organometallics</i> , 2012, 31, 505-512.	1.1	33
2520	Metal free hydrogenation reaction on carbon doped boron nitride fullerene: A DFT study on the kinetic issue. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 14336-14342.	3.8	94

#	ARTICLE	IF	CITATIONS
2521	DFT study on the abstraction and addition of Cl atom with toluene. Computational and Theoretical Chemistry, 2012, 996, 44-50.	1.1	10
2522	A theoretical study on intramolecular anion radical [2+2] cyclobutanation of bis(enones): Dramatic effects of the electron-deficient enone partners on the yielding of cyclobutane ring systems. Computational and Theoretical Chemistry, 2012, 996, 110-116.	1.1	3
2523	A computational study on the structures and energetics of isobutanol pyrolysis. Computational and Theoretical Chemistry, 2012, 997, 94-102.	1.1	9
2524	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
2525	Facile synthesis of dihydrochalcones via the AlCl <sub>3</sub> -promoted tandem Friedel-Crafts acylation and alkylation of arenes with 2-alkenoyl chlorides. Journal of Molecular Catalysis A, 2012, 365, 203-211.	4.8	20
2526	Neutral Metal Atoms Acting as a Leaving Group in Gas-Phase S <sub>N</sub> 2 Reactions: M(CH <sub>3</sub> ) <sup>+</sup> + NH <sub>3</sub> → CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup> + M (M = Zn, Cd, Hg). Organometallics, 2012, 31, 3816-3824.	1.1	32
2527	Ring-Opening Polymerization of Epoxides Catalyzed by Uranyl Complexes: An Experimental and Theoretical Study of the Reaction Mechanism. Inorganic Chemistry, 2012, 51, 9132-9140.	1.9	23
2528	Experimental and theoretical study of the [3 + 2] cycloaddition of carbonyl ylides with alkynes. Organic and Biomolecular Chemistry, 2012, 10, 8434.	1.5	12
2529	The reaction force constant: an indicator of the synchronicity in double proton transfer reactions. Physical Chemistry Chemical Physics, 2012, 14, 11125.	1.3	54
2530	Theoretical Study on Cyclopropanation of <i>endo</i> -Dicyclopentadiene with Zinc Carbenoids: Effects of Solvent and (ICH <sub>2</sub> ) <sub>2</sub> Zn. Journal of Organic Chemistry, 2012, 77, 10065-10072.	1.7	19
2531	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. Physical Chemistry Chemical Physics, 2012, 14, 12992.	1.3	32
2532	A Study of the Atmospherically Important Reactions between Dimethyl Selenide (DMSe) and Molecular Halogens (X <sub>2</sub> = Cl <sub>2</sub> , Br <sub>2</sub> , and I <sub>2</sub> ) with <i>ab initio</i> Calculations. Journal of Physical Chemistry A, 2012, 116, 5595-5603.	1.1	3
2533	A theoretical study of the reaction of N(4S) with nitrogen dioxide on the N <sub>2</sub> O <sub>2</sub> potential energy surface. Russian Journal of Physical Chemistry A, 2012, 86, 1438-1446.	0.1	2
2534	Concerted, highly asynchronous, enzyme-catalyzed [4 + 2] cycloaddition in the biosynthesis of spinosyn A; computational evidence. Organic and Biomolecular Chemistry, 2012, 10, 7503.	1.5	44
2535	Binding of anticancer drug Ru(II)-6-C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> OH)Cl <sub>2</sub> (DAPTA) to DNA purine bases and amino acid residues: a theoretical study. Structural Chemistry, 2012, 23, 1931-1940.	1.0	5
2536	Deactivation mechanism of AuCl <sub>3</sub> catalyst in acetylene hydrochlorination reaction: a DFT study. RSC Advances, 2012, 2, 4814.	1.7	84
2537	A DFT-Based Analysis of the Gold-Catalyzed Cycloisomerization of 1-Siloxy 1,5-Enynes to Cyclohexadienes. Journal of Organic Chemistry, 2012, 77, 6231-6238.	1.7	18
2538	Local Control of the <i>Cis</i> → <i>Trans</i> Isomerization and Backbone Dihedral Angles in Peptides Using Trifluoromethylated Pseudoprolines. Journal of Physical Chemistry B, 2012, 116, 4069-4079.	1.2	24

#	ARTICLE	IF	CITATIONS
2539	Untethered 4,1,2-MC2B10 supraicosahedral metallocarboranes, their C,C-dimethyl 4,1,6-, 4,1,8- and 4,1,12-MC2B10 analogues, and DFT study of the (4,1,2)- to (4,1,6)-isomerisations of C2B11 carboranes and MC2B10 metallocarboranes. Dalton Transactions, 2012, 41, 10957.	1.6	12
2540	Mechanism of the Acid-Promoted Intramolecular Schmidt Reaction: Theoretical Assessment of the Importance of Lone Pair-Cation, Cation- $\pi$ , and Steric Effects in Controlling Regioselectivity. Journal of Organic Chemistry, 2012, 77, 640-647.	1.7	41
2541	Pt(II)-Mediated Imine-Nitrile Coupling Leading to Symmetrical (1,3,5,7,9-Pentaaza-1,3,6,8-tetraenato)Pt(II) Complexes Containing the Incorporated 1,3-Diiminoisoindoline Moiety. Inorganic Chemistry, 2012, 51, 10774-10786.	1.9	15
2542	Theoretical Study of H-Abstraction Reactions from CH <sub>3</sub> Cl and CH <sub>3</sub> Br Molecules by ClO and BrO Radicals. Journal of Physical Chemistry A, 2012, 116, 4396-4408.	1.1	8
2543	DFT-Based Insights into Pd-Zn Cooperative Effects in Oxidative Addition and Reductive Elimination Processes Relevant to Negishi Cross-Couplings. Organometallics, 2012, 31, 2053-2058.	1.1	53
2545	Theoretical Investigations toward the [4 + 2] Cycloaddition of Ketenes with <i>N</i> -Benzoyldiazenes Catalyzed by N-Heterocyclic Carbenes: Mechanism and Enantioselectivity. Journal of Organic Chemistry, 2012, 77, 10729-10737.	1.7	57
2546	Mechanism of ketone hydrosilylation using NHC-Cu(I) catalysts: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	17
2547	Synthesis and evaluation of new guanidine-thiourea organocatalyst for the nitro-Michael reaction: Theoretical studies on mechanism and enantioselectivity. Beilstein Journal of Organic Chemistry, 2012, 8, 1485-1498.	1.3	36
2548	Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events. , 0, , .		1
2549	Quantum Information-Theoretical Analyses of Systems and Processes of Chemical and Nanotechnological Interest. , 2012, , .		0
2550	Active role of hydrogen bond and ambient water in Meyer-Schuster rearrangements in high-temperature water. International Journal of Quantum Chemistry, 2012, 112, 647-652.	1.0	2
2551	A DFT study on the mechanisms for the cycloaddition reactions between 1-azabenzonallene cations and carbodiimides. International Journal of Quantum Chemistry, 2012, 112, 809-822.	1.0	3
2552	A theoretical study on the reaction mechanisms of O( <sup>3</sup> P)+1-butene. International Journal of Quantum Chemistry, 2012, 112, 858-872.	1.0	10
2553	Multichannel RRKM study on the mechanism and kinetics of the CH <sub>3</sub> Cl + OH reaction. International Journal of Quantum Chemistry, 2012, 112, 1307-1315.	1.0	3
2554	Theoretical study on the reaction of butadiynyl radical (C <sub>4</sub> H) with ethylene (C <sub>2</sub> H <sub>4</sub> ) to form C <sub>6</sub> H <sub>4</sub> and H. International Journal of Quantum Chemistry, 2012, 112, 1913-1925.	1.0	3
2555	Theoretical study on HO <sub>2</sub> -initiated atmospheric oxidation of halogenated carbonyls. International Journal of Quantum Chemistry, 2012, 112, 1926-1935.	1.0	4
2556	Mechanistic study on Mo(CO) <sub>6</sub> -catalyzed intramolecular [2+2] or [2+2+1] cycloaddition reaction of 5-alkenylalkynes. Journal of Physical Organic Chemistry, 2012, 25, 21-31.	0.9	2
2557	Quantum chemical study on the mechanism of intramolecular cyclization of 2-benzyloxyphenyl trimethylsilyl ketone to give the benzofuran derivatives. Journal of Physical Organic Chemistry, 2012, 25, 400-408.	0.9	7

#	ARTICLE	IF	CITATIONS
2558	Aza-Diels-Alder reaction between cyclopentadiene and protonated <i>N</i> -phenylethyliminoacetates of 8-phenylmenthol and 8-phenylneomenthol: a density functional theory study. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 515-522.	0.9	4
2559	Mechanism and regioselectivity of the 1,3-dipolar cycloaddition of thiocarbonyl <i>S</i> -imide with cyclopent-1,2-dione and methoxyethene: a density functional theory approach. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 748-753.	0.9	3
2560	Comparative theoretical investigation of the formation of DNA interstrand crosslinks induced by two kinds of <i>N</i> -nitroso compounds: nitrosoureas and nitrosamines. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 1153-1167.	0.9	13
2561	A proline mimetic for enantioselective aldol reaction: a quantum chemical study of a catalytic reaction with a sterically hindered <i>l</i> -prolinamide derivative. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 971-978.	0.9	3
2562	Substituent effect on the reaction mechanism of proton transfer in formamide. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2378-2381.	1.0	18
2563	Multistep conformational interconversion mechanism of cyclododecane. A simple and fast analysis using potential energy curves. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2382-2391.	1.0	2
2564	Influence of the methylation degree on the rate constants of the $\text{C}^{\text{OH}}$ addition to alkenes and its temperature dependence. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3479-3483.	1.0	8
2565	Mechanisms and rate constants in the atmospheric oxidation of saturated esters by hydroxyl radicals: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3508-3515.	1.0	16
2566	$\text{O}(\text{C}^{\text{P}}) + \text{CH}_3\text{SH}$ reactions: Structures, energetics, and kinetics. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3269-3275.	1.0	18
2567	Theoretical study of the conformational energy hypersurface of cyclotrisarcosyl. <i>Open Chemistry</i> , 2012, 10, 248-255.	1.0	6
2568	Mechanisms for the Reaction of Thiophene and Methylthiophene with Singlet and Triplet Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4934-4946.	1.1	42
2569	On the Mechanism of the $[\text{Cp}_2\text{Mo}(\text{OH})(\text{OH})_2]_{\text{Cp}}^+$ -Catalyzed Nitrile Hydration to Amides: A Theoretical Study. <i>Organometallics</i> , 2012, 31, 1618-1626.	1.1	22
2570	Unveiling the Role of Molecule-Assisted Homolysis: A Mechanistic Probe into the Chemistry of a Bicyclic Peroxide. <i>Journal of Organic Chemistry</i> , 2012, 77, 2134-2141.	1.7	4
2571	Reverse Cope Elimination of Hydroxylamines and Alkenes or Alkynes: Theoretical Investigation of Tether Length and Substituent Effects. <i>Journal of the American Chemical Society</i> , 2012, 134, 2434-2441.	6.6	67
2572	Understanding the origin of the asynchronicity in bond-formation in polar cycloaddition reactions. A DFT study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-benzoquinones. <i>RSC Advances</i> , 2012, 2, 1334-1342.	1.7	53
2573	Elusive Fluoro Sulfinyl Nitrite, $\text{FS}(\text{O})\text{NO}$ , Produced by Photolysis of Matrix-Isolated $\text{FS}(\text{O})_2\text{N}$ . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, 526-533.	0.6	25
2574	Elucidation of the reaction mechanisms and diastereoselectivities of phosphine-catalyzed [4 + 2] annulations between allenolates and ketones or aldimines. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7689.	1.5	45
2575	Dehydrative Cyclocondensation Mechanisms of Hydrogen Thioperoxide and of Alkanesulfenic Acids. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8031-8039.	1.1	8

#	ARTICLE	IF	CITATIONS
2576	Understanding the Physics and Chemistry of Reaction Mechanisms from Atomic Contributions: A Reaction Force Perspective. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7419-7423.	1.1	20
2577	Dyotropic Rearrangements of Fused Tricyclic $\beta$ -Lactones: Application to the Synthesis of ( $\alpha$ )-Curcumanolide A and ( $\alpha$ )-Curcumalactone. <i>Journal of the American Chemical Society</i> , 2012, 134, 13348-13356.	6.6	74
2578	Density functional theory study of 1,2-dioxetanone decomposition in condensed phase. <i>Journal of Computational Chemistry</i> , 2012, 33, 2118-2123.	1.5	12
2579	Gas-phase reactions of $\text{SiH}_n$ ( $n = 1, 2$ ) with $\text{NF}_3$ : A computational investigation on the detailed mechanistic aspects. <i>Journal of Computational Chemistry</i> , 2012, 33, 1918-1926.	1.5	3
2580	The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. <i>Journal of Computational Chemistry</i> , 2012, 33, 2292-2302.	1.5	39
2581	Aromatic C-H bond activation revealed by infrared multiphoton dissociation spectroscopy. <i>Journal of Mass Spectrometry</i> , 2012, 47, 460-465.	0.7	19
2582	Fragmentation of oxime and silyl oxime ether odd-electron positive ions by the McLafferty rearrangement: new insights on structural factors that promote $\beta$ , $\gamma$ fragmentation. <i>Journal of Mass Spectrometry</i> , 2012, 47, 676-686.	0.7	11
2583	Structure and reactivity of thiosulfonic acids and their anions: A theoretical study. <i>Heteroatom Chemistry</i> , 2012, 23, 329-339.	0.4	1
2584	Prereactive Complexes in Chlorination of Benzene, Triazine, and Tetrazine: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1298-1306.	1.1	19
2585	Probing O-dealkylation and deamination aging processes in tabun-conjugated AChE: a computational study. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	2
2586	Ring splitting of azetidin-2-ones via radical anions. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 7928.	1.5	13
2593	C $\beta$ -N and C $\beta$ -C Bond Formations in the Thermal Reactions of $\text{Cp}^*\text{Ni}(\text{NH}_2)_2$ with $\text{C}_2\text{H}_4$ : Mechanistic Insight on the Metal-Mediated Hydroamination of an Unactivated Olefin. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3483-3488.	7.2	24
2594	Experimental Observation of the 16-Electron Molecules SPN, SNP, and Cyclic PSN. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3334-3339.	7.2	22
2595	Direct Conversion of Methane into Formaldehyde Mediated by $[\text{Al}_2\text{O}_3]$ at Room Temperature. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3703-3707.	7.2	98
2596	Thermal Reactions of $\text{YAlO}_3$ with Methane: Increasing the Reactivity of $\text{Y}_2\text{O}_3$ and the Selectivity of $\text{Al}_2\text{O}_3$ by Doping. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5991-5994.	7.2	69
2597	Sequential Methyl-Fluorine Exchange Reactions of Siloxide Ions in the Gas-Phase. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 8632-8635.	7.2	2
2598	Thermal Ammonia Activation by Cationic Transition-Metal Hydrides of the First Row "Small but Mighty". <i>Chemistry - an Asian Journal</i> , 2012, 7, 1214-1220.	1.7	17
2599	Conformational preferences of 4-chloroproline residues. <i>Biopolymers</i> , 2012, 97, 629-641.	1.2	7

#	ARTICLE	IF	CITATIONS
2600	Mechanism of the Transition-Metal-Catalyzed Hydroarylation of Bromo-Alkynes Revisited: Hydrogen versus Bromine Migration. <i>Chemistry - A European Journal</i> , 2012, 18, 5401-5415.	1.7	52
2601	Control over the Chemoselectivity of Pd-Catalyzed Cyclization Reactions of (2-Iodoanilino)carbonyl Compounds. <i>Chemistry - A European Journal</i> , 2012, 18, 6950-6958.	1.7	20
2602	Gold-Catalyzed 1,2-Bis-acetoxy Migration of 1,4-Bis-propargyl Acetates: A Mechanistic Study. <i>Chemistry - A European Journal</i> , 2012, 18, 6811-6824.	1.7	50
2603	Theoretical Study of the Oxidation of Histidine by Singlet Oxygen. <i>Chemistry - A European Journal</i> , 2012, 18, 8437-8447.	1.7	31
2604	Sustainable Heck-Matsuda Reaction with Catalytic Amounts of Diazonium Salts: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2012, 18, 7210-7218.	1.7	41
2605	Origin of Selectivity of Tsuji-Trost Allylic Alkylation of Lactones: Highly Ordered Transition States with Lithium-Containing Enolates. <i>Chemistry - A European Journal</i> , 2012, 18, 10408-10418.	1.7	16
2606	Reactivity Control of C-H Bond Activation over Vanadium-Silver Bimetallic Oxide Cluster Cations. <i>Chemistry - A European Journal</i> , 2012, 18, 10998-11006.	1.7	24
2607	Mechanism of Silver(I)-Catalyzed Enantioselective Synthesis of Axially Chiral Allenes Based on Propargylamines. <i>Chinese Journal of Chemistry</i> , 2012, 30, 951-958.	2.6	18
2608	Structures and Reactivity of Oxygen-Rich Scandium Cluster Anions $\text{ScO}_3^{5-}$ . <i>ChemPhysChem</i> , 2012, 13, 1282-1288.	1.0	29
2609	Scandium-Catalyzed Preparation of Cytotoxic 3-Functionalized Quinolinones: Regioselective Ring Enlargement of Isatins or Imino Isatins. <i>ChemPlusChem</i> , 2012, 77, 563-569.	1.3	24
2610	Catalytic Adaptive Recognition of Thiol (SH) and Selenol (SeH) Groups Toward Synthesis of Functionalized Vinyl Monomers. <i>Journal of the American Chemical Society</i> , 2012, 134, 6637-6649.	6.6	97
2611	Computational Study of the Mechanism of the Photochemical and Thermal Ring-Opening/Closure Reactions and Solvent Dependence in Spirooxazines. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8148-8158.	1.1	17
2612	Substituent Effects in Thermal Reactions of a Silene with Silyl-Substituted Alkynes: A Theoretical Study. <i>Organometallics</i> , 2012, 31, 4737-4747.	1.1	7
2613	Syntheses and Crystal Structures of the closo-Borate $\text{M}[\text{B}_8\text{H}_9]$ ( $\text{M} = [\text{PPh}_4]^+$ and $[\text{N}(\text{n-Bu}_4)]^+$ ). <i>Inorganic Chemistry</i> , 2012, 51, 5111-5117.	1.9	7
2614	A Negative Ion Mass Spectrometry Approach to Identify Cross-Linked Peptides Utilizing Characteristic Disulfide Fragmentations. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 1364-1375.	1.2	15
2615	Hydrolysis mechanism of anticancer Pd(II) complexes with coumarin derivatives: a theoretical investigation. <i>Structural Chemistry</i> , 2012, 23, 831-839.	1.0	22
2616	Theoretical study on germylenoid $\text{H}_2\text{GeFBef}$ . <i>Structural Chemistry</i> , 2012, 23, 867-871.	1.0	11
2617	Mechanistic and kinetic study the reaction of $\text{O}(\text{3P})\text{A}\text{H}_3\text{CFCH}_2$ . <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	8

#	ARTICLE	IF	CITATIONS
2618	Coordinate reduction for exploring chemical reaction paths. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
2619	Theoretical studies on models of lysine-arginine cross-links derived from $\alpha$ -oxoaldehydes: a new mechanism for glucosepane formation. <i>Journal of Molecular Modeling</i> , 2012, 18, 1645-1659.	0.8	9
2620	Assessing the reactivation efficacy of hydroxylamine anion towards VX-inhibited AChE: a computational study. <i>Journal of Molecular Modeling</i> , 2012, 18, 1801-1808.	0.8	12
2621	Theoretical study of BN <sub>4</sub> : potential precursors of high energy density materials (HEDMs). <i>Journal of Molecular Modeling</i> , 2012, 18, 1927-1934.	0.8	5
2622	Gas-phase thermolysis reaction of formaldehyde diperoxide. Kinetic study and theoretical mechanisms. <i>Chemical Physics</i> , 2012, 393, 37-45.	0.9	5
2623	Computational study of the reaction mechanism and kinetics of ethyl acrylate ozonolysis in atmosphere. <i>Chemical Physics</i> , 2012, 402, 6-13.	0.9	8
2624	Proton exchange in acid-base complexes induced by reaction coordinates with heavy atom motions. <i>Chemical Physics</i> , 2012, 402, 105-112.	0.9	1
2625	Mechanism and electronic transition in the reaction: On the fly dynamics simulations with multi-reference potentials. <i>Chemical Physics Letters</i> , 2012, 535, 44-48.	1.2	10
2626	What is the mechanism of the OSO ring formation in sulfur tetroxide (SO <sub>4</sub> (C <sub>2v</sub> )) molecule?. <i>Chemical Physics Letters</i> , 2012, 538, 10-13.	1.2	3
2627	C-H bond activation by nanosized scandium oxide clusters in gas-phase. <i>International Journal of Mass Spectrometry</i> , 2012, 310, 57-64.	0.7	112
2628	Intracluster ion-molecule reactions between V <sup>+</sup> and methyl acetate or ethyl acetate clusters. <i>International Journal of Mass Spectrometry</i> , 2012, 315, 15-21.	0.7	4
2629	Mechanistic and kinetic study of the gas-phase reaction of vinyl acetate with ozone. <i>Atmospheric Environment</i> , 2012, 49, 197-205.	1.9	10
2630	Density functional calculations on the effect of sulfur substitution for 2-hydroxypropyl-p-nitrophenyl phosphate: C-O vs. P-O bond cleavage. <i>Bioorganic Chemistry</i> , 2012, 40, 99-107.	2.0	2
2631	Role of bifunctional catalyst 2-pyridone in the aminolysis of p-nitrophenyl acetate with n-butylamine: A computational study. <i>Journal of Molecular Catalysis A</i> , 2012, 355, 102-112.	4.8	12
2632	Diels-Alder reactions for the rational design of benzo[b]thiophenes: DFT-based guidelines for synthetic chemists. <i>Journal of Molecular Structure</i> , 2012, 1010, 158-168.	1.8	2
2633	Experimental and DFT study of cyclodehydration and acetylation of ferrocenyl diols. <i>Journal of Molecular Structure</i> , 2012, 1019, 7-15.	1.8	3
2634	A change from stepwise to concerted mechanism in the acid-catalysed benzidine rearrangement: a theoretical study. <i>Tetrahedron</i> , 2012, 68, 2161-2165.	1.0	18
2635	A quantum chemical study on the thermal degradation reaction of polyesters. <i>Polymer Degradation and Stability</i> , 2012, 97, 941-947.	2.7	15



#	ARTICLE	IF	CITATIONS
2636	Probing the simulant behavior of PNPDP toward parathion and paraoxon: A computational study. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 34, 10-17.	1.3	16
2637	The mechanism of copper-catalyzed azide-alkyne cycloaddition reaction: A quantum mechanical investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 34, 101-107.	1.3	20
2638	Reaction of aniline with ammonium persulphate and concentrated hydrochloric acid: Experimental and DFT studies. <i>Chemical Papers</i> , 2012, 66, .	1.0	10
2639	A theoretical study of kinetics and mechanism of the oxa 6π electrocyclization of naphthoquinones as antimalarial drugs. <i>Russian Journal of Physical Chemistry A</i> , 2012, 86, 1220-1225.	0.1	0
2640	Highly Diastereoselective Construction of Fused Carbocycles from Cyclopropane-1,1-dicarboxylates and Cyclic Enol Silyl Ethers: Scope, Mechanism, and Origin of Diastereoselectivity. <i>Chemistry - A European Journal</i> , 2012, 18, 2196-2201.	1.7	74
2641	Alder-ene reaction: Aromaticity and activation-strain analysis. <i>Journal of Computational Chemistry</i> , 2012, 33, 509-516.	1.5	93
2642	Formic Acid Catalyzed Gas-Phase Reaction of H <sub>2</sub> O with SO <sub>3</sub> and the Reverse Reaction: A Theoretical Study. <i>ChemPhysChem</i> , 2012, 13, 323-329.	1.0	77
2643	Gas-phase oxidation of cresol isomers initiated by OH or NO <sub>3</sub> radicals in the presence of NO <sub>2</sub> . <i>International Journal of Chemical Kinetics</i> , 2012, 44, 165-178.	1.0	9
2644	Linking Ion and Neutral Chemistry in C-H Bond Electrophilic Activation: Generation and Detection of HO <sub>2</sub> <sup>•</sup> Reactive Radicals in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 1455-1458.	7.2	6
2645	Theoretical study of the ozonolysis of allyl acetate: mechanism and kinetics. <i>Structural Chemistry</i> , 2012, 23, 201-208.	1.0	12
2646	Mechanistic and kinetic study on the ozonolysis of ethyl vinyl ether and propyl vinyl ether. <i>Structural Chemistry</i> , 2012, 23, 499-514.	1.0	10
2647	Quantum chemical investigation of the thermal pyrolysis reactions of the carboxylic group in a brown coal model. <i>Journal of Molecular Modeling</i> , 2012, 18, 359-365.	0.8	37
2648	Mechanism of intermolecular hydroacylation of vinylsilanes catalyzed by a rhodium(I) olefin complex: a DFT study. <i>Journal of Molecular Modeling</i> , 2012, 18, 1229-1239.	0.8	9
2649	Theoretical study of the pH-dependent antioxidant properties of vitamin C. <i>Journal of Molecular Modeling</i> , 2013, 19, 1945-1952.	0.8	10
2650	A density functional theory investigation on the formation mechanisms of DNA interstrand crosslinks induced by chloroethylnitrosoureas. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1299-1306.	1.0	15
2651	The role of benzoic acid in proline-catalyzed asymmetric michael addition: A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1339-1348.	1.0	6
2652	Novel theoretical studies of the dehydrogenation of LiBH <sub>2</sub> NH <sub>3</sub> . <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1358-1364.	1.0	6
2653	Reaction mechanism on the activation of ethane C-H and C-C bonds by a diplatinum cluster. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	10

#	ARTICLE	IF	CITATIONS
2654	The catalytic mechanism of intramolecular alkylation of $\hat{\pm}$ -diimine by rare earth complexes: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	9
2655	A theoretical investigation of the reaction mechanism for hydrogenated furan formation under Prins reaction conditions in trifluoroacetic acid medium. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2013, 109, 301-313.	0.8	2
2656	DFT Studies on the Reaction Mechanisms of 1,4-Dithio 1,3-Dienes with Nitriles. <i>Organometallics</i> , 2013, 32, 2059-2068.	1.1	8
2657	Mechanism and Stereoselectivity of Biologically Important Oxygenation Reactions of the 7-Dehydrocholesterol Radical. <i>Journal of Organic Chemistry</i> , 2013, 78, 7023-7029.	1.7	7
2658	DFT study of the stereo-selectivity of oxygenated heterocycles from 10 to 12 links. <i>Canadian Journal of Chemistry</i> , 2013, 91, 811-820.	0.6	0
2659	Formal Syntheses of ( $\hat{\pm}$ )-Platensimycin and ( $\hat{\pm}$ )-Platencin via a Dual-Mode Lewis Acid Induced Cascade Cyclization Approach. <i>Journal of Organic Chemistry</i> , 2013, 78, 7912-7929.	1.7	33
2660	Reaction of Dimethyl Ether with Hydroxyl Radicals: Kinetic Isotope Effect and Prereactive Complex Formation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8343-8351.	1.1	47
2661	Multichannel RRKM-TST and Direct-Dynamics CVT Study of the Reaction of Hydrogen Sulfide with Ozone. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6744-6756.	1.1	13
2662	Mechanistic aspects of the reaction of dimedone derivatives with sulfenic acids and other sulfur compounds—a computational study. <i>Tetrahedron</i> , 2013, 69, 7243-7252.	1.0	7
2663	Computational study on mechanism of Rh(iii)-catalyzed oxidative Heck coupling of phenol carbamates with alkenes. <i>Dalton Transactions</i> , 2013, 42, 4175.	1.6	57
2664	Theoretical study on the cracking reaction catalyzed by a solid acid with zeolitic structure: The catalytic cracking of 1-hexene on the surface of H-ZSM-5. <i>Applied Catalysis A: General</i> , 2013, 455, 65-70.	2.2	28
2665	Experimental and theoretical studies on polar Diels–Alder reactions of 1-nitronaphthalene developed in ionic liquids. <i>RSC Advances</i> , 2013, 3, 13825.	1.7	10
2666	Association reaction between SiH <sub>3</sub> and H <sub>2</sub> O <sub>2</sub> : a computational study of the reaction mechanism and kinetics. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	7
2667	Modeling the mechanism of glycosylation reactions between ethanol, 1,2-ethanediol and methoxymethanol. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14026.	1.3	6
2668	Reactivity and properties of dications generated by photoionization of 2,5-norbornadiene. <i>International Journal of Mass Spectrometry</i> , 2013, 336, 17-26.	0.7	5
2669	New Mechanism for the Ring-Opening Polymerization of Lactones? Uranyl Aryloxide-Induced Intermolecular Catalysis. <i>Inorganic Chemistry</i> , 2013, 52, 9077-9086.	1.9	45
2670	Mechanistic Study of Palladium-Catalyzed Chemoselective C(sp <sup>3</sup> )–H Activation of Carbamoyl Chloride. <i>Organometallics</i> , 2013, 32, 4165-4173.	1.1	23
2671	Production of ions at high energy and its role in extraterrestrial environments. <i>Rendiconti Lincei</i> , 2013, 24, 53-65.	1.0	45

#	ARTICLE	IF	CITATIONS
2672	Hydrogen adsorption and dissociation on small Al <sub>n</sub> Au clusters: an electronic structure density functional study. <i>European Physical Journal D</i> , 2013, 67, 1.	0.6	6
2673	Controlled Heterocyclization/Cross-Coupling Domino Reaction of $\hat{I}^2, \hat{I}^3$ -Allendiols and $\hat{I}^{\pm}$ -Allenic Esters: Method and Mechanistic Insight for the Preparation of Functionalized Buta-1,3-dienyl Dihydropyrans. <i>Chemistry - A European Journal</i> , 2013, 19, 14233-14244.	1.7	11
2674	Synthesis of 3,3-Disubstituted Oxindoles by Palladium-Catalyzed Asymmetric Intramolecular $\hat{I}^{\pm}$ -Arylation of Amides: Reaction Development and Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2013, 19, 11916-11927.	1.7	88
2675	A Theoretical Study of Formation Routes and Dimerization of Methanimine and Implications for the Aerosols Formation in the Upper Atmosphere of Titan. <i>Lecture Notes in Computer Science</i> , 2013, , 47-56.	1.0	16
2676	Theoretical studies on the unimolecular decomposition of nitroglycerin. <i>Journal of Molecular Modeling</i> , 2013, 19, 1617-1626.	0.8	14
2677	Evolution of a Multicomponent System: Computational and Mechanistic Studies on the Chemo- and Stereoselectivity of a Divergent Process. <i>Chemistry - A European Journal</i> , 2013, 19, 13355-13361.	1.7	15
2678	Mechanism and diastereoselectivity of arsenic ylide mediated cyclopropanation: a theoretical study. <i>RSC Advances</i> , 2013, 3, 17793.	1.7	5
2679	Memory Effects in Carbocation Rearrangements: Structural and Dynamic Study of the Norborn-2-en-7-ylmethyl-X Solvolysis Case. <i>Journal of Organic Chemistry</i> , 2013, 78, 9041-9050.	1.7	13
2680	Aggregation and Cooperative Effects in the Aldol Reactions of Lithium Enolates. <i>Chemistry - A European Journal</i> , 2013, 19, 13761-13773.	1.7	17
2681	Heteroleptic Tin(II) Initiators for the Ring-Opening (Co)Polymerization of Lactide and Trimethylene Carbonate: Mechanistic Insights from Experiments and Computations. <i>Chemistry - A European Journal</i> , 2013, 19, 13463-13478.	1.7	56
2682	An Iterative, Bimodular Nonribosomal Peptide Synthetase that Converts Anthranilate and Tryptophan into Tetracyclic Asperlicins. <i>Chemistry and Biology</i> , 2013, 20, 870-878.	6.2	20
2683	Theoretic study of DNA base guanine and adenine and protein residues <sup>TM</sup> binding mode of the trans geometries of new antitumor non-classical platinum complexes containing pyridine and picoline ligand. <i>Structural Chemistry</i> , 2013, 24, 2137-2148.	1.0	1
2684	Systematic kinetic study of H <sub>2</sub> release from the dimer of lithium amidoborane (LiNH <sub>2</sub> BH <sub>3</sub> ) <sub>2</sub> . <i>Structural Chemistry</i> , 2013, 24, 1527-1536.	1.0	7
2685	Theoretical study on the gas phase reaction mechanism of acetylene with nitrous oxide. <i>Structural Chemistry</i> , 2013, 24, 1513-1526.	1.0	5
2686	Atmospheric ozonolysis study of methyl acrylate and methyl 3-methyl acrylate. <i>Structural Chemistry</i> , 2013, 24, 1451-1460.	1.0	4
2687	Computational mechanistic study of methanol and molecular oxygen reaction on the triplet and singlet potential energy surfaces. <i>Structural Chemistry</i> , 2013, 24, 1051-1062.	1.0	5
2688	Theoretical studies on the interaction mechanisms between tetrachloro-p-benzoquinone and hydrogen peroxide. <i>Structural Chemistry</i> , 2013, 24, 1253-1264.	1.0	6
2689	A computational investigation on the potential energy surface of thiosulfeno with O(3P) reaction. <i>Structural Chemistry</i> , 2013, 24, 517-522.	1.0	4

#	ARTICLE	IF	CITATIONS
2690	Computational study on the reaction mechanism of atmospheric oxidation of ethanol with ozone. <i>Structural Chemistry</i> , 2013, 24, 611-621.	1.0	6
2691	Theoretical study on the reaction mechanism of NO and CO catalyzed by Rh atom. <i>Structural Chemistry</i> , 2013, 24, 13-23.	1.0	9
2692	Theoretical study on the mechanism and kinetics of acetaldehyde and hydroperoxyl radical: An important atmospheric reaction. <i>Chemical Physics Letters</i> , 2013, 583, 190-197.	1.2	8
2693	Theoretical studies on structures and stabilities of C <sub>4</sub> H <sub>2</sub> + isomers. <i>Chemical Research in Chinese Universities</i> , 2013, 29, 150-153.	1.3	6
2694	A DFT study on the reaction mechanisms of isocyanide-based multicomponent synthesis of polysubstituted cyclopentenes. <i>Computational and Theoretical Chemistry</i> , 2013, 1018, 85-90.	1.1	3
2695	Experimental and theoretical studies of Diels-Alder reaction between methyl (Z)-2-nitro-3-(4-nitrophenyl)-2-propenoate and cyclopentadiene. <i>Monatshefte für Chemie</i> , 2013, 144, 327-335.	0.9	11
2696	Oxidation reactivity of zinc-cysteine clusters in metallothionein. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 333-342.	1.1	13
2697	Theoretical investigation of Co(0)-catalyzed intramolecular hydroacylation of 4-pentenal. <i>Journal of Molecular Modeling</i> , 2013, 19, 2225-2234.	0.8	5
2698	DFT comparison of the OH-initiated degradation mechanisms for five chlorophenoxy herbicides. <i>Journal of Molecular Modeling</i> , 2013, 19, 2249-2263.	0.8	28
2699	Role of gold in a complex cascade reaction involving two electrocyclization steps. <i>Journal of Molecular Modeling</i> , 2013, 19, 1981-1984.	0.8	1
2700	Ethylene dimerization catalyzed by mixed phosphine-iminophosphorane nickel(II) complexes: a DFT investigation. <i>Journal of Molecular Modeling</i> , 2013, 19, 2107-2118.	0.8	15
2701	Mechanistic investigations of Al(OH) <sub>3</sub> oligomerization mechanisms. <i>Journal of Molecular Modeling</i> , 2013, 19, 1565-1572.	0.8	11
2702	DFT studies of the adsorption and dissociation of H <sub>2</sub> O on the Al <sub>13</sub> cluster: origins of this reactivity and the mechanism for H <sub>2</sub> release. <i>Journal of Molecular Modeling</i> , 2013, 19, 1789-1799.	0.8	22
2703	Electronic structure and decomposition reaction mechanism of cyclopropanone, phenylcyclopropanone and their sulfur analogues: a theoretical study. <i>Journal of Molecular Modeling</i> , 2013, 19, 1339-1353.	0.8	4
2704	A Highly Oxidizing and Isolable Oxoruthenium(V) Complex [Ru <sup>V</sup> (N <sub>4</sub> O)(O)] <sup>2+</sup> : Electronic Structure, Redox Properties, and Oxidation Reactions Investigated by DFT Calculations. <i>Chemistry - an Asian Journal</i> , 2013, 8, 2046-2056.	1.7	12
2705	Theoretical Study on Ruthenium-Catalyzed Hydrocarboxylative Dimerization of Phenylacetylene with Acetic Acid Leading to (1 <i>E</i> ,3 <i>E</i> )-1,4-Diphenyl-1,3-butadienyl Acetate. <i>Organometallics</i> , 2013, 32, 5201-5211.	1.1	8
2706	Negative ion fragmentations of disulfide-containing cross-linking reagents are competitive with aspartic acid side-chain-induced cleavages. <i>Rapid Communications in Mass Spectrometry</i> , 2013, 27, 238-248.	0.7	6
2707	Molecular Catch Bonds and the Anti-Hammond Effect in Polymer Mechanochemistry. <i>Journal of the American Chemical Society</i> , 2013, 135, 12722-12729.	6.6	118

#	ARTICLE	IF	CITATIONS
2708	Mechanism of Copper(I)-Catalyzed Allylic Alkylation of Phosphorothioate Esters: Influence of the Leaving Group on $\pm$ Regioselectivity. <i>Chemistry - A European Journal</i> , 2013, 19, 14126-14142.	1.7	14
2709	Formation of Guanine-6-sulfonate from 6-Thioguanine and Singlet Oxygen: A Combined Theoretical and Experimental Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 4509-4515.	6.6	34
2710	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. <i>Computational and Theoretical Chemistry</i> , 2013, 1025, 58-66.	1.1	5
2711	The OH-initiated atmospheric oxidation of cyclopentene: A coupled-cluster study of the potential energy surface. <i>Chemical Physics Letters</i> , 2013, 579, 35-39.	1.2	7
2712	Density functional calculations on alcoholysis and thiolysis of phosphate triesters: Stepwise or concerted?. <i>Computational and Theoretical Chemistry</i> , 2013, 1017, 60-71.	1.1	10
2713	A Theoretical DFT-Based and Experimental Study of the Transmetalation Step in Au/Pd-Mediated Cross-Coupling Reactions. <i>Chemistry - A European Journal</i> , 2013, 19, 15290-15303.	1.7	49
2714	Theoretical study on the molecular mechanism of the [5 + 2] vs. [4 + 2] cyclization mediated by Lewis acid in the quinone system. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 8357.	1.5	2
2715	Interstate Crossing-Induced Chemiexcitation as the Reason for the Chemiluminescence of Dioxetanones. <i>ChemPhysChem</i> , 2013, 14, 1071-1079.	1.0	26
2716	Investigation on the mechanism of water-assisted palladium-catalyzed benzylic C-H amination by N-fluorobenzenesulfonimide. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 7923.	1.5	14
2717	Borylated Tetrazoles from Cycloaddition of Azide Anions to Nitrilium Derivatives of <i>closo</i> -Decaborate Clusters. <i>Organometallics</i> , 2013, 32, 6576-6586.	1.1	30
2718	Rearrangement Reactions of Lithiated Oxiranes. <i>Journal of Organic Chemistry</i> , 2013, 78, 10776-10783.	1.7	9
2719	How the Bicyclo[4.1.0] Substrate Isomerizes into 4,5-Dihydrobenzo[b]furan: The Contribution from W(CO) <sub>5</sub> and NEt <sub>3</sub> . <i>Journal of Organic Chemistry</i> , 2013, 78, 10812-10820.	1.7	4
2720	Autoxidation of Organic Compounds in the Atmosphere. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3513-3520.	2.1	444
2721	Double-Ended Surface Walking Method for Pathway Building and Transition State Location of Complex Reactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5745-5753.	2.3	98
2722	Modular Mesoionics: Understanding and Controlling Regioselectivity in 1,3-Dipolar Cycloadditions of M <sup>1/4</sup> anchnone Derivatives. <i>Journal of the American Chemical Society</i> , 2013, 135, 17349-17358.	6.6	58
2723	Reactivity of Stoichiometric Lanthanum Oxide Cluster Cations in C-H Bond Activation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17548-17556.	1.5	24
2724	Direct dynamics study on the hydrogen abstraction reaction of fluoromethanes with vinyl radical. <i>Computational and Theoretical Chemistry</i> , 2013, 1020, 143-150.	1.1	2
2725	Understanding C-C bond formation in polar reactions. An ELF analysis of the Friedel-Crafts reaction between indoles and nitroolefins. <i>RSC Advances</i> , 2013, 3, 7520.	1.7	23

#	ARTICLE	IF	CITATIONS
2726	Reactivity of ethanol with ground state Ni+(2D) in the gas phase: A density functional study. Computational and Theoretical Chemistry, 2013, 1023, 29-37.	1.1	2
2727	Ion chemistry of sulfuryl fluoride: An experimental and theoretical study on gas-phase reactions involving neutral and ionized SO <sub>2</sub> F <sub>2</sub> . International Journal of Mass Spectrometry, 2013, 354-355, 46-53.	0.7	0
2728	Excitation of Nucleobases from a Computational Perspective I: Reaction Paths. Topics in Current Chemistry, 2013, 355, 57-97.	4.0	66
2729	DFT Investigation on Mechanisms and Stereoselectivities of [2 + 2 + 2] Multimolecular Cycloaddition of Ketenes and Carbon Disulfide Catalyzed by N-Heterocyclic Carbenes. Journal of Organic Chemistry, 2013, 78, 11849-11859.	1.7	38
2730	A theoretical study of H- and I-abstraction reactions from CH <sub>3</sub> I molecule by I (2P <sub>3/2</sub> ) atom and IO radical. Computational and Theoretical Chemistry, 2013, 1012, 72-83.	1.1	4
2731	Nickel/zinc-catalyzed decarbonylative addition of anhydrides to alkynes: A DFT study. Journal of Molecular Modeling, 2013, 19, 4545-4554.	0.8	5
2732	Theoretical Study of the X-Abstraction Reactions (X = H, Br, or I) from CH <sub>2</sub> I <sub>2</sub> by OH Radicals: Implications for Atmospheric Chemistry. Zeitschrift Fur Physikalische Chemie, 2013, , 130613021201008.	1.4	6
2733	Theoretical studies of the ring opening metathesis reaction of 3,3-dimethyl cyclopropene with molybdenum catalyst. Computational and Theoretical Chemistry, 2013, 1024, 1-8.	1.1	6
2734	DFT study on reaction mechanisms of propylamine and dimethyl acetylenedicarboxylate with 1,3-dimethylalloxan. Computational and Theoretical Chemistry, 2013, 1004, 47-55.	1.1	7
2735	Enantioselective Michael addition of aldehydes to maleimides organocatalysed by chiral 1,2-diamines: an experimental and theoretical study. Tetrahedron: Asymmetry, 2013, 24, 1531-1535.	1.8	26
2736	Theoretical investigation on the kinetics and branching ratio of the gas phase reaction of sevoflurane with Cl atom. Journal of Molecular Modeling, 2013, 19, 4815-4822.	0.8	13
2737	Theoretical investigations on the synthesis mechanism of cyanuric acid from NH <sub>3</sub> and CO <sub>2</sub> . Journal of Molecular Modeling, 2013, 19, 5037-5043.	0.8	7
2738	Quantum chemical study of $\beta$ -dimerization reaction of 1-silacycloprop-2-enes. Russian Chemical Bulletin, 2013, 62, 622-633.	0.4	1
2739	Theoretical Study on Copper-Catalyzed S-Arylation of Thiophenols with Aryl Halides: Evidence Supporting the LCu(I)-SPh Active Catalyst and Halogen Atom Transfer Mechanism. Organometallics, 2013, 32, 4944-4951.	1.1	26
2740	One Site Is Enough: A Theoretical Investigation of Iron-Catalyzed Dehydrogenation of Formic Acid. Chemistry - A European Journal, 2013, 19, 11869-11873.	1.7	29
2741	Acid-Activated Carbon Materials: Cheaper Alternative Catalysts for the Synthesis of Substituted Quinolines. ChemCatChem, 2013, 5, 3736-3742.	1.8	24
2742	Synthesis of Densely Functionalised 5-Halogen-1,3-Oxazin-2-ones by Halogen-Mediated Regioselective Cyclisation of N-Cbz-Protected Propargylic Amines: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2013, 19, 14852-14860.	1.7	24
2743	Theoretical Prediction of Rare Gas Containing Hydride Cations: HRgBF <sup>+</sup> (Rg = He, Ar, Kr, Xe). J. Phys. Chem. A, 2013, 117, 10784-10791.	1.1	37

#	ARTICLE	IF	CITATIONS
2744	Role of Metal Ion in Specific Recognition of Pyrophosphate Ion under Physiological Conditions and Hydrolysis of the Phosphoester Linkage by Alkaline Phosphatase. <i>Inorganic Chemistry</i> , 2013, 52, 11034-11041.	1.9	60
2745	Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes. <i>Organometallics</i> , 2013, 32, 4423-4430.	1.1	47
2746	Fluxional Cyclic Seleninate Ester: NMR and Computational Studies, Glutathione Peroxidase-like Behavior, and Unexpected Rearrangement. <i>Journal of Organic Chemistry</i> , 2013, 78, 10369-10382.	1.7	20
2747	New Delhi Metallo- $\beta$ -Lactamase I: Substrate Binding and Catalytic Mechanism. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11596-11607.	1.2	34
2748	Oxazolone-Based Photoswitches: Synthesis and Properties. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 6611-6618.	1.2	36
2749	Theoretical and Experimental Analysis of the Reaction Mechanism of MrTPS2, a Triquinane-Forming Sesquiterpene Synthase from Chamomile. <i>Chemistry - A European Journal</i> , 2013, 19, 13590-13600.	1.7	30
2750	DFT Study of a 5-endo-trig-Type Cyclization of 3-Alkenoic Acids by Using Pd-Spiro-bis(isoxazoline) as Catalyst: Importance of the Rigid Spiro Framework for Both Selectivity and Reactivity. <i>Chemistry - A European Journal</i> , 2013, 19, 9518-9525.	1.7	15
2751	Gas-Phase Reactions of OH with Methyl Amines in the Presence or Absence of Molecular Oxygen. An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10736-10745.	1.1	48
2752	Theoretical Study on the Gas Phase Reaction of Allyl Alcohol with Hydroxyl Radical. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6629-6640.	1.1	25
2753	Theoretical studies on the kinetics and mechanism of the reaction of atomic hydrogen with carbon dioxide. <i>Kinetics and Catalysis</i> , 2013, 54, 671-676.	0.3	1
2754	Kinetics and mechanism of intramolecular aldol condensation of 2,5-hexadione, a DFT and MP2 study. <i>Russian Journal of Physical Chemistry B</i> , 2013, 7, 540-547.	0.2	1
2755	Catalytic oxidation of CO by N <sub>2</sub> O conducted via the neutral oxide cluster couple VO <sub>2</sub> /VO <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10429.	1.3	35
2756	Synthesis, characterization and computational study of heterobimetallic CoFe complexes for mimicking hydrogenase. <i>RSC Advances</i> , 2013, 3, 3557.	1.7	14
2757	Hydrothermal synthesis of an ortho-metallated Co(III) complex anchored by a carboxylate group with a selective oxidation catalytic property. <i>Dalton Transactions</i> , 2013, 42, 4313.	1.6	5
2758	ReaxFF molecular dynamics simulations of non-catalytic pyrolysis of triglyceride at high temperatures. <i>RSC Advances</i> , 2013, 3, 6401.	1.7	23
2759	Two-step radical reactions that switch low multiplicity channels leading to the carbene and carbyne species detected for Ru(5F) + CH <sub>4</sub> <sup>n</sup> (n = 2-4) interactions under matrix isolation conditions. <i>RSC Advances</i> , 2013, 3, 11607.	1.7	10
2760	Exploration of the reactivity of N <sub>2</sub> O <sub>5</sub> with two Si(OH) <sub>4</sub> monomers using electronic structure methods. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1633-1640.	1.0	5
2761	Revisiting the reactivity of different carbon bases: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2471-2477.	1.0	12

#	ARTICLE	IF	CITATIONS
2762	A microiterative intrinsic reaction coordinate method for large QM/MM systems. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14188.	1.3	10
2763	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5140.	1.3	26
2764	Cyclopalladation of dimesityl selenide: synthesis, reactivity, structural characterization, isolation of an intermediate complex with C $\delta^+$ -H $\delta^-$ -Pd intra-molecular interaction and computational studies. <i>Dalton Transactions</i> , 2013, 42, 10828.	1.6	11
2765	On the method-dependence of transition state asynchronicity in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5108.	1.3	76
2766	Role of conformational structures and torsional anharmonicity in controlling chemical reaction rates and relative yields: butanal + HO <sub>2</sub> reactions. <i>Chemical Science</i> , 2013, 4, 200-212.	3.7	40
2767	An experimental and theoretical study on the reaction of Cl with CF <sub>3</sub> CF <sub>2</sub> CH <sub>2</sub> OH. <i>Molecular Physics</i> , 2013, 111, 753-763.	0.8	7
2768	Annuloselectivity in Cycloadditions of Ketenes with Imines: A DFT Study. <i>Journal of Organic Chemistry</i> , 2013, 78, 347-355.	1.7	32
2769	First diastereoselective [3 + 2] cycloaddition reaction of diethyl isocyanomethylphosphonate and maleimides. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 1640.	1.5	16
2770	Modified McFadyen-Stevens reaction for a versatile synthesis of aliphatic/aromatic aldehydes: design, optimization, and mechanistic investigations. <i>Chemical Science</i> , 2013, 4, 1111.	3.7	12
2771	Tentative mechanisms of 1,2-dihydropyridine and 4H-pyran formation via the reaction of 3-trimethylsilyl-2-propyn-1-al with 2-aminopyridine and water: experimental and quantum chemistry studies. <i>Tetrahedron</i> , 2013, 69, 2357-2368.	1.0	9
2772	Theory of the Formation and Decomposition of N $\delta^-$ -Heterocyclic Aminoxy-carbenes through Metal-Assisted [2+3] Dipolar Cycloaddition/Retro-Cycloaddition. <i>Chemistry - A European Journal</i> , 2013, 19, 2874-2888.	1.7	48
2773	Chemiluminescence of 1,2-dioxetanone studied by a closed-shell DFT approach. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1709-1716.	1.0	6
2774	Mechanism for Repair of Thymine Dimers by Photoexcitation of Proximal 8-Oxo-7,8-dihydroguanine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1240-1253.	1.1	19
2775	Quantum chemistry studies of the catalysis mechanism differences between the two isoforms of glutamic acid decarboxylase. <i>Journal of Molecular Modeling</i> , 2013, 19, 705-714.	0.8	2
2776	Theoretical investigation of molecular hydrogen adsorption and dissociation on Al <sub>n</sub> V <sub>(n-1)</sub> clusters. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 3640-3649.	3.8	25
2778	On the Origin of the Surprisingly Sluggish Redox Reaction of the N <sub>2</sub> O/CO Couple Mediated by [Y <sub>2</sub> O <sub>2</sub> ] <sup>+</sup> and [YAlO <sub>2</sub> ] <sup>+</sup> Cluster Ions in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 1226-1230.	7.2	57
2779	Theoretical kinetic investigation of thermal decomposition of methylcyclohexane. <i>Computational and Theoretical Chemistry</i> , 2013, 1026, 38-45.	1.1	11
2780	Theoretical studies on acetylene cyclotrimerization into benzene catalyzed by Cp <sub>2</sub> Zr fragment. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 29-35.	0.8	24



#	ARTICLE	IF	CITATIONS
2781	Theoretical studies on the reaction mechanism of CF <sub>3</sub> CF <sub>2</sub> with OH. Computational and Theoretical Chemistry, 2013, 1013, 15-22.	1.1	16
2782	Reaction mechanism of low-temperature fast pyrolysis of fructose to produce 5-hydroxymethyl furfural. Journal of Fuel Chemistry and Technology, 2013, 41, 1070-1076.	0.9	19
2783	Probing the role of solvation in predicting the $\beta$ -facial selectivity of 5-Fluoro-2-methyleneadamantane with per-acid: A case study. Computational and Theoretical Chemistry, 2013, 1026, 46-54.	1.1	0
2784	Reinvestigation of homoaromaticity of cyclohepta-1,3,5-triene. Computational and Theoretical Chemistry, 2013, 1017, 72-77.	1.1	6
2785	Thermochemistry and kinetics of isobutanol oxidation by the OH radical. Fuel, 2013, 106, 431-436.	3.4	10
2786	Computational investigations on the electronic and structural properties of germacyclopropylidenoids. Computational and Theoretical Chemistry, 2013, 1023, 24-28.	1.1	3
2787	Theoretical studies on the kinetics and mechanism of multi-channel gas-phase unimolecular reaction of ethyl acetate. Computational and Theoretical Chemistry, 2013, 1009, 43-49.	1.1	11
2788	The location of stationary points in the reaction of fluoroformyloxyl radical (FCO <sub>2</sub> (C <sub>2</sub> V)) with atomic hydrogen: A computational study on the pathways of the singlet and triplet reaction and intersystem crossing. Computational and Theoretical Chemistry, 2013, 1022, 86-93.	1.1	2
2789	Thermochemistry and kinetics of the $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si24.gif" overflow="scroll" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi mathvariant="italic" \rangle trans} \langle \text{mml:mi} \rangle \langle \text{mml:mtext} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle N \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle$ reaction. Chemical Physics Letters, 2013, 557, 37-42.	1.2	13
2790	Theoretical study on the reaction mechanism of CO <sub>2</sub> hydrogenation to methanol. Computational and Theoretical Chemistry, 2013, 1023, 59-64.	1.1	19
2791	Titanocene-catalyzed dehydrocoupling of the adduct Me <sub>2</sub> NH $\hat{A}$ BH <sub>3</sub> via competitive pathways: A DFT study. Journal of Organometallic Chemistry, 2013, 745-746, 479-486.	0.8	6
2792	Conformers of Cysteine and Cysteine Sulfinic Acid and Mechanisms of the Reaction of Cysteine Sulfinic Acid with 5,5-Dimethyl-1,3-cyclohexanedione (Dimedone). Journal of Physical Chemistry B, 2013, 117, 16000-16012.	1.2	12
2793	Insights into the Mechanism of the Reaction between Tetrachloro $\hat{A}$ Benzoquinone and Hydrogen Peroxide and their Implications in the Catalytic Role of Water Molecules in Producing the Hydroxyl Radial. ChemPhysChem, 2013, 14, 2737-2743.	1.0	18
2794	Bifunctional mesoporous MCF materials as catalysts in the Friedl $\hat{A}$ nder condensation. Catalysis Today, 2013, 218-219, 70-75.	2.2	23
2795	Computer modeling on the tautomerization of sulbactam intermediate in SHV-1 $\hat{I}^2$ -lactamases: E166A mutant vs. wild type. Journal of Molecular Graphics and Modelling, 2013, 40, 131-139.	1.3	0
2796	Thermal and photochemical reactions of phenylethynyltris-(trimethylsilyl)germane. Journal of Organometallic Chemistry, 2013, 727, 50-59.	0.8	3
2797	Theoretical study on the reaction mechanisms of HXC <sub>N</sub> (X=1,2) with nitrate radical. Chemical Physics, 2013, 412, 68-71.	0.9	3
2798	Advances in mechanistic understanding of iodine behaviour in PHEBUS-FP tests with the help of ab initio calculations. Annals of Nuclear Energy, 2013, 61, 170-178.	0.9	21

#	ARTICLE	IF	CITATIONS
2799	A density functional theory study of the hydrolysis mechanism of phosphodiester catalyzed by a mononuclear Zn(II) complex. <i>Journal of Molecular Catalysis A</i> , 2013, 368-369, 53-60.	4.8	2
2800	Branching ratio of gas-phase reaction of $\text{CH}_3\text{C}(\text{O})\text{CHCl}_2 + \text{OH}$ : A theoretical dynamic study. <i>Computational and Theoretical Chemistry</i> , 2013, 1008, 61-66.	1.1	3
2801	Gas-phase reactivity of sulfate esters and analogs: Why is the sulfur center unreactive?. <i>International Journal of Mass Spectrometry</i> , 2013, 354-355, 326-332.	0.7	1
2802	The reaction of 2,5-dimethylfuran with hydrogen atoms – An experimental and theoretical study. <i>Proceedings of the Combustion Institute</i> , 2013, 34, 233-239.	2.4	40
2803	The addition mechanism of TMS-CN into N-acetylpyridinium to give 2-cyanoacetylpyridinium: The roles of $\text{TpW}(\text{NO})(\text{PMe}_3)$ and DABCO. <i>Journal of Organometallic Chemistry</i> , 2013, 724, 117-128.	0.8	2
2804	Why Do Five-Membered Heterocyclic Compounds Sometimes Not Participate in Polar Diels-Alder Reactions?. <i>Journal of Organic Chemistry</i> , 2013, 78, 2462-2471.	1.7	45
2805	Polymerization of cyclic esters using N-heterocyclic carbene carboxylate catalysts. <i>Polymer Chemistry</i> , 2013, 4, 2414.	1.9	43
2806	Gas-Phase Reactions Regarding GaN Crystal Growth in a Carbon-Based Transport System: A Quantum Chemical Study. <i>Crystal Growth and Design</i> , 2013, 13, 1445-1457.	1.4	5
2807	Theoretical Studies on the Mechanism of the C-H Amination of Silyl Cyclopropenes by Azodicarboxylates. <i>Journal of Organic Chemistry</i> , 2013, 78, 988-995.	1.7	17
2808	Neighboring Effect in Fragmentation Pathways of Cage Guanidylhydrazones in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2242-2252.	1.1	5
2809	Reaction Path Optimization without NEB Springs or Interpolation Algorithms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1305-1310.	2.3	85
2810	Aminoxyl (Nitroxyl) Radicals in the Early Decomposition of the Nitramine RDX. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2233-2241.	1.1	25
2811	On the Mechanism of the Dehydroaromatization of Hexane to Benzene by an Iridium Pincer Catalyst. <i>Chemistry - A European Journal</i> , 2013, 19, 4069-4077.	1.7	20
2812	Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene. <i>Journal of Computational Chemistry</i> , 2013, 34, 646-655.	1.5	17
2813	A DFT Study of the [3 + 2] versus [4 + 2] Cycloaddition Reactions of 1,5,6-Trimethylpyrazinium-3-olate with Methyl Methacrylate. <i>Journal of Organic Chemistry</i> , 2013, 78, 1621-1629.	1.7	28
2814	Asymmetric 1,4-Michael Addition Reactions Catalyzed by a Cinchona Alkaloid Derived Primary Amine: A Theoretical Investigation of the Reaction Mechanism and Enantioselectivity. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 1706-1715.	1.2	13
2815	Selective Nucleophilic Oxygenation of Palladium-Bound Isocyanide Ligands: Route to Imine Complexes That Serve as Efficient Catalysts for Copper-/Phosphine-Free Sonogashira Reactions. <i>Organometallics</i> , 2013, 32, 1979-1987.	1.1	23
2816	Photo-assisted cyanation of transition metal nitrates coupled with room temperature C-C bond cleavage of acetonitrile. <i>Chemical Communications</i> , 2013, 49, 1906.	2.2	17

#	ARTICLE	IF	CITATIONS
2817	Stereoretentive Chlorination of Cyclic Alcohols Catalyzed by Titanium(IV) Tetrachloride: Evidence for a Front Side Attack Mechanism. <i>Journal of Organic Chemistry</i> , 2013, 78, 2118-2127.	1.7	14
2818	How the Conical Intersection Seam Controls Chemical Selectivity in the Photocycloaddition of Ethylene and Benzene. <i>Journal of Organic Chemistry</i> , 2013, 78, 1874-1886.	1.7	28
2819	Complex consequences: Substituent effects on metal $\pi$ -arylmethyl cation interactions. <i>Journal of Organometallic Chemistry</i> , 2013, 748, 68-74.	0.8	6
2820	MCl <sub>2</sub> (M = Hg, Au, Ru; $n = 2, 3$ ) catalyzed hydrochlorination of acetylene – A density functional theory study. <i>Canadian Journal of Chemistry</i> , 2013, 91, 120-125.	0.6	56
2821	Palladium(II)-Catalyzed Regioselective Arylation of Naphthylamides with Aryl Iodides Utilizing a Quinolinamide Bidentate System. <i>Journal of Organic Chemistry</i> , 2013, 78, 3030-3038.	1.7	80
2822	Catalytic Cycle for N $\equiv$ CN Bond Cleavage by Molybdenum Silyl Catalyst: A DFT Study. <i>Organometallics</i> , 2013, 32, 2725-2735.	1.1	12
2823	Electrophilic monoiodination of terminal alkenes. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2891.	1.5	6
2824	Mechanistic Study of a Ru-Xantphos Catalyst for Tandem Alcohol Dehydrogenation and Reductive Aryl-Ether Cleavage. <i>ACS Catalysis</i> , 2013, 3, 963-974.	5.5	42
2825	Asymmetric Organocatalytic Thio-Diels-Alder Reactions via Trienamine Catalysis. <i>Journal of the American Chemical Society</i> , 2013, 135, 5200-5207.	6.6	84
2826	Determinants of Regioselectivity and Chemoselectivity in Fosfomycin Resistance Protein FosA from QM/MM Calculations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1326-1336.	1.2	12
2827	Mechanism of Alkoxy Groups Substitution by Grignard Reagents on Aromatic Rings and Experimental Verification of Theoretical Predictions of Anomalous Reactions. <i>Journal of the American Chemical Society</i> , 2013, 135, 6633-6642.	6.6	24
2828	Photochemistry and photophysics of the amino and imino tautomers of 1-methylcytosine: tautomerisation as a side product of the radiationless decay. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1401-1408.	1.6	22
2829	Reactivity of Atomic Oxygen Radical Anions Bound to Titania and Zirconia Nanoparticles in the Gas Phase: Low-Temperature Oxidation of Carbon Monoxide. <i>Journal of the American Chemical Society</i> , 2013, 135, 2991-2998.	6.6	73
2830	Why Do Cycloaddition Reactions Involving C <sub>60</sub> Prefer [6,6] over [5,6] Bonds?. <i>Chemistry - A European Journal</i> , 2013, 19, 7416-7422.	1.7	100
2831	A quantum chemical study on polymerization catalysts for polyesters: Catalytic performance of chelated complexes of titanium. <i>Polymer</i> , 2013, 54, 3297-3305.	1.8	13
2832	Isomer-Selective Thermal Activation of Methane in the Gas Phase by [HMO] <sup>+</sup> and [M(OH)] <sup>+</sup> (M=Ti and V). <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6097-6101.	7.2	38
2833	Interpretation and Application of Reaction Class Transition State Theory for Accurate Calculation of Thermokinetic Parameters Using Isodesmic Reaction Method. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3279-3291.	1.1	15
2834	Role of F $\pi$ in the hydrolysis-condensation mechanisms of silicon alkoxide Si(OCH <sub>3</sub> ) <sub>4</sub> : a DFT investigation. <i>New Journal of Chemistry</i> , 2013, 37, 1371.	1.4	10

#	ARTICLE	IF	CITATIONS
2835	Assessing the viability of biosynthetic pathways for calophyline A formation—are pericyclic reactions involved?. <i>Tetrahedron Letters</i> , 2013, 54, 2952-2955.	0.7	6
2836	Sulfur(IV)-Mediated Transformations: From Ylide Transfer to Metal-Free Arylation of Carbonyl Compounds. <i>Journal of the American Chemical Society</i> , 2013, 135, 7312-7323.	6.6	137
2837	A joint experimental/theoretical investigation of the MMA polymerization initiated by yttrium phenoxyamine complexes. <i>Dalton Transactions</i> , 2013, 42, 9226.	1.6	4
2838	Mechanisms and Risk Assessments on the N-Nitration of <i>N</i> -Acetylhexahydro- <i>s</i> -triazines: Understanding the Preparation of RDX (2). <i>Journal of Physical Chemistry A</i> , 2013, 117, 5007-5014.	1.1	3
2839	stretchy="false">(</mml:mo><mml:msup><mml:mrow><mml:mtext>HN</mml:mtext></mml:mrow><mml:mrow><mml:mo>+</mml:mo><mml:msub><mml:mrow><mml:mtext>OH</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>	1.1	5
2840	Computational Interactions of the aquated forms of the anticancer drug AMD443 with DNA purine bases: A detailed computational approach. <i>Inorganica Chimica Acta</i> , 2013, 400, 130-141.	1.2	4
2841	Understanding the formation of [3+2] and [2+4] cycloadducts in the Lewis acid catalysed reaction between methyl glyoxylate oxime and cyclopentadiene: a theoretical study. <i>RSC Advances</i> , 2013, 3, 447-457.	1.7	20
2842	The chemical fate of paroxetine metabolites. Dehydration of radicals derived from 4-(4-fluorophenyl)-3-(hydroxymethyl)piperidine. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 4232.	1.5	6
2843	Mechanism and Kinetics of the Atmospheric Oxidative Degradation of Dimethylphenol Isomers Initiated by OH Radical. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4611-4626.	1.1	26
2844	Improved Predictor–Corrector Integrators For Evaluating Reaction Path Curvature. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1481-1488.	2.3	27
2845	Conformational preference and mechanism of decarboxylation of levodopa. A quantum dynamics/quantum mechanics study. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1966-1974.	1.0	3
2846	Caryolene-forming carbocation rearrangements. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 323-331.	1.3	23
2847	Theoretical and experimental study of the OH radical reaction with HCN. <i>Molecular Physics</i> , 2013, 111, 1589-1598.	0.8	8
2848	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 7311.	1.3	53
2849	A Detailed Look at the Reaction Mechanisms of Substituted Carbenes with Water. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1991-1999.	1.1	25
2850	Carbocyclization versus Oxycyclization on the Metal-Catalyzed Reactions of Oxyallenyl C3-Linked Indoles. <i>Journal of Organic Chemistry</i> , 2013, 78, 6688-6701.	1.7	39
2851	First-Principles Study of Molecular Hydrogen Adsorption and Dissociation on Al <sub>n</sub> Cr ( <i>n</i> = 1–13) Clusters. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3458-3466.	1.1	27
2852	A first principles investigation of aging processes in soman conjugated AChE. <i>Chemico-Biological Interactions</i> , 2013, 204, 185-190.	1.7	13

#	ARTICLE	IF	CITATIONS
2853	Mechanism of AMPPD Chemiluminescence in a Different Voice. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2300-2312.	2.3	44
2854	Heuristic control of kinetic energy in dynamic reaction coordinate calculations. <i>Journal of Computational Chemistry</i> , 2013, 34, 1835-1841.	1.5	11
2855	DFT Study on the Mechanism and Stereochemistry of the Petasis-Ferrier Rearrangements. <i>Journal of Organic Chemistry</i> , 2013, 78, 6947-6955.	1.7	26
2856	Mechanism of the Deamination Reaction of Isoguanine: A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5715-5725.	1.1	9
2857	Click-Like Reactions with the Inert HCB <sub>11</sub> Cl <sub>11</sub> <sup>+</sup> Anion Lead to Carborane-Fused Heterocycles with Unusual Aromatic Character. <i>Inorganic Chemistry</i> , 2013, 52, 6223-6229.	1.9	50
2858	Aromatic Claisen Rearrangements of <i>o</i> -Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2823-2831.	1.2	18
2859	Theoretical study on the proton shuttle mechanism of saccharopine dehydrogenase. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 17-25.	1.3	5
2860	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. <i>Journal of Molecular Modeling</i> , 2013, 19, 2689-2697.	0.8	36
2861	Global and local reactivity indices for electrophilic/nucleophilic free radicals. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 4350.	1.5	136
2862	Strong Spin-Orbit Coupling Facilitates C-H Activation in the Reactions of Os <sup>+</sup> with CH <sub>3</sub> F: Theoretical Investigations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1087-1092.	2.3	8
2863	Single and Double N-H Bond Activation of Ammonia by [Al <sub>2</sub> O <sub>3</sub> ] <sup>+</sup> : Room Temperature Formation of the Aminyl Radical and Nitrene. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 9513-9517.	7.2	7
2864	Theoretical calculations of rate of NDMA formation from gramine. <i>Canadian Journal of Chemistry</i> , 2013, 91, 275-282.	0.6	0
2865	Matrix Isolation Study of the Ozonolysis of 1,3- and 1,4-Cyclohexadiene: Identification of Novel Reaction Pathways. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4174-4182.	1.1	12
2866	Noyori Hydrogenation: Aromaticity, Synchronicity, and Activation Strain Analysis. <i>Journal of Organic Chemistry</i> , 2013, 78, 5669-5676.	1.7	44
2867	Understanding the regioselectivity in hetero Diels-Alder reactions. An ELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. <i>Tetrahedron</i> , 2013, 69, 107-114.	1.0	52
2868	Theoretical Study of the Catalytic Mechanism of E1 Subunit of Pyruvate Dehydrogenase Multienzyme Complex from <i>Bacillus stearothermophilus</i> . <i>Biochemistry</i> , 2013, 52, 8079-8093.	1.2	15
2869	Mechanism of Proton Transport in Ionic-Liquid-Doped Perfluorosulfonic Acid Membranes. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14449-14456.	1.2	23
2870	Structure, stability, and dissociation of small ionic silicon oxide clusters [SiO <sub>n</sub> <sup>+</sup> (n = 3, 4)]: Insight from density functional and topological exploration. <i>Journal of Chemical Physics</i> , 2013, 139, 234303.	1.2	7

#	ARTICLE	IF	CITATIONS
2871	Atmospheric Reactivity of CH <sub>2</sub> Cl with OH Radicals: High-Level OVOS CCSD(T) Calculations for the X-Abstraction Pathways (X = H, Cl, or I). <i>Journal of Physical Chemistry A</i> , 2013, 117, 771-782.	1.1	15
2872	Reactivity of First-Row Transition Metal Monocations (Sc <sup>+</sup> , Ti <sup>+</sup> ,) <i>Journal of Physical Chemistry A</i> , 2013, 117, 2932-2943.	1.1	8
2873	Adsorption of TiCl <sub>4</sub> and electron donor on defective MgCl <sub>2</sub> surfaces and propylene polymerization over Ziegler-Natta catalyst: A DFT study. <i>Chinese Journal of Polymer Science (English Edition)</i> , 2013, 31, 591-600.	2.0	27
2874	Kinetics Studies of the Reactions of Main Fourth-Period Monocations (Ga <sup>+</sup> ,) <i>Journal of Physical Chemistry A</i> , 2013, 117, 7742-7753.	1.1	2
2875	Time-Resolved and Mechanistic Study of the Photochemical Uncaging Reaction of the <i>o</i> -Hydroxycinnamic Caged Compound. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7767-7775.	1.1	5
2876	Vinylnitrene Formation from 3,5-Diphenyl-isoxazole and 3-Benzoyl-2-phenylazirine. <i>Journal of Organic Chemistry</i> , 2013, 78, 11349-11356.	1.7	31
2877	Computational studies on the thermal decomposition of the CH <sub>2</sub> FOCHFO radical. <i>Molecular Physics</i> , 2013, 111, 3756-3761.	0.8	7
2878	A theoretical study on mechanism of the anticancer drug camptothecin's E-ring-opening. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 43, 58-65.	1.3	11
2879	Catalytic H/D Exchange of Unactivated Aliphatic C-H Bonds. <i>Organometallics</i> , 2013, 32, 6599-6604.	1.1	24
2880	Ab initio study on the paths of oxygen abstraction of hydrogen trioxide (HO <sub>3</sub> ) molecule in the HO <sub>3</sub> + SO <sub>2</sub> reaction. <i>Journal of Chemical Sciences</i> , 2013, 125, 927-932.	0.7	0
2881	Theoretical Views on Activation of Methane Catalyzed by Hf <sup>2+</sup> and Oxidation of CO (x <sup>1</sup> Σ <sup>+</sup> ) by N <sub>2</sub> O (x <sup>1</sup> Σ <sup>+</sup> ) Catalyzed by HfO <sub>2</sub> <sup>+</sup> and TaO <sub>2</sub> <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2013, 117, 8843-8854.	1.1	9
2882	Theoretical Investigation of Lactide Ring-Opening Polymerization Induced by a Dinuclear Indium Catalyst. <i>Organometallics</i> , 2013, 32, 6950-6956.	1.1	54
2883	Double C-H Bond Activation of Hydrocarbons by a Gas Phase Neutral Oxide Cluster: The Importance of Spin State. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2294-2301.	1.1	27
2884	Theoretical Study on the Mechanism of Palladium-Catalyzed Dearomatization Reaction of Chloromethylnaphthalene. <i>Organometallics</i> , 2013, 32, 52-62.	1.1	14
2885	Formation of Acene-Based Polymers: Mechanistic Computational Study. <i>Journal of Organic Chemistry</i> , 2013, 78, 10058-10068.	1.7	9
2886	Theoretical Study on the Water-Assisted Reaction of NCO with HCHO. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6883-6892.	1.1	41
2887	Structure and Chemistry of the Heteronuclear Oxo-Cluster [VPO <sub>4</sub> ] <sup>+</sup> : A Model System for the Gas-Phase Oxidation of Small Hydrocarbons. <i>Journal of the American Chemical Society</i> , 2013, 135, 3711-3721.	6.6	66
2888	Triple Shifts and Thioether Assistance in Rearrangements Associated with an Unusual Biomethylation of the Sterol Side Chain. <i>Journal of Organic Chemistry</i> , 2013, 78, 935-941.	1.7	12

#	ARTICLE	IF	CITATIONS
2889	Catalytic Mechanism of Hyaluronate Lyase from <i>Spectrooccus pneumonia</i> : Quantum Mechanical/Molecular Mechanical and Density Functional Theory Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10161-10172.	1.2	10
2890	The Electronic Nature of the 1,4-Glycosidic Bond and Its Chemical Environment: DFT Insights into Cellulose Chemistry. <i>Chemistry - A European Journal</i> , 2013, 19, 16282-16294.	1.7	84
2891	A Computational Study of Detoxification of Lewisite Warfare Agents by British Anti-lewisite: Catalytic Effects of Water and Ammonia on Reaction Mechanism and Kinetics. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3496-3506.	1.1	19
2892	Quantum chemistry studies of adenosine 2503 methylation by S-adenosylmethionine-dependent enzymes. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1409-1415.	1.0	2
2893	COMPUTATIONAL MODELING STUDY ON METABOLISM MECHANISM OF OSELTAMIVIR. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350037.	1.8	0
2894	Generation and reactivity of putative support systems, Ce-Al neutral binary oxide nanoclusters: CO oxidation and C-H bond activation. <i>Journal of Chemical Physics</i> , 2013, 139, 194313.	1.2	22
2895	Inherent dynamical preferences in carbocation rearrangements leading to terpene natural products. <i>Pure and Applied Chemistry</i> , 2013, 85, 1949-1957.	0.9	28
2896	THEORETICAL STUDY ON THE BINDING OF THE ANTICANCER DRUGS Cis/Trans-[PtCl <sub>2</sub> (NH <sub>3</sub> ){HN = C(CH <sub>3</sub> ) <sub>2</sub> }] AND Cis/Trans-[PtCl <sub>2</sub> {HN = C(CH <sub>3</sub> ) <sub>2</sub> } <sub>2</sub> ] TO PURINE BASES. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350020.	1.8	1
2897	Theoretical Study of the <sup>1</sup> CF <sub>2</sub> + <sup>3</sup> O <sub>2</sub> Reaction on the Singlet Potential Surface. <i>Advanced Materials Research</i> , 2013, 641-642, 140-143.	0.3	0
2898	N <sub>2</sub> and CO Desorption from Interaction between NO and Nitrogen-Containing Char. <i>Advanced Materials Research</i> , 0, 860-863, 985-988.	0.3	0
2899	THEORETICAL INVESTIGATION OF SUBSTITUTION EFFECT ON THE PROTON TRANSFER MECHANISM IN 3-MERCAPTO-PROPENETHIAL. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1350045.	1.8	0
2900	A Theoretical Study of the OH + HN <sub>2</sub> Reaction. <i>Applied Mechanics and Materials</i> , 2013, 321-324, 314-317.	0.2	0
2901	Theoretical Investigation of the Decarbonylation of Acetaldehyde by Ni <sup>+2</sup> Using Density Functional Theory. <i>Applied Mechanics and Materials</i> , 2013, 446-447, 168-171.	0.2	0
2902	A Theoretical Study of the O <sub>3</sub> P + HCONH <sub>2</sub> Reaction. <i>Applied Mechanics and Materials</i> , 0, 316-317, 933-936.	0.2	0
2903	Ethylenediamine Catalyzed Decarboxylation of Oxaloacetic Acid: A DFT Investigation. <i>Advanced Materials Research</i> , 2013, 781-784, 253-258.	0.3	0
2904	Disposal of Dangerous Chemicals in Urban Areas and Mega Cities. <i>NATO Science for Peace and Security Series C: Environmental Security</i> , 2013, , .	0.1	10
2905	Theoretical Investigation of Product Channels in the CH <sub>3</sub> OO <sub>2</sub> + CN Reaction. <i>Applied Mechanics and Materials</i> , 0, 380-384, 4307-4310.	0.2	0
2906	A DFT study on the effect of functional groups on the formation kinetics of 1,2,3-triazolo-1,4-benzoxazine via intramolecular 1,3-dipolar cycloaddition. <i>Progress in Reaction Kinetics and Mechanism</i> , 2013, 38, 191-196.	1.1	0

#	ARTICLE	IF	CITATIONS
2907	A DFT Study on the 1,3-Dipolar Cycloaddition of Benzonitrile Oxide and N-Ethylmaleimide. Progress in Reaction Kinetics and Mechanism, 2013, 38, 316-322.	1.1	0
2908	Mechanism and Thermodynamics of Multichannel 1:1 Ammonia and Ozone Tropospheric Oxidation Reaction. Progress in Reaction Kinetics and Mechanism, 2013, 38, 266-282.	1.1	7
2909	Theoretical study of a reaction mechanism of tropospheric interest: CH <sub>3</sub> CH <sub>2</sub> F + OH. Progress in Reaction Kinetics and Mechanism, 2013, 38, 342-358.	1.1	0
2910	The Oxidative Mechanism in Electrophilic C <sub>2</sub> H Activation: The Case of CH <sub>2</sub> F <sub>2</sub> and CH <sub>2</sub> Cl <sub>2</sub> . Chemistry - an Asian Journal, 2013, 8, 588-595.	1.7	5
2911	Theoretical study on the mechanism of Pd(OAc) <sub>2</sub> catalyzed dehydrogenative cross-coupling of two heteroarenes. RSC Advances, 2013, 3, 20772.	1.7	5
2912	Gas-Phase Reactions of Cationic Vanadium-Phosphorus Oxide Clusters with C <sub>2</sub> H <sub>x</sub> (x = 4, 6): A DFT-Based Analysis of Reactivity Patterns. Chemistry - A European Journal, 2013, 19, 3017-3028.	1.7	24
2913	Thermal Activation of Ammonia by Transition-Metal Hydroxide Cations. ChemPlusChem, 2013, 78, 952-958.	1.3	3
2914	Global reaction route mapping of isomerization pathways of exotic C <sub>6</sub> H molecular species. Journal of Chemical Physics, 2013, 139, 224311.	1.2	18
2915	Dehydrogenation of N <sub>2</sub> H <sub>x</sub> (x = 2-4) by nitrogen atoms: Thermochemical and kinetics. Journal of Chemical Physics, 2013, 139, 194301.	1.2	8
2916	Thermal Methane Activation by a Binary V-Nb Transition-Metal Oxide Cluster Cation: A Further Example for the Crucial Role of Oxygen-Centered Radicals. Chemistry - A European Journal, 2013, 19, 11496-11501.	1.7	29
2917	THE MECHANISM OF ACID-CATALYZED DECARBOXYLATION OF PYRROLE-2-CARBOXYLIC ACID: INSIGHTS FROM CLUSTER-CONTINUUM MODEL CALCULATIONS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350017.	1.8	2
2918	Selective Activation of C-Cl and C-F Bonds by SO <sub>3</sub> <sup>+</sup> Radical Cations: An Experimental and Computational Study. ChemPlusChem, 2013, 78, 1065-1072.	1.3	7
2919	The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. Physical Chemistry Chemical Physics, 2013, 15, 18921.	1.3	26
2920	Tuning of the Dienophilic Reactivity of Imidazo[1,2-a]pyridine: A Comparison of DFT and Dispersion-Corrected DFT Calculations. Bulletin of the Chemical Society of Japan, 2013, 86, 57-66.	2.0	1
2921	Mechanistic Aspects of Gas-Phase Hydrogen-Atom Transfer from Methane to [CO] <sub>3</sub> <sup>+</sup> and [SiO] <sub>3</sub> <sup>+</sup> : Why Do They Differ?. Chemistry - A European Journal, 2013, 19, 6662-6669.	1.7	23
2923	The Roles of Counterion and Water in a Stereoselective Cysteine-Catalyzed Rauhut-Currier Reaction: A Challenge for Computational Chemistry. Chemistry - A European Journal, 2013, 19, 14245-14253.	1.7	33
2926	The Concerted Nature of the Cyclization of Squalene Oxide to the Protosterol Cation. Angewandte Chemie - International Edition, 2013, 52, 11029-11033.	7.2	25
2927	Ring opening of 2-aza-3-borabicyclo[2.2.0]hex-5-ene, the Dewar form of 1,2-dihydro-1,2-azaborine: stepwise versus concerted mechanisms. Beilstein Journal of Organic Chemistry, 2013, 9, 761-766.	1.3	9



#	ARTICLE	IF	CITATIONS
2928	Second-Row Transition-Metal Doping of (ZnSi) <sub>i</sub> , i = 12, 16 Nanoclusters: Structural and Magnetic Properties. <i>Computation</i> , 2013, 1, 31-45.	1.0	5
2929	Comprehensive Theoretical Studies on the Reaction of 1-Bromo-3,3,3-trifluoropropene with OH Free Radicals. <i>Molecules</i> , 2013, 18, 7873-7885.	1.7	3
2930	Theoretical Investigation on the Absence of Spore Photoproduct Analogue at Cytosine-Thymine Site. <i>Chinese Journal of Chemical Physics</i> , 2013, 26, 661-668.	0.6	1
2931	Prediction of Tetraoxygen Reaction Mechanism with Sulfur Atom on the Singlet Potential Energy Surface. <i>Scientific World Journal</i> , The, 2014, 2014, 1-8.	0.8	1
2932	Understanding the Polar Character Trend in a Series of Diels-Alder Reactions Using Molecular Quantum Similarity and Chemical Reactivity Descriptors. <i>Journal of Quantum Chemistry</i> , 2014, 2014, 1-19.	0.6	11
2934	Theoretical Study on Dissociation Mechanisms of Di-ethyl Berylliums and Di-t-butyl Berylliums. <i>Chinese Journal of Chemical Physics</i> , 2014, 27, 168-174.	0.6	1
2935	A computational investigation into the substituent effect on the chemo- and stereoselectivity of crossed intermolecular radical anion [2 + 2] cycloadditions of enones. <i>RSC Advances</i> , 2014, 4, 63475-63484.	1.7	2
2936	Acyclic and cyclic nitrene cycloadditions to 1-cinnamoyl-1-piperidine: A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450071.	1.8	1
2937	Sequential bond energies and structures of the Cr + $\hat{\alpha} \dots (N_2)_n$ , n = 1 $\hat{\alpha}$ 4. <i>Journal of Chemical Sciences</i> , 2014, 126, 1743-1751.	0.7	1
2938	Theoretical study on the C-H activation in decarbonylation of acetaldehyde by NiL <sub>2</sub> (L=SO <sub>3</sub> CH <sub>3</sub> ) using density functional theory. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2014, 29, 1170-1172.	0.4	0
2939	A computational study on the formation of pyridin-2(1H)-one and pyridine-2(1H)-thione from the reaction of cobaltacyclopentadiene with isocyanate and isothiocyanate. <i>Journal of Organometallic Chemistry</i> , 2014, 770, 101-115.	0.8	8
2940	A Molecular Modeling Study of N <sub>2</sub> Desorption from NO Heterogeneous Reduction on Char. <i>Energy Sources, Part A: Recovery, Utilization and Environmental Effects</i> , 2014, 36, 158-166.	1.2	18
2941	Formation of cyanates in low-valent uranium chemistry: a synergistic experimental/theoretical study. <i>Dalton Transactions</i> , 2014, 43, 11202-11208.	1.6	18
2942	Tautomeric transformations and reactivity of isoindole and sila-indole: A computational study. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450041.	1.8	10
2943	Quantum chemical study on the atmospheric photooxidation of ethyl acetate. <i>Canadian Journal of Chemistry</i> , 2014, 92, 814-820.	0.6	2
2944	Highly regioselective hydride transfer, oxidative dehydrogenation, and hydrogen-atom abstraction in the thermal gas-phase chemistry of [Zn(OH)] <sup>+</sup> /C <sub>3</sub> H <sub>8</sub> . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26617-26623.	1.3	11
2945	New insights into the gas-phase unimolecular fragmentations of [Cysteine-Ca] <sup>2+</sup> complexes. <i>Computational and Theoretical Chemistry</i> , 2014, 1047, 38-46.	1.1	2
2946	Mechanisms and Reaction Pathways in MEA Degradation; A Computational Study. <i>Energy Procedia</i> , 2014, 63, 1115-1121.	1.8	8

#	ARTICLE	IF	CITATIONS
2947	Theoretical investigation of atomic oxygen erosion mechanisms of 1,3-didecyl cyclopentane, 1,3-dioctyldecyl cyclopentane and alkylated cyclopentane. RSC Advances, 2014, 4, 50486-50493.	1.7	4
2948	Theoretical Insight into the Coordination of Cyclic $\hat{I}^2$ -Glucose to $[Al(OH)(aq)]^{2+}$ and $[Al(OH)_2(aq)]^{1+}$ Ions. Journal of Physical Chemistry B, 2014, 118, 13890-13902.	1.2	23
2949	Effects of $PAr_3$ Ligands on Direct Arylation of Heteroarenes with Isolated $[Pd(2,6-Me_2C_6H_3)(\frac{1}{4}O_2CMe)(PAr_3)]_4$ Complexes. Organometallics, 2014, 33, 6247-6252.		28
2950	Oxidative Degradation of Thiaproline Derivatives in Aqueous Solutions Induced by $\cdot OH$ Radicals. Israel Journal of Chemistry, 2014, 54, 321-332.	1.0	7
2951	A finite difference Davidson procedure to sidestep full <i>ab initio</i> hessian calculation: Application to characterization of stationary points and transition state searches. Journal of Chemical Physics, 2014, 140, 164115.	1.2	25
2952	Quantum chemical investigation of the primary thermal pyrolysis reactions of the sodium carboxylate group in a brown coal model. Journal of Molecular Modeling, 2014, 20, 2523.	0.8	3
2953	A computational study on the mechanism and kinetics of the reaction between $CH_3CH_2S$ and $OH$ . RSC Advances, 2014, 4, 62835-62843.	1.7	2
2954	A Twist on Facial Selectivity of Hydride Reductions of Cyclic Ketones: Twist-Boat Conformers in Cyclohexanone, Piperidone, and Tropinone Reactions. Journal of Organic Chemistry, 2014, 79, 11609-11618.	1.7	21
2955	The Oxidation of Sulfur Dioxide by Single and Double Oxygen Transfer Paths. ChemPhysChem, 2014, 15, 2723-2731.	1.0	10
2956	A density functional theory study on lewis acid catalyzed transesterification of $\hat{I}^2$ oxodithioesters. International Journal of Quantum Chemistry, 2014, 114, 862-868.	1.0	2
2957	Theoretical Chemistry in Belgium. Highlights in Theoretical Chemistry, 2014, , .	0.0	1
2958	The exothermic $HCl + OH \cdot (H_2O)$ reaction: Removal of the $HCl + OH$ barrier by a single water molecule. Journal of Chemical Physics, 2014, 140, 124316.	1.2	8
2959	Density Functional Calculations on the Alkaline Hydrolysis of Phosphate Triesters. Advanced Materials Research, 0, 900, 327-332.	0.3	1
2960	A theoretical study of the role of carbenes in the kinetics and mechanism of the reactions of synthesis and pyrolysis of carbon suboxide. Russian Journal of Physical Chemistry B, 2014, 8, 829-840.	0.2	1
2961	Theoretical study on the gas phase reaction of allyl chloride with hydroxyl radical. Journal of Chemical Physics, 2014, 140, 084309.	1.2	5
2962	Computational Mechanistic Study of the Gas Phase Oxidation of Methanol with Ozone. Progress in Reaction Kinetics and Mechanism, 2014, 39, 171-185.	1.1	3
2963	A DFT Study of 1,3-dipolar Cycloaddition Reaction of Benzonitrile Oxide and <i>N</i> -aryl-2,4,6-heptatrien-1-imine. Progress in Reaction Kinetics and Mechanism, 2014, 39, 292-298.	1.1	2
2964	Effect of Fluorine Substitution on the Reaction between Methylene and Acetone: A DFT Study. Progress in Reaction Kinetics and Mechanism, 2014, 39, 53-61.	1.1	4

#	ARTICLE	IF	CITATIONS
2965	Pathways, kinetics and thermochemistry of methyl-ester peroxy radical decomposition in the low-temperature oxidation of methyl butanoate: A computational study of a biodiesel fuel surrogate. <i>Combustion and Flame</i> , 2014, 161, 2270-2287.	2.8	29
2966	A novel, non-metallic graphitic carbon nitride catalyst for acetylene hydrochlorination. <i>Journal of Catalysis</i> , 2014, 311, 288-294.	3.1	148
2967	Density functional theory study of side-chain alkylation of toluene with formaldehyde over alkali-exchanged zeolite. <i>Microporous and Mesoporous Materials</i> , 2014, 196, 129-135.	2.2	17
2968	1,3-Dipolar cycloaddition between substituted phenyl azide and 2,3-dihydrofuran. <i>Chemical Papers</i> , 2014, 68, .	1.0	7
2969	Activation of propane C-H and C-C bonds by a diplatinum cluster: potential energy surfaces and reaction mechanisms. <i>Structural Chemistry</i> , 2014, 25, 471-481.	1.0	9
2970	Theoretical study on the mechanism and kinetics for the ozonolysis of vinyl propionate. <i>Structural Chemistry</i> , 2014, 25, 285-291.	1.0	7
2971	Insight into detailed mechanism of the atmospheric reaction of imidogen with hydroxyl: a computational study. <i>Structural Chemistry</i> , 2014, 25, 169-175.	1.0	5
2972	Mechanisms and kinetics of the ozonolysis reaction of cis-3-hexenyl acetate and trans-2-hexenyl acetate in atmosphere: a theoretical study. <i>Structural Chemistry</i> , 2014, 25, 71-83.	1.0	8
2973	Theoretic studies on the kinetics and mechanism of multi-channel gas-phase unimolecular reactions of 1-chloropropane and 2-chloropropane. <i>Structural Chemistry</i> , 2014, 25, 21-28.	1.0	4
2974	Tautomerism in pyridazin-3(2H)-one: A theoretical study using implicit/explicit solvation models. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 49, 47-54.	1.3	23
2975	2,3-Dihydro-1H-1,3-diazepin-2-ones: synthesis and novel rearrangements into pyrrole derivatives. <i>Tetrahedron Letters</i> , 2014, 55, 1416-1420.	0.7	9
2976	A computational investigation of product channels in the CH <sub>3</sub> O <sub>2</sub> +F reaction. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 112-115.	1.1	4
2977	Theoretical studies of ruthenium hydride-catalyzed addition reactions of benzaldehydes to isoprenes leading to $\alpha,\beta$ -unsaturated ketones: The role of the ligands hydride, carbonyl, chloride, and triphenylphosphine of the catalyst. <i>Journal of Organometallic Chemistry</i> , 2014, 753, 1-8.	0.8	6
2978	A DFT study of the unimolecular decomposition of 1,2,4-butanetriol trinitrate. <i>Journal of Molecular Modeling</i> , 2014, 20, 2081.	0.8	7
2979	DFT study of the mechanism and stereoselectivity of the 1,3-dipolar cycloaddition between pyrroline-1-oxide and methyl crotonate. <i>Journal of Chemical Sciences</i> , 2014, 126, 283-292.	0.7	14
2980	Theoretical investigation on mechanism of asymmetric Michael addition of trans-1-nitro-2-phenylethylene to 2-methylpropionaldehyde catalyzed by a Cinchona alkaloid-derived primary amine. <i>Structural Chemistry</i> , 2014, 25, 1343-1357.	1.0	5
2981	1, 3-dipolar cycloaddition of C-phenyl carbamoyl-N-phenyl nitrene with some dialkyl-substituted 2-benzylidenecyclopropane-1,1-dicarboxylates: theoretical analysis of mechanism and regioselectivity. <i>Journal of the Iranian Chemical Society</i> , 2014, 11, 1459-1465.	1.2	5
2982	Theoretical study on the gas phase reaction of acrylonitrile with atomic hydrogen. <i>Structural Chemistry</i> , 2014, 25, 1217-1227.	1.0	4

#	ARTICLE	IF	CITATIONS
2983	A two-step reaction scheme leading to singlet carbene species that can be detected under matrix conditions for the reaction of $Zr(\sup>3\sup>F)$ with either $CH_3F$ or $CH_3CN$ . <i>Journal of Computational Chemistry</i> , 2014, 35, 883-890.	1.5	9
2984	Ene-Reactions: Activation Strain Analysis and the Role of Aromaticity. <i>Chemistry - A European Journal</i> , 2014, 20, 10791-10801.	1.7	56
2985	Enantioselective synthesis of hexahydrofuro[3,2-c]quinolines through a multicomponent process. A new aromatic sandwich-model for BINOL-phosphoric acid catalyzed reactions. <i>Chemical Science</i> , 2014, 5, 996-1007.	3.7	82
2986	A DFT study of the domino reactions between imidazole NHC, ketenimines and DMAD or MP acetylene derivatives yielding spiro-pyrroles. <i>Computational and Theoretical Chemistry</i> , 2014, 1030, 25-32.	1.1	4
2987	A theoretical study on the competing mechanisms and regioselectivity of the intermolecular radical anion [2+2] cycloadditions of phenyl vinyl sulfone with enones. <i>Computational and Theoretical Chemistry</i> , 2014, 1028, 27-33.	1.1	2
2988	Thermal Ethane Activation by Bare $[V_2O_5]^+$ and $[Nb_2O_5]^+$ Cluster Cations: on the Origin of Their Different Reactivities. <i>Chemistry - A European Journal</i> , 2014, 20, 6672-6677.	1.7	24
2989	Ligand effect on the CuI-catalyzed C-S coupling reaction: A density functional theoretical study. <i>Computational and Theoretical Chemistry</i> , 2014, 1038, 40-48.	1.1	4
2990	Theoretical investigation on mechanisms and kinetics of the reactions of Cl atom with $CH_3OOH$ and $CH_3CH_2OOH$ . <i>Computational and Theoretical Chemistry</i> , 2014, 1038, 33-39.	1.1	11
2991	Reactions of n-butyl acrylate and ethyl methacrylate with ozone in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2014, 1039, 33-39.	1.1	2
2992	Mechanism of $AuCl_3$ -catalyzed cyclization of 1-(Indol-2-yl)-3-alkyn-1-ols: a DFT study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2239.	0.8	2
2993	Longphyllinesides A and B: natural Diels-Alder adducts from <i>Daphniphyllum longeracemosum</i> ?. <i>Tetrahedron</i> , 2014, 70, 4017-4021.	1.0	14
2994	Hydrazinolysis of 3-R-[1,2,4]Triazino[2,3-c]quinazolin-2-ones. <i>Synthetic and Theoretical Aspects. Journal of Physical Chemistry A</i> , 2014, 118, 1895-1905.	1.1	18
2996	Mechanisms of the $PtCl_2$ -Catalyzed Intramolecular Cyclization of o-Isopropyl-Substituted Aryl Alkynes for the Synthesis of Indenes and Comparison of Three $sp^3$ C-H Bond Activation Modes. <i>Journal of Organic Chemistry</i> , 2014, 79, 5684-5696.	1.7	31
2997	Neutral Compounds with Xenon-Germanium Bonds: A Theoretical Investigation on $FXeGeF$ and $FXeGeF_3$ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 3326-3334.	1.1	21
2998	The Photochemical Reaction of Vinylaziridines and Vinylazetidines with Chromium(0) and Molybdenum(0) (Fischer) Carbene Complexes. <i>Chemistry - A European Journal</i> , 2014, 20, 1359-1366.	1.7	14
2999	On the Importance of Decarbonylation as a Side-Reaction in the Ruthenium-Catalysed Dehydrogenation of Alcohols: A Combined Experimental and Density Functional Study. <i>Chemistry - A European Journal</i> , 2014, 20, 4141-4155.	1.7	39
3000	Cyclodimerization versus Polymerization of Methyl Methacrylate Induced by $N$ -Heterocyclic Carbenes: A Combined Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2014, 20, 3989-3997.	1.7	37
3001	The mechanism of ionic Diels-Alder reactions. A DFT study of the oxa-Povarov reaction. <i>RSC Advances</i> , 2014, 4, 16567-16577.	1.7	26

#	ARTICLE	IF	CITATIONS
3002	DFT study on the reaction mechanisms and stereoselectivities of NHC-catalyzed [2 + 2] cycloaddition between arylalkylketenes and electron-deficient benzaldehydes. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 6374.	1.5	36
3003	(E)-2-(Benzo[d]thiazol-2-yl)-3-heteroarylacrylonitriles as efficient Michael acceptors for cysteine: Real application in biological imaging. <i>Sensors and Actuators B: Chemical</i> , 2014, 193, 391-399.	4.0	8
3004	Mechanism and kinetic study of 3-fluoropropene with hydroxyl radical reaction. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 48, 18-27.	1.3	10
3005	Mechanism and Regioselectivity of C=N Bond Cleavage and Ring Expansion of N-Heterocyclic Carbenes. <i>Organometallics</i> , 2014, 33, 53-60.	1.1	32
3006	Understanding the mechanisms of [3+2] cycloaddition reactions. The pseudoradical versus the zwitterionic mechanism. <i>Tetrahedron</i> , 2014, 70, 1267-1273.	1.0	95
3007	Biosynthetic consequences of multiple sequential post-transition-state bifurcations. <i>Nature Chemistry</i> , 2014, 6, 104-111.	6.6	128
3008	A density functional theory study of the Cu+·(NO) <sub>n</sub> complexes (n=1-2). <i>Monatshefte für Chemie</i> , 2014, 145, 241-252.	0.9	3
3009	A DFT study on the NHC catalysed Michael addition of enols to $\hat{1},\hat{2}$ -unsaturated acyl-azoliums. A base catalysed C=C bond-formation step. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 895-904.	1.5	30
3010	New insight into the potential energy landscape and relaxation pathways of photoexcited aniline from CASSCF and XMCQDPT2 electronic structure calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3122-3133.	1.3	32
3011	Combined Experimental/Computational Study of Iridium and Palladium Hydride PP(O)P Pincer Complexes. <i>Organometallics</i> , 2014, 33, 571-577.	1.1	19
3012	Origin of the "endo rule" in Diels-Alder reactions. <i>Journal of Computational Chemistry</i> , 2014, 35, 371-376.	1.5	75
3013	Cyclic amine-borane adducts [C <sub>n</sub> H <sub>2n+1</sub> NBH <sub>3</sub> ] <sub>n</sub> (n = 2-6) as chemical hydrogen storage systems: a computational analysis. <i>RSC Advances</i> , 2014, 4, 1352-1361.	1.7	15
3014	The Viability of Nitrene-Alkene (3 + 2) Cycloadditions in Alkaloid Biosynthesis. <i>Journal of Organic Chemistry</i> , 2014, 79, 432-435.	1.7	28
3015	An application of the reaction class transition state theory to the kinetics of hydrogen abstraction reactions of hydrogen with methyl esters at the methoxy group. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 103-111.	1.1	24
3016	Substituent-Controlled Selective Synthesis of N-Acyl 2-Aminothiazoles by Intramolecular Zwitterion-Mediated C=N Bond Cleavage. <i>Journal of Organic Chemistry</i> , 2014, 79, 11146-11154.	1.7	22
3017	Conformationally locked bicyclo[4.3.0]nonane carbanucleosides: synthesis and bio-evaluation. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 9439-9445.	1.5	6
3018	Eco-Friendly Catalytic Systems Based on Carbon-Supported Magnesium Oxide Materials for the Friedländer Condensation. <i>ChemCatChem</i> , 2014, 6, 3440-3447.	1.8	16
3019	1,3-Dipolar Cycloaddition Reactions between Ethyl Diazoacetate and Substituted Alkynes: A Density Functional Theory Study. <i>Progress in Reaction Kinetics and Mechanism</i> , 2014, 39, 233-248.	1.1	5

#	ARTICLE	IF	CITATIONS
3020	Gas-Phase Reaction of $CeV_2O_7$ with $C_2H_4$ : Activation of $C-C$ and $C-H$ Bonds. <i>ChemPhysChem</i> , 2014, 15, 4117-4125.	1.0	9
3021	Understanding the selectivity in the formation of $\beta$ -lactams vs. $\gamma$ -lactams in the Staudinger reactions of chloro-cyan-ketene with unsaturated imines. A DFT study. <i>RSC Advances</i> , 2014, 4, 58559-58566.	1.7	14
3022	Theoretical studies of palladium-catalyzed cycloaddition of alkynyl aryl ethers and alkynes. <i>Journal of Molecular Modeling</i> , 2014, 20, 2514.	0.8	5
3023	The role of $NH_3$ and hydrocarbon mixtures in GaN pseudo-halide CVD: a quantum chemical study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2473.	0.8	4
3024	Facile Smiles-type rearrangement in radical cations of $N$ -acyl arylsulfonamides and analogs. <i>Rapid Communications in Mass Spectrometry</i> , 2014, 28, 829-834.	0.7	8
3025	A theoretical study on diastereoselective oxidative dearomatization by iodoxybenzoic acid. <i>Journal of Molecular Modeling</i> , 2014, 20, 2342.	0.8	11
3026	Importance of Ligand Exchanges in Pd(II)-Brønsted Acid Cooperative Catalytic Approach to Spirocyclic Rings. <i>Journal of the American Chemical Society</i> , 2014, 136, 15998-16008.	6.6	61
3027	Polarizability of neutral copper clusters. <i>Journal of Molecular Modeling</i> , 2014, 20, 2410.	0.8	13
3028	The structures and stability of silylenoids $RBrsiLi_2$ ( $R=CH_3$ , $C(SiH_3)_3$ ). <i>Journal of Molecular Modeling</i> , 2014, 20, 2462.	0.8	0
3029	Highly diastereoselective 1,3-dipolar cycloadditions of chiral non-racemic nitrones to 1,2-diaza-1,3-dienes: an experimental and computational investigation. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8888-8901.	1.5	14
3030	Reduction of an Fe(i) mesityl complex induced by $\beta$ -acid ligands. <i>Dalton Transactions</i> , 2014, 43, 9032.	1.6	11
3031	Heterolytic cleavage of $Si-H$ bonds: reduction of imines using silane/high-valent oxo-molybdenum $MoO_2Cl_2$ as a catalyst. <i>Catalysis Science and Technology</i> , 2014, 4, 43-46.	2.1	6
3032	Theoretical and kinetic study of the hydrogen atom abstraction reactions of ethyl esters with hydrogen radicals. <i>Chemical Physics Letters</i> , 2014, 616-617, 109-114.	1.2	28
3033	Pentalene formation mechanisms redux. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 887-894.	1.5	24
3034	An environmentally benign, mild, and catalyst-free reaction of quinones with heterocyclic ketene aminals in ethanol: site-selective synthesis of rarely fused [1,2-a]indolone derivatives via an unexpected anti-Nenitzescu strategy. <i>Green Chemistry</i> , 2014, 16, 4359-4370.	4.6	50
3035	Combined activation strain model and energy decomposition analysis methods: a new way to understand pericyclic reactions. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7662-7671.	1.3	85
3036	Origin of Reactivity Trends of Noble Gas Endohedral Fullerenes $Ng_2@C_{60}$ ( $Ng = He, Ne, Ar, Kr, Xe, Rn$ ). <i>Journal of Physical Chemistry C</i> , 2014, 118, 10000-10006.	2.3	34
3037	Understanding the mechanism of the Povarov reaction. A DFT study. <i>RSC Advances</i> , 2014, 4, 25268.	1.7	54

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3038	Theoretical mechanism for selective catalysis of double hydrophosphination of terminal arylacetylenes by an iron complex. <i>Dalton Transactions</i> , 2014, 43, 4813.	1.6	10
3039	Palladium Complexes with Chelating Bis-NHC Ligands in the Mizoroki-Heck Reaction Mechanism and Electronic Effects, a DFT Study. <i>Journal of Organic Chemistry</i> , 2014, 79, 12096-12105.	1.7	35
3040	Trans-Cis Isomerization of Vinylketones through Triplet 1,2-Biradicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10433-10447.	1.1	14
3041	Ab initio chemical kinetics for the unimolecular decomposition of Si <sub>2</sub> H <sub>5</sub> radical and related reverse bimolecular reactions. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 278-288.	1.0	6
3042	A density functional theory study on the catalytic mechanism of hydroxycinnamoyl-CoA hydratase-lyase. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 249-254.	1.0	7
3043	Theoretical study on the reaction of (Z)-CF <sub>3</sub> CH=CHCF <sub>3</sub> with OH radicals. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 176-182.	1.0	9
3044	A theoretical study of the catalytic mechanism of oxalyl-CoA decarboxylase, an enzyme for treating urolithiasis. <i>RSC Advances</i> , 2014, 4, 35777.	1.7	10
3045	Mechanistic insights into <i>trans</i> -proline-catalyzed transamidation of carboxamide with benzylamine from density functional theory calculations. <i>RSC Advances</i> , 2014, 4, 30108-30117.	1.7	13
3046	Computational insights into carbon-carbon homocoupling reactions mediated by organolanthanide(III) complexes. <i>Dalton Transactions</i> , 2014, 43, 4520.	1.6	10
3047	Halogen-abstraction reactions from chloromethane and bromomethane molecules by alkaline-earth monocations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16121-16136.	1.3	2
3048	Predicting pathways for terpene formation from first principles - routes to known and new sesquiterpenes. <i>Chemical Science</i> , 2014, 5, 1555.	3.7	26
3049	Combined DFT and experimental studies of C-C and C-X elimination reactions promoted by a chelating phosphine-alkene ligand: the key role of penta-coordinate PdII. <i>Dalton Transactions</i> , 2014, 43, 11165.	1.6	14
3050	Mechanistic understanding of domino cyclization between gem-dialkylthio vinylallenes and benzylamine towards economic synthesis: a computational study. <i>Green Chemistry</i> , 2014, 16, 2653.	4.6	27
3051	A Computational Study of Allene Synthesis via the Zn <sub>2</sub> -Promoted Alkylation of Terminal Alkynes (ATA Reaction). <i>Asian Journal of Organic Chemistry</i> , 2014, 3, 309-313.	1.3	11
3052	Towards a comprehensive understanding of the chemical vapor deposition of titanium nitride using Ti(NMe <sub>2</sub> ) <sub>4</sub> : a density functional theory approach. <i>Dalton Transactions</i> , 2014, 43, 8877.	1.6	8
3053	Spiropyran as a reusable chemosensor for selective colorimetric detection of aromatic thiols. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12137-12142.	1.3	36
3054	NO <sub>2</sub> bond cleavage by MoL <sub>3</sub> complexes. <i>Dalton Transactions</i> , 2014, 43, 1620-1629.	1.6	3
3055	A DFT study on the reaction mechanism of dimerization of methyl methacrylate catalyzed by N-heterocyclic carbene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20001-20008.	1.3	21

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3056	The mechanism of catalytic methylation of 2-phenylpyridine using di-tert-butyl peroxide. Dalton Transactions, 2014, 43, 10183-10201.	1.6	12
3057	Degradation of methyl salicylate through Cl initiated atmospheric oxidation – a theoretical study. RSC Advances, 2014, 4, 23464.	1.7	26
3058	Reaction mechanism and kinetics of the degradation of bromoxynil initiated by OH radical. RSC Advances, 2014, 4, 7749.	1.7	7
3059	Hydroaminomethylation of Styrene Catalyzed by Rhodium Complexes Containing Chiral Diphosphine Ligands and Mechanistic Studies: Why Is There a Lack of Asymmetric Induction?. ACS Catalysis, 2014, 4, 435-447.	5.5	29
3060	Reactivity of CHI <sub>3</sub> with OH Radicals: X-Abstraction Reaction Pathways (X = H, I), Atmospheric Chemistry, and Nuclear Safety. Journal of Physical Chemistry A, 2014, 118, 9512-9520.	1.1	3
3061	Quantum chemical and steered molecular dynamics studies for one pot solution to reactivate aged acetylcholinesterase with alkylator oxime. Chemico-Biological Interactions, 2014, 223, 58-68.	1.7	13
3062	Mechanism of N-heterocyclic carbene-catalyzed chemical fixation of CO <sub>2</sub> with aziridines: a theoretical study. RSC Advances, 2014, 4, 17236-17244.	1.7	24
3063	Spiroaminals - Crystal Structure and Computational Investigation of Conformational Preferences and Tautomerization Reactions. European Journal of Organic Chemistry, 2014, 2014, 5476-5486.	1.2	3
3064	Controlling the oxidative addition of aryl halides to Au(I). Journal of Computational Chemistry, 2014, 35, 2140-2145.	1.5	65
3065	Experimental and Computational Studies on the Mechanism of Zwitterionic Ring-Opening Polymerization of $\delta$ -Valerolactone with N-Heterocyclic Carbenes. Journal of Physical Chemistry B, 2014, 118, 6553-6560.	1.2	57
3066	The activation strain model and molecular orbital theory: understanding and designing chemical reactions. Chemical Society Reviews, 2014, 43, 4953-4967.	18.7	604
3067	Photoelectron Spectroscopy of Co <sub>2</sub> H <sub>2</sub> <sup>+</sup> and Density Functional Study of Co <sub>n</sub> C <sub>2</sub> H <sub>2</sub> (n = 1-3) Anion and Neutral Clusters. Journal of Physical Chemistry A, 2014, 118, 6757-6762.	1.1	7
3068	Diels-Alder Reaction on Free C <sub>68</sub> Fullerene and Endohedral Sc <sub>3</sub> N@C <sub>68</sub> Fullerene Violating the Isolated Pentagon Rule: Importance of Pentagon Adjacency. Chemistry - an Asian Journal, 2014, 9, 2604-2611.	1.7	20
3069	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
3070	A quantum chemical topological analysis of the C-C bond formation in organic reactions involving cationic species. Physical Chemistry Chemical Physics, 2014, 16, 14108.	1.3	15
3071	Photophysical and Photochemical Properties of 4-Thiouracil: Time-Resolved IR Spectroscopy and DFT Studies. Journal of Physical Chemistry B, 2014, 118, 5864-5872.	1.2	40
3072	Photoreaction Study of Methanol Adsorption Complexes on VO <sub>2</sub> (VO <sub>2</sub> ) <sub>n</sub> <sup>+</sup> (n = 1-3) Clusters at 355 nm. Journal of Physical Chemistry C, 2014, 118, 18488-18495.	1.5	15
3073	Theoretical study on the bifunctional substitution reactions between gold(III) dithiocarbamate derivative Au(DMDT)Cl <sub>2</sub> (DMDT=N,N-dimethyldithiocarbamate) and target molecules. Computational and Theoretical Chemistry, 2014, 1048, 84-94.	1.1	6



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3074	Switching the Enantioselectivity in Catalytic [4 + 1] Cycloadditions by Changing the Metal Center: Principles of Inverting the Stereochemical Preference of an Asymmetric Catalysis Revealed by DFT Calculations. <i>Journal of the American Chemical Society</i> , 2014, 136, 9414-9423.	6.6	21
3075	Formation of Bare $UO_2^{2+}$ and $NUO^{+}$ by Fragmentation of Gas-Phase Uranyl $\pi$ -Acetonitrile Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7838-7846.	1.1	35
3076	Investigation of the Cycloisomerization of 1,6-Enynes Catalyzed by Gold Nanoparticles with First-Principles Calculations: Mechanism and Selectivity. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18510-18520.	1.5	13
3077	DFT Study of the Mechanism and Stereochemistry of the Rh(I)-Catalyzed Diels $\pi$ -Alder Reactions between Electronically Neutral Dienes and Dienophiles. <i>Journal of Organic Chemistry</i> , 2014, 79, 11949-11960.	1.7	36
3078	Kinetics and mechanism for chlorine-initiated atmospheric oxidation of ethyl formate. <i>Canadian Journal of Chemistry</i> , 2014, 92, 598-604.	0.6	3
3079	CO Oxidation Promoted by Gold Atoms Supported on Titanium Oxide Cluster Anions. <i>Journal of the American Chemical Society</i> , 2014, 136, 3617-3623.	6.6	121
3080	Catalytic effect of water, water dimer, or formic acid on the tautomerization of nitroguanidine. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 90-96.	1.1	21
3081	Triplet Sensitized Photolysis of a Vinyl Azide: Direct Detection of a Triplet Vinyl Azide and Nitrene. <i>Journal of Organic Chemistry</i> , 2014, 79, 9325-9334.	1.7	20
3082	Physical Quenching in Competition with the Formation of Cyclobutane Pyrimidine Dimers in DNA Photolesion. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9105-9112.	1.1	6
3083	$CH_2NH_2 + O_2$ and $CH_3CHNH_2 + O_2$ Reaction Kinetics: Photoionization Mass Spectrometry Experiments and Master Equation Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2176-2186.	1.1	52
3084	Dissociation of H <sub>2</sub> on carbon doped aluminum cluster Al <sub>6</sub> C. <i>Journal of Chemical Physics</i> , 2014, 141, 064302.	1.2	21
3085	Understanding the polar mechanism of the ene reaction. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7581-7590.	1.5	36
3086	Lifetimes of carbocations encountered along reaction coordinates for terpene formation. <i>Chemical Science</i> , 2014, 5, 3301.	3.7	33
3087	Nitrogen $\pi$ -Doped Pitch $\pi$ -Based Spherical Active Carbon as a Nonmetal Catalyst for Acetylene Hydrochlorination. <i>ChemCatChem</i> , 2014, 6, 2339-2344.	1.8	55
3088	Kinetics and mechanism of the water-assisted reaction of NCO with CH <sub>3</sub> OH: A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 55-61.	1.1	5
3089	Theoretical study on the nickel(0)-mediated coupling of carbon dioxide and benzyldenecyclopropane: Mechanism and selectivity. <i>Computational and Theoretical Chemistry</i> , 2014, 1044, 44-54.	1.1	5
3090	A Contribution to the Direct Observation of Transient Phosphanylidene Complexes [RP=W(CO) <sub>5</sub> ] (R: Me, Ph): A Revisited Approach to Their Electronic Structure by UV $\pi$ -Photoelectron Spectroscopy. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 1694-1705.	1.0	4
3091	Experimental and Theoretical Study of Gold(III)-Catalyzed Hydration of Alkynes. <i>Organometallics</i> , 2014, 33, 3823-3830.	1.1	27

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3092	Reactivity of Metal Catalysts in Glucose→Fructose Conversion. <i>Chemistry - A European Journal</i> , 2014, 20, 12298-12309.	1.7	25
3093	Mechanistic Investigation on the Cleavage of Phosphate Monoester Catalyzed by Unsymmetrical Macrocyclic Dinuclear Complexes: The Selection of Metal Centers and the Intrinsic Flexibility of the Ligand. <i>Inorganic Chemistry</i> , 2014, 53, 3354-3361.	1.9	28
3094	Theoretical Insights into Mechanisms for Copper(I)-Catalyzed C→P Coupling of Diarylphosphines with Aryl Halides: A Combined Solvent and Ancillary Ligand Effect on the Identity of Active Catalyst and Reaction Mechanism. <i>Organometallics</i> , 2014, 33, 5263-5271.	1.1	13
3095	Parallel Optimization of a Reactive Force Field for Polycondensation of Alkoxysilanes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10966-10978.	1.2	37
3096	Theoretical study on the gas phase reaction of propargyl alcohol with hydroxyl radical. <i>Journal of Computational Chemistry</i> , 2014, 35, 1646-1656.	1.5	7
3097	Reactions of Benzene and 3-Methylpyrrole with the →OH and →OOH Radicals: An Assessment of Contemporary Density Functional Theory Methods. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2667-2682.	1.1	7
3098	Mechanistic Insights on Cooperative Asymmetric Multicatalysis Using Chiral Counterions. <i>Journal of Organic Chemistry</i> , 2014, 79, 7600-7606.	1.7	44
3099	Recent developments in methods for identifying reaction coordinates. <i>Molecular Simulation</i> , 2014, 40, 784-793.	0.9	64
3100	Cyclic and Acyclic Fructose Conformers in the Gas Phase: A Large-Scale Second-Order Perturbation Theory Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7925-7938.	1.1	11
3101	All the 2p-block elements in a molecule: experimental and theoretical studies of FBNCO and FBNCO+. <i>Chemical Communications</i> , 2014, 50, 13900-13903.	2.2	4
3102	Theoretical investigations toward the tandem reactions of N-aziridinyl imine compounds forming triquinanes via trimethylenemethane diyls: mechanisms and stereoselectivity. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 1220-1231.	1.5	6
3103	Mechanistic insights into the stereoselective C2-functionalization of 1-substituted imidazoles with cyanophenylacetylene and aldehydes. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 35-41.	1.1	5
3104	Insights into the Formation of Borabenzene Adducts via Ligand Exchange Reactions and TMSCl Elimination from Boracyclohexadiene Precursors. <i>Organometallics</i> , 2014, 33, 3596-3606.	1.1	24
3105	The origin of exo-stereoselectivity of norbornene in hetero Diels→Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8079-8086.	1.5	14
3106	Neutral Au <sub>n</sub> (n = 3→10) clusters catalyze acetylene hydrochlorination: a density functional theory study. <i>RSC Advances</i> , 2014, 4, 38466-38473.	1.7	33
3107	Thermal decomposition and isomerization of 1-heptyl radical: a computational investigation. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
3108	The mechanistic study of the hydroxyl radical reaction with trans-2-chlorovinylchloroarsine. <i>Journal of Molecular Modeling</i> , 2014, 20, 2335.	0.8	4
3109	The reaction mechanisms and kinetics of CF <sub>3</sub> CHFOCH <sub>3</sub> and CHF <sub>2</sub> CHFOCF <sub>3</sub> with atomic chlorine: a computational study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2435.	0.8	2

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3110	Thermochemical and kinetics studies of the CH <sub>3</sub> SH+S (3P) hydrogen abstraction and insertion reactions. <i>Journal of Molecular Modeling</i> , 2014, 20, 2449.	0.8	3
3111	Theoretical studies on the effect of sulfur substitution for the methanolysis of cyclic and acyclic phosphate esters. <i>Computational and Theoretical Chemistry</i> , 2014, 1048, 35-45.	1.1	2
3112	Siderophore Receptor-Mediated Uptake of Lactivicin Analogues in Gram-Negative Bacteria. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 3845-3855.	2.9	50
3113	Mechanism for the decomposition of 5-aza-2'-deoxycytidine: a theoretical study using Monte Carlo simulation plus local microhydration model. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	1
3114	Reaction mechanism of oxidative desulfurization of heterocyclic organic sulfides: a computational study. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	10
3115	Mechanism of OH-initiated atmospheric oxidation of E/Z-CF <sub>3</sub> CF = CFCF <sub>3</sub> : a quantum mechanical study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2179.	0.8	26
3116	Theoretical study of the gas-phase thermolysis of 3-methyl-1,2,4,5-tetroxane. <i>Journal of Molecular Modeling</i> , 2014, 20, 2224.	0.8	1
3117	Mechanistic exploration of the catalytic cycles for the CO oxidation by O <sub>2</sub> over FeO <sub>1</sub> application of the energetic span model. <i>Journal of Molecular Modeling</i> , 2014, 20, 2301.	0.8	2
3118	Hetero-Diels-Alder reaction of aromatic aldehydes catalyzed by titanium tetrachloride: computational and experimental results. <i>Tetrahedron</i> , 2014, 70, 735-741.	1.0	8
3119	Density functional theory study of the regio and stereoselectivity in 1,3-dipolar cycloaddition reactions between N-methyl methylenitrone and fluorinated dipolarophiles. <i>Journal of Fluorine Chemistry</i> , 2014, 162, 60-65.	0.9	12
3120	Mechanistic Insight into the (NHC)copper(I)-Catalyzed Hydrosilylation of Ketones. <i>Organometallics</i> , 2014, 33, 1953-1963.	1.1	70
3121	Comparison of the Photochemistry of 3-Methyl-2-phenyl-2-azirine and 2-Methyl-3-phenyl-2-azirine. <i>Journal of Organic Chemistry</i> , 2014, 79, 653-663.	1.7	30
3122	Can hydroxylamine be a more potent nucleophile for the reactivation of tabun-inhibited AChE than prototype oxime drugs? An answer derived from quantum chemical and steered molecular dynamics studies. <i>Molecular BioSystems</i> , 2014, 10, 2368.	2.9	15
3123	One-Pot Synthesis of 1,3,5-Triazine Derivatives via Controlled Cross-Cyclotrimerization of Nitriles: A Mechanism Approach. <i>Journal of Organic Chemistry</i> , 2014, 79, 7012-7024.	1.7	38
3124	Understanding the domino retro [3+2] cycloaddition/cyclization reaction of bicyclic isoxazolidines in the synthesis of spirocyclic alkaloids. A DFT study. <i>Journal of Molecular Modeling</i> , 2014, 20, 2347.	0.8	4
3125	Carboxylic Group and Its Tetrazolyl Isostere in One Molecule. Matrix Isolation FTIR and DFT Studies on Thermal Decomposition and Photochemistry of (Tetrazol-5-yl)acetic Acid. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2072-2082.	1.1	13
3126	Catalytic combustion of dichloromethane over NaFAU and HFAU zeolites: a combined experimental and theoretical study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2014, 112, 249-265.	0.8	7
3127	Mechanism and kinetics of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical: a theoretical study. <i>Structural Chemistry</i> , 2014, 25, 1773-1783.	1.0	3

#	ARTICLE	IF	CITATIONS
3128	Sonochemical degradation of diclofenac: byproduct assessment, reaction mechanisms and environmental considerations. <i>Environmental Science and Pollution Research</i> , 2014, 21, 5929-5939.	2.7	37
3129	Computational mechanistic investigation of the gas phase C <sub>2</sub> H <sub>4</sub> +CO reaction on the singlet and triplet potential energy surfaces. <i>Journal of the Iranian Chemical Society</i> , 2014, 11, 781-790.	1.2	1
3130	A DFT study on CO oxidation catalyzed by subnanometer AlCu <sub>n</sub> (n = 1-3) clusters. <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 1113-1123.	0.1	3
3131	On-Demand Selection of the Reaction Path from Imino Diels-Alder to Ene-Type Cyclization: Synthesis of Epiminopyrimido[4,5-b]azepines. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 660-669.	1.2	15
3132	C-H Bond Activation with Trier Metals: Indium and Gallium Zwitterions through Internal Hydride Abstraction in Rigid Salan Ligands. <i>Chemistry - A European Journal</i> , 2014, 20, 7706-7717.	1.7	8
3133	Experimental and Theoretical Studies on the Platinum-Mediated Selective C(sp)-Si Bond Cleavage of Alkynylsilanes. <i>Organometallics</i> , 2014, 33, 1878-1889.	1.1	11
3134	Computational Study on the Kinetics and Mechanism of the Carbaryl + OH Reaction. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7776-7781.	1.1	3
3135	Single- versus Multi-Proton-Coupled Rydberg-State Electron Transfer in Amine Clusters. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18861-18867.	1.5	12
3136	A Reaction Mechanism of Methane Coupling on a Silica-Supported Single-Site Tantalum Catalyst. <i>Organometallics</i> , 2014, 33, 2172-2181.	1.1	7
3137	Catalytic role of borane and alane in hydrogen release from cyclic amine adducts C <sub>n</sub> H <sub>2n</sub> +1N·XH <sub>3</sub> [X = B, Al; n = 2-5]: a theoretical interpretation. <i>RSC Advances</i> , 2014, 4, 21924.	1.7	8
3138	Mechanistic and kinetic investigations on the ozonolysis of isopropenyl acetate and propenyl acetate in atmosphere. <i>Computational and Theoretical Chemistry</i> , 2014, 1049, 42-50.	1.1	4
3139	Atmospheric formation of the NO <sub>3</sub> radical from gas-phase reaction of HNO <sub>3</sub> acid with the NH <sub>2</sub> radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19437-19445.	1.3	17
3140	Origins of Diastereoselectivity in Lewis Acid Promoted Ketene-Alkene [2 + 2] Cycloadditions. <i>Organic Letters</i> , 2014, 16, 5168-5171.	2.4	28
3141	A theoretical study on the mechanisms of the reactions between 1,3-dialkynes and ammonia derivatives for the formation of five-membered N-heterocycles. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7503-7514.	1.5	27
3142	Mechanism of C-H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium(I). <i>Organometallics</i> , 2014, 33, 715-721.	1.1	26
3143	Factors Controlling the Facility of Transannular Diels-Alder Reactions of Macrocyclic Bis-enones. <i>Journal of Organic Chemistry</i> , 2014, 79, 7162-7168.	1.7	1
3144	The mechanism and regioselectivity of gold(I) or platinum(II) catalyzed intramolecular hydroarylation to pyrrolopyridinones and pyrroloazepinones. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8433-8441.	1.5	8
3146	Dimetal hydride generated from dimetalated glycine: Formation mechanism and electronic structure. <i>International Journal of Mass Spectrometry</i> , 2014, 363, 32-39.	0.7	4

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3147	Oâ€“H anharmonic vibrational motions in Clâˆ“âˆ“(CH <sub>3</sub> OH) <sub>1</sub> âˆ“ <sup>2</sup> ionic clusters. Combined IRPD experiments and AIMD simulations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 119, 12-17.	2.0	14
3148	Enantioselective Michael addition of isobutyraldehyde to nitroalkenes organocatalyzed by chiral primary amine-guanidines. <i>Tetrahedron: Asymmetry</i> , 2014, 25, 462-467.	1.8	27
3149	Computational study on the mechanism and kinetics of Cl-initiated oxidation of vinyl acetate. <i>Atmospheric Environment</i> , 2014, 94, 63-73.	1.9	11
3150	Dioxygen activation at room temperature during controllable and highly efficient acetaldehyde-to-acetic acid oxidation using a simple iron(III)â€“acetonitrile complex. <i>Catalysis Today</i> , 2014, 233, 140-146.	2.2	5
3151	Phosphoranide production and decomposition in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2014, 362, 18-23.	0.7	2
3152	A theoretical investigation of NO <sub>3</sub> -initiated oxidation of toluene. <i>Computational and Theoretical Chemistry</i> , 2014, 1037, 63-69.	1.1	8
3153	Electrochemical reduction of 2-chloro-N-phenylacetamides at carbon and silver cathodes in dimethylformamide. <i>Electrochimica Acta</i> , 2014, 127, 159-166.	2.6	11
3154	Mechanism of Mo-catalyzed Câ€“S cleavage of thiophene. <i>Journal of Organometallic Chemistry</i> , 2014, 749, 275-286.	0.8	5
3155	Structure and potential energy surface of Na <sup>+</sup> /Oâˆ“(O <sub>2</sub> ) <sub>n</sub> (n=1â€“3) complexes. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 62-72.	1.1	5
3156	The intrinsic mechanism of methane oxidation under explosion condition: A combined ReaxFF and DFT study. <i>Fuel</i> , 2014, 124, 85-90.	3.4	90
3158	Ring opening of monocyclic dimethyl cyclopropene via metathesis by tungsten catalystâ€“ A computational study. <i>Journal of Chemical Sciences</i> , 2014, 126, 691-700.	0.7	2
3159	Mechanism for Activation of the Câ€“CN Bond of Nitriles by a Cationic CpRh <sup>III</sup> â€“Silyl Complex: A Systematic DFT Study. <i>Organometallics</i> , 2014, 33, 3030-3039.	1.1	17
3160	Mechanisms of the InCl <sub>3</sub> -Catalyzed Type-I, II, and III Cycloisomerizations of 1,6-Enynes. <i>Journal of Organic Chemistry</i> , 2014, 79, 3809-3820.	1.7	24
3161	Exploring Water Catalysis in the Reaction of Thioformic Acid with Hydroxyl Radical: A Global Reaction Route Mapping Perspective. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4019-4029.	1.1	19
3162	Branching Out from the Bisaboyl Cation. Unifying Mechanistic Pathways to Barbatene, Bazzanene, Chamigrene, Chamipinene, Cumacrene, Cuprenene, Dunniene, Isobazzanene, Iso- <sup>13</sup> -bisabolene, Isochamigrene, Laurene, Microbiotene, Sesquithujene, Sesquisabinene, Thujopsene, Trichodiene, and Widdradiene Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 2450-2463.	6.6	95
3163	Quantum mechanical/effective fragment potential (QM/EFP) study of phosphate diester cleavage in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2014, 1043, 5-12.	1.1	3
3164	DFT Study on the Mechanisms and Diastereoselectivities of Lewis Acid-Promoted Keteneâ€“Alkene [2 + 2] Cycloadditions: What is the Role of Lewis Acid in the Ketene and C = X (X = O, CH <sub>2</sub> ), and NH [2 + 2] Cycloaddition Reactions?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4288-4300.	1.1	46
3165	Alkynol polymerization catalysed by Grubbs-type and Hoveydaâ€“Grubbs ruthenium alkylidene complexes: A computational study. <i>Journal of Organometallic Chemistry</i> , 2014, 767, 6-15.	0.8	9

#	ARTICLE	IF	CITATIONS
3166	Density functional theory study on mechanisms of epoxy-phenol curing reaction. <i>Journal of Computational Chemistry</i> , 2014, 35, 1630-1640.	1.5	16
3167	Theoretical Elucidation of the Mechanism of the Cycloaddition between Nitrone Ylides and Electron-Deficient Alkenes. <i>Journal of Organic Chemistry</i> , 2014, 79, 2189-2202.	1.7	15
3168	Experimental and Theoretical Insights into the Mechanisms of Sulfate and Sulfamate Ester Hydrolysis and the End Products of Type I Sulfatase Inactivation by Aryl Sulfamates. <i>Journal of Organic Chemistry</i> , 2014, 79, 1995-2005.	1.7	32
3169	Nonadiabatic reaction mechanisms of the O(3P) with cyclopentene. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 51, 184-192.	1.3	4
3170	A DFT Study: Why Do $[\text{Ni}(\text{P}(\text{R})_2)_2\text{N}(\text{R}')_2]^2+$ Complexes Facilitate the Electrocatalytic Oxidation of Formate?. <i>Inorganic Chemistry</i> , 2014, 53, 3281-3289.	1.9	15
3171	Theoretical study on the atmospheric reaction of SO <sub>2</sub> with the HO <sub>2</sub> and HO <sub>2</sub> -H <sub>2</sub> O complex formation HSO <sub>4</sub> and H <sub>2</sub> SO <sub>3</sub> . <i>Chemical Physics Letters</i> , 2014, 608, 272-276.	1.2	20
3172	Tandem Michael addition of amines to maleic anhydride and 1,3-prototropic shift: experimental and theoretical results. <i>Tetrahedron</i> , 2014, 70, 5052-5056.	1.0	6
3173	Computational study on the mechanism and thermodynamic of atmospheric oxidation of HCN with ozone. <i>Structural Chemistry</i> , 2014, 25, 267-274.	1.0	2
3174	Reactivity of Oxygen Radical Anions Bound to Scandia Nanoparticles in the Gas Phase: C-H Bond Activation. <i>Chemistry - A European Journal</i> , 2014, 20, 1167-1175.	1.7	22
3175	Catalytic Mechanism of H <sub>2</sub> Activation by a Carbenoid Aluminum Complex. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26598-26604.	1.5	27
3176	Computational Studies of the Gas Phase Reactions of Ethers with Anions: Kinetic Barriers, Isotope Effects, Consecutive Eliminations and Site Selectivity. <i>European Journal of Mass Spectrometry</i> , 2015, 21, 141-147.	0.5	0
3177	Is the reaction between formic acid and protonated aminomethanol a possible source of glycine precursors in the interstellar medium?. <i>Astronomy and Astrophysics</i> , 2015, 579, A125.	2.1	15
3178	Hydrolysis of ammonia borane and metal amidoboranes: A comparative study. <i>Journal of Chemical Physics</i> , 2015, 143, 194305.	1.2	13
3179	Photodissociation at Various Wavelengths: Fragmentation Studies of Oxazine 170 Using Nanosecond Laser Pulses. <i>European Journal of Mass Spectrometry</i> , 2015, 21, 599-608.	0.5	4
3180	Theoretical study of kinetics and isomerization mechanism of dimethyladamantane carbocations. <i>Doklady Physical Chemistry</i> , 2015, 463, 141-144.	0.2	2
3181	Exploring the metastability and the pathways for polyanionic isomerization in the dianions and trianions of doubly- and triply-deprotonated benzene. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	8
3182	Theoretical Studies of the Reactions $\text{CF}_3\text{H}^+\text{COOR}+\text{Cl}$ and $\text{CF}_3\text{COOCH}_3+\text{OH}$ . <i>ChemPhysChem</i> , 2015, 16, 1768-1776.	1.0	16
3183	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl Sulfoxide Reductase with Mo and W. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 3580-3589.	1.0	23

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3184	A Joint Experimentalâ€“Computational Comparative Study of the Pd <sup>0</sup> â€“Catalysed Reactions of Aryl Iodides and Aldehydes with N, O, and S Tethers. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3935-3942.	1.2	8
3185	Reaction of $\text{OH}^\bullet$ radical and ozone with methyl salicylate â€“ a $\text{DFT}$ study. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 542-553.	0.9	11
3186	Hydroxylamine synthesis by oxygen insertion into $\text{Re}\xi\text{NH}_2$ bond via Baeyerâ€“Villiger oxidation: a Theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 690-694.	0.9	0
3187	Stereoselective [3+2] Carbocyclization of Indoleâ€“Derived Imines and Electronâ€“Rich Alkenes: A Divergent Synthesis of Cyclopenta[ <i>b</i> ]indole or Tetrahydroquinoline Derivatives. <i>Chemistry - A European Journal</i> , 2015, 21, 16769-16774.	1.7	16
3189	Mechanistic Understanding of the Divergent Cyclizations of $\alpha$ -Alkynylbenzaldehyde Acetals and Thioacetals Catalyzed by Metal Halides. <i>Chemistry - A European Journal</i> , 2015, 21, 17256-17268.	1.7	10
3191	A Family of Highâ€“Efficiency Hydrogenâ€“Generation Catalysts Based on Ammonium Species. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9328-9332.	7.2	55
3192	$\text{Rh}^{\text{V}}$ â€“Nitrenoid as a Key Intermediate in $\text{Rh}^{\text{III}}$ â€“Catalyzed Heterocyclization by $\text{C}\xi\text{H}$ Activation: A Computational Perspective on the Cycloaddition of Benzamide and Diazo Compounds. <i>Chemistry - A European Journal</i> , 2015, 21, 9209-9218.	1.7	85
3193	Factors Controlling $\beta$ -Elimination Reactions in Groupâ€“10 Metal Complexes. <i>Chemistry - A European Journal</i> , 2015, 21, 14362-14369.	1.7	36
3194	Theoretical Investigation of the Reaction Mechanism of the Photoisomerization of 1,2â€“Dihydroâ€“1,2â€“Azaborine. <i>ChemPhysChem</i> , 2015, 16, 1670-1675.	1.0	10
3195	From Gasâ€“Phase to Liquidâ€“Water Chemical Reactions: The Fluorine Atom Plus Water Trimer System. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11223-11226.	7.2	11
3196	Ferrocenylâ€“Substituted Pyrimidine Nucleobases: An Experimental and Computational Study of Regioselective Acylation of Uracil, Thymine, and 5â€“Fluorouracil. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 5424-5431.	1.2	6
3197	A Computational Study of the Kinetics and Mechanism for the $\text{C}_2\text{H}_3 + \text{CH}_3\text{OH}$ Reaction. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 764-772.	1.0	3
3198	Theoretical study on the atmospheric reaction of $\text{CH}_3\text{O}_2$ with OH. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1181-1186.	1.0	10
3199	Steric Enhancement of the Chemiluminescence of Luminols. <i>Chemistry - A European Journal</i> , 2015, 21, 9975-9979.	1.7	24
3200	Mass spectrometric study of the decomposition pathways of canonical amino acids and $\beta$ -lactones in the gas phase. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 635-644.	0.9	5
3201	Unmasking the Action of Phosphinous Acid Ligands in Nitrile Hydration Reactions Catalyzed by Areneâ€“Ruthenium(II) Complexes. <i>Chemistry - A European Journal</i> , 2015, 21, 16874-16886.	1.7	42
3202	Microwaveâ€“Assisted Organocatalyzed Rearrangement of Propargyl Vinyl Ethers to Salicylaldehyde Derivatives: An Experimental and Theoretical Study. <i>Chemistry - A European Journal</i> , 2015, 21, 18280-18289.	1.7	14
3203	Why Is the Spontaneous Deprotonation of $[\text{Cu}(\text{uracil})_2]^{2+}$ Complexes Accompanied by Enolization of the System?. <i>ChemPhysChem</i> , 2015, 16, 2375-2382.	1.0	2

#	ARTICLE	IF	CITATIONS
3204	Enantioselective Arylation of <i>N</i> -Tosylimines by Phenylboronic Acid Catalysed by a Rhodium/Diene Complex: Reaction Mechanism from Density Functional Theory. <i>Chemistry - A European Journal</i> , 2015, 21, 9753-9768.	1.7	19
3205	Ligand-Controlled CO <sub>2</sub> Activation Mediated by Cationic Titanium Hydride Complexes, [L <sup>+</sup> TiH] (L=Cp <sub>2</sub> , O). <i>Chemistry - A European Journal</i> , 2015, 21, 8483-8490.	1.7	38
3206	Depolymerization of Free Radical Polymers with Spin Migrations. <i>ChemPhysChem</i> , 2015, 16, 3308-3312.	1.0	11
3207	The <i>in situ</i> gas-phase formation of a C-glycoside ion obtained during electrospray ionization tandem mass spectrometry. A unique intramolecular mechanism involving an ion-molecule reaction. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1717-1732.	0.7	2
3208	Theoretical Studies on the Mechanism of the Michael Addition Reaction Catalyzed by a Thiourea-Cinchona-Amine: Triple Activation. <i>Asian Journal of Organic Chemistry</i> , 2015, 4, 904-911.	1.3	6
3209	Theoretical study of the mechanism generating azomethine ylide from formaldehyde and glycine. <i>Journal of Structural Chemistry</i> , 2015, 56, 1262-1267.	0.3	1
3210	A DFT Study on the Degradation of Chlorobenzene to p-chlorophenol via Stable Hydroxo Intermediate Promoted by Iron and Manganese Monoxides. , 2015, 05, .		0
3211	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. , 2015, , 169-201.		0
3212	On the Dehydrocoupling of Alkenylacetylenes Mediated by Various Samarocene Complexes: A Charming Story of Metal Cooperativity Revealing a Novel Dual Metal $\sigma$ -Bond Metathesis Type of Mechanism (DM $\sigma$ -BM). <i>Inorganics</i> , 2015, 3, 573-588.	1.2	2
3213	Computational Study of a Model System of Enzyme-Mediated [4+2] Cycloaddition Reaction. <i>PLoS ONE</i> , 2015, 10, e0119984.	1.1	18
3214	Dimerization of methanimine and its charged species in the atmosphere of Titan and interstellar/cometary ice analogs. <i>Astronomy and Astrophysics</i> , 2015, 584, A76.	2.1	48
3215	Theoretical investigation on H abstraction reaction mechanisms and rate constants of Isoflurane with the OH radical. <i>Molecular Physics</i> , 2015, 113, 3663-3672.	0.8	5
3216	An experimental and theoretical study of the kinetics of the reaction between 3-hydroxy-3-methyl-2-butanone and OH radicals. <i>RSC Advances</i> , 2015, 5, 26559-26568.	1.7	12
3217	Oxidation of Olefins with Benzeneseleninic Anhydride in the Presence of TMSOTf. <i>Journal of Organic Chemistry</i> , 2015, 80, 6052-6061.	1.7	4
3218	Theoretical insight into the effect of fluorine substituents on the rearrangement step in Fischer indolisations. <i>Tetrahedron</i> , 2015, 71, 7199-7203.	1.0	2
3219	Theoretical studies on gas-phase kinetics and mechanism of H-abstraction reaction from methanol by ClO and BrO radicals. <i>RSC Advances</i> , 2015, 5, 39110-39121.	1.7	9
3220	Pathways for the OH + Cl <sub>2</sub> $\rightarrow$ HOCl + Cl and HOCl + Cl $\rightarrow$ HCl + ClO Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7802-7809.	1.1	5
3221	Simulations of Chemical Reactions with the Frozen Domain Formulation of the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3053-3064.	2.3	26



#	ARTICLE	IF	CITATIONS
3222	A theoretical investigation on palladium-catalyzed one-pot coupling of aryl iodides, alkynes, and amines through C≡N bond cleavage for the synthesis of indole derivatives. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 361-368.	1.0	2
3223	Mechanisms and stereoselectivities of the Rh( <i>κ</i> )-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 6587-6597.	1.5	36
3224	Effect of water on carbonation of mineral aerosol surface models of kaolinite: a density functional theory study. <i>Environmental Earth Sciences</i> , 2015, 73, 7053-7060.	1.3	12
3225	Theoretical investigations of the reaction between 1,4-dithiane-2,5-diol and azomethine imines: mechanisms and diastereoselectivity. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 7558-7569.	1.5	19
3226	Activation of Methane by the Pyridine Radical Cation and its Substituted Forms in the Gas Phase. <i>Journal of the American Society for Mass Spectrometry</i> , 2015, 26, 1382-1387.	1.2	4
3227	A Theoretical Study on the Functionalisation Process of C <sub>18</sub> Fullerene Through its Open [5,5] Cycloaddition with 4-Pyridine Nitrile Oxide. <i>Progress in Reaction Kinetics and Mechanism</i> , 2015, 40, 169-176.	1.1	8
3228	Theoretical study of water gas shift reaction on Cu <sub>n</sub> Ni <sub>n</sub> (n = 1–12) clusters. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2015, 51, 740-755.	0.3	1
3229	Variable-Cell Double-Ended Surface Walking Method for Fast Transition State Location of Solid Phase Transitions. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4885-4894.	2.3	58
3230	Catalytic dehydrochlorination of 1,2-dichloroethane to produce vinyl chloride over N-doped coconut activated carbon. <i>RSC Advances</i> , 2015, 5, 104071-104078.	1.7	32
3231	Noble Gas Inserted Protonated Silicon Monoxide Cations: HN <sub>g</sub> OSi <sup>+</sup> (N <sub>g</sub> = He, Ne, Ar, Kr,) <i>Tj ETQq1 1 0,784314 rgBT /Overle</i>	1.1	14
3232	Fluxional behaviour of tricyclo[2.2.1.0 <sup>2,6</sup> ]heptaphosphide trisanion: a DFT investigation. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2015, 70, 871-878.	0.3	1
3233	Effect of Cr <sup>1</sup> R <sup>2</sup> P <sup>+</sup> R <sup>1</sup> R <sup>2</sup> Exchange on the Degenerate Cope Rearrangement of Barbaralane. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2015, 190, 2255-2266.	0.8	0
3234	Theoretical study of the BINOL-zinc complex-catalyzed asymmetric inverse-electron-demand imino Diels-Alder reaction: mechanism and stereochemistry. <i>RSC Advances</i> , 2015, 5, 93318-93330.	1.7	2
3235	Modulation of inherent dynamical tendencies of the bisabolyl cation via preorganization in epi-isozizaene synthase. <i>Chemical Science</i> , 2015, 6, 2347-2353.	3.7	32
3236	Diels-Alder <i>versus</i> 1,3-dipolar cycloaddition pathways in the reaction of C <sub>20</sub> fullerene and 2-furan nitrile oxide. <i>Progress in Reaction Kinetics and Mechanism</i> , 2015, 40, 383-390.	1.1	15
3237	Kinetics and mechanism for OH-initiated gas-phase chemistry of $\pm$ -terpineol. <i>RSC Advances</i> , 2015, 5, 95096-95103.	1.7	5
3238	Adsorption and dissociation of H <sub>2</sub> on B12C6N6 cage. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 16347-16354.	3.8	7
3239	Theoretical study on the nitrate radical oxidation of methyl vinyl ether. <i>Computational and Theoretical Chemistry</i> , 2015, 1072, 72-78.	1.1	2

#	ARTICLE	IF	CITATIONS
3240	Enantioselective addition of aryl ketones and acetone to nitroalkenes organocatalyzed by carbamate-monoprotected cyclohexa-1,2-diamines. <i>Tetrahedron: Asymmetry</i> , 2015, 26, 970-979.	1.8	11
3241	Toward Understanding the Decomposition of Carbonyl Diazide (N <sub>3</sub> ) <sub>2</sub> O and Formation of Diazirone <i>cycl</i> -N <sub>2</sub> CO: Experiment and Computations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8903-8911.	1.1	14
3242	Quantum chemical study of mechanisms of organic reactions. <i>Russian Chemical Bulletin</i> , 2015, 64, 511-517.	0.4	4
3243	Computational Study on the "Heteroatom Bond Formation via Stille Cross-Coupling Reaction: Differences between Organoheterostannanes Me <sub>3</sub> SnAsPh <sub>2</sub> vs Me <sub>3</sub> SnPPH <sub>2</sub> . <i>Organometallics</i> , 2015, 34, 159-166.	1.1	9
3244	Theoretical study for OH radical-initiated atmospheric oxidation of ethyl acrylate. <i>Chemosphere</i> , 2015, 119, 626-633.	4.2	25
3245	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2034-2043.	1.5	15
3246	The multieffects of DMF and DBU on the [5+1] benzannulation of nitroethane and $\alpha$ -alkenyl ketene acetals: Hydrogen bonding and electrostatic interactions. <i>Journal of Computational Chemistry</i> , 2015, 36, 731-738.	1.5	6
3247	High-resolution XPS and DFT investigations into Al-modified Phillips CrOx/SiO <sub>2</sub> catalysts. <i>Journal of Molecular Catalysis A</i> , 2015, 401, 1-12.	4.8	19
3248	Theoretical study of the dimerization of aqueous beryllium cations. <i>Journal of Molecular Modeling</i> , 2015, 21, 6.	0.8	18
3249	Theoretical study of the reaction mechanism of CH <sub>3</sub> NO <sub>2</sub> with NO <sub>2</sub> , NO and CO: the bimolecular reactions that cannot be ignored. <i>Journal of Molecular Modeling</i> , 2015, 21, 13.	0.8	8
3250	<i>Ab Initio</i> Study of the Reaction of Ozone with Bromide Ion. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4482-4488.	1.1	13
3251	Effects of Helix Macrodipole and Local Interactions on Catalysis of Acyl Transfer by $\alpha$ -Helical Peptides. <i>ACS Catalysis</i> , 2015, 5, 1617-1622.	5.5	10
3252	Decomposition of fluorophosphoryl diazide: a joint experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6433-6439.	1.3	10
3253	The mechanism, electronic and ligand effects for reductive elimination from arylPd( $\eta$ -trifluoromethyl) complexes: a systematic DFT study. <i>Dalton Transactions</i> , 2015, 44, 4613-4622.	1.6	26
3254	Effect of CH/P Exchange on the Fluxional Behavior of Bullvalene, Semibullvalene, and Barbaralane: A DFT Investigation. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2015, 190, 1-10.	0.8	12
3255	A DFT study on the difference of C-H bond activation by Pd(II) and Pd(IV) complex. <i>Computational and Theoretical Chemistry</i> , 2015, 1056, 41-46.	1.1	6
3256	A computational investigation of the hydrogenation of imines catalyzed by rhodium thiolate complexes. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1-5.	1.0	6
3257	Theoretical Study of Mechanism and Stereoselectivity of Catalytic Kinugasa Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 2649-2660.	1.7	48

#	ARTICLE	IF	CITATIONS
3258	Theoretical investigation on the mechanism and dynamics of oxo exchange of neptunyl( $\nu$ ) hydroxide in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7537-7547.	1.3	2
3259	Restricted Hartree Fock using complex-valued orbitals: A long-known but neglected tool in electronic structure theory. <i>Journal of Chemical Physics</i> , 2015, 142, 024104.	1.2	26
3260	Role of Fluoride in Accelerating the Reactions of Dialkylstannylene Acetals. <i>Journal of Organic Chemistry</i> , 2015, 80, 2989-3002.	1.7	6
3261	Photoremoval of Protecting Groups: Mechanistic Aspects of 1,3-Dithiane Conversion to a Carbonyl Group. <i>Journal of Organic Chemistry</i> , 2015, 80, 2733-2739.	1.7	17
3262	Axial Coordination Dichotomy in Dirhodium Carbenoid Catalysis: A Curious Case of Cooperative Asymmetric Dual-Catalytic Approach toward Amino Esters. <i>Journal of Organic Chemistry</i> , 2015, 80, 2192-2197.	1.7	26
3263	Ab Initio Study of Guanine Damage by Hydroxyl Radical. <i>Journal of Physical Chemistry A</i> , 2015, 119, 377-382.	1.1	12
3264	Mechanistic Insight into the Dehydro-Diels-Alder Reaction of Styrene. <i>Journal of Organic Chemistry</i> , 2015, 80, 11686-11698.	1.7	47
3265	Theoretical Study on the Reactions of $(CF_3)_2CFOCH_3 + OH/Cl$ and Reaction of $(CF_3)_2CFOCHO$ with Cl Atom. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1256-1266.	1.1	15
3266	Bicyclobutonium Ions in Biosynthesis – Interconversion of Cyclopropyl-Containing Sterols from Orchids. <i>Journal of the American Chemical Society</i> , 2015, 137, 2085-2088.	6.6	22
3267	Direct and solvent-assisted keto-enol tautomerism and hydrogen-bonding interactions in 4-(m-chlorobenzylamino)-3-phenyl-4,5-dihydro-1H-1,2,4-triazol-5-one: a quantum-chemical study. <i>Journal of Molecular Modeling</i> , 2015, 21, 19.	0.8	11
3268	Efficient Synthesis of 5-Chalcogenyl-1,3,4-oxazin-2-ones by Chalcogen-Mediated Yne-Carbamate Cyclization: An Experimental and Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 1020-1027.	1.2	16
3269	A DFT Study of the CO Oxidation Mechanism on Al <sub>n</sub> Au (n = 1-12) Clusters. <i>Journal of Cluster Science</i> , 2015, 26, 505-527.	1.7	4
3270	Trichloroalane addition to bis(silyl)amino-silyliminoborines: a theoretical study. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 183-190.	1.2	0
3271	Uncovering the Mechanism of Homogeneous Methyl Methacrylate Formation with P,N Chelating Ligands and Palladium: Favored Reaction Channels and Selectivities. <i>Organometallics</i> , 2015, 34, 438-449.	1.1	57
3272	Hydrative trimerization of acetylene into 2-vinyl-1,3-butadiene in the KOH/DMSO system: a quantum chemical insight. <i>Tetrahedron Letters</i> , 2015, 56, 1063-1066.	0.7	5
3273	Solvent-Induced Reversal of Enantioselectivity in the Synthesis of Succinimides by the Addition of Aldehydes to Maleimides Catalysed by Carbamate-Monoprotected 1,2-Diamines. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 1218-1225.	1.2	44
3274	Deprotonated Purine Dissociation: Experiments, Computations, and Astrobiological Implications. <i>Journal of Physical Chemistry A</i> , 2015, 119, 334-343.	1.1	7
3275	Kinetics and mechanism of the reactions of OH radicals with p-nitroaniline in gas-phase and aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2015, 1055, 68-77.	1.1	11

#	ARTICLE	IF	CITATIONS
3276	New insights into dissociation of deprotonated 2,4-dinitrotoluene by combined high-resolution mass spectrometry and density functional theory calculations. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 29-34.	0.7	2
3277	An automated method to find transition states using chemical dynamics simulations. <i>Journal of Computational Chemistry</i> , 2015, 36, 222-234.	1.5	158
3278	An experimental and theoretical study of the gas phase kinetics of atomic chlorine reactions with CH <sub>3</sub> NH <sub>2</sub> , (CH <sub>3</sub> ) <sub>2</sub> NH, and (CH <sub>3</sub> ) <sub>3</sub> N. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 911-917.	1.3	29
3279	Theoretical mechanism for selective catalysis of ruthenium complex catalyzed hydroboration of terminal alkynes to Z-vinylboronates. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 59-67.	1.0	5
3280	CO <sub>2</sub> Capture and Separation from N <sub>2</sub> /CH <sub>4</sub> Mixtures by Co <sub>8</sub> /Co <sub>8</sub> <sup>+</sup> and M <sub>9</sub> /M <sub>9</sub> <sup>+</sup> (M = Ir, Rh, Ru) Clusters: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 796-805.	1.1	31
3281	Conformational composition, molecular structure and decomposition of difluorophosphoryl azide in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8784-8791.	1.3	15
3282	A Computational Study of the Mechanism and Kinetics for Gas-Phase Decomposition and Reactivity of the C <sub>4</sub> F <sub>9</sub> OCH <sub>2</sub> O Radical between 200 and 400 K. <i>Progress in Reaction Kinetics and Mechanism</i> , 2015, 40, 59-68.	1.1	1
3283	Understanding the Reactivity of Endohedral Metallofullerenes: C <sub>78</sub> versus Sc <sub>3</sub> N@C <sub>78</sub> . <i>Chemistry - A European Journal</i> , 2015, 21, 5760-5768.	1.7	45
3284	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. <i>Tetrahedron</i> , 2015, 71, 2421-2427.	1.0	24
3285	Regio- and diastereoselectivity of the 1,3-dipolar cycloaddition of $\hat{\pm}$ -aryl nitrene with methacrolein. A theoretical investigation. <i>RSC Advances</i> , 2015, 5, 22126-22134.	1.7	4
3286	Ab initio study in the hydration process of metaphosphoric acid: the importance of the pnictogen interactions. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	7
3287	On the mechanism of the preferential oxidation of carbon monoxide over Cu n Pd (n=3-12) catalysts. <i>Transition Metal Chemistry</i> , 2015, 40, 207-216.	0.7	2
3288	Mechanistic investigation of the reaction of thiourea with dialkyl acetylenedicarboxylates: a theoretical study. <i>Journal of Sulfur Chemistry</i> , 2015, 36, 422-433.	1.0	3
3289	Theoretical investigation of the mechanism of tritiated methane dehydrogenation reaction using nickel-based catalysts. <i>Fusion Engineering and Design</i> , 2015, 95, 91-98.	1.0	2
3290	Mechanistic Insights into the Cu(I)- and Cu(II)-Catalyzed Cyclization of <i>o</i> -Alkynylbenzaldehydes: The Solvent DMF and Oxidation State of Copper Affect the Reaction Mechanism. <i>Journal of Organic Chemistry</i> , 2015, 80, 6553-6563.	1.7	21
3291	A Theoretical Study of the Kinetics of the Hydrogen Atom Abstraction Reactions from Cyclopropane by H, O ( <sup>3</sup> P), and Cl ( <sup>2</sup> P <sub>3/2</sub> ) Atoms and OH Radicals. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 232-245.	1.0	3
3292	Computational investigation on NO <sub>3</sub> -initiated degradation of p,p'-DDE in atmosphere: Mechanism and kinetics. <i>Computational and Theoretical Chemistry</i> , 2015, 1068, 21-29.	1.1	1
3293	Unraveling the intramolecular cyclization mechanism of oxidized tryptophan in aqueous solution as a function of pH. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 8695-8702.	1.5	4

#	ARTICLE	IF	CITATIONS
3294	Fine-Tuning of $\hat{I}^2$ -Substitution to Modulate the Lowest Triplet Excited States: A Bioinspired Approach to Design Phosphorescent Metalloporphyrinoids. <i>Journal of the American Chemical Society</i> , 2015, 137, 10745-10752.	6.6	41
3295	Computational study of the gas phase reaction of hydrogen azide and corannulene: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2015, 1070, 94-101.	1.1	4
3296	The Gilded Edge in Acetylenic Scaffolding II: A Computational Study of the Transmetalation Processes Involved in Palladium-Catalyzed Cross-Couplings of Gold(I) Acetylides. <i>Organometallics</i> , 2015, 34, 3678-3685.	1.1	3
3297	Decomposition of O,S-dimethyl methylphosphonothiolate by ammonia on magnesium oxide: a theoretical study of catalytic detoxification of a chemical warfare agent. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20231-20249.	1.3	3
3298	Computational insights into the mechanism of iron carbonyl-catalyzed ethylene hydrosilylation or dehydrogenative silylation. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 66-76.	1.1	6
3299	Comprehensive Study of Methylation on the Silicon (100)-2 $\hat{A}$ -1 Surface: A Density Functional Approach. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4939-4952.	1.1	2
3300	Quantum Chemical Studies on Detail Mechanism of Nitrosylation of NAMI-A-HSA Adduct. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10456-10465.	1.2	3
3301	Theoretical Study on Internal Alkyne/Vinylidene Isomerization in Group 8 Transition-Metal Complexes. <i>Organometallics</i> , 2015, 34, 3934-3943.	1.1	26
3302	Hydrogen-release mechanisms in $\text{LiNH}_2\text{BH}_3\hat{A}\cdot\text{NH}_3\text{BH}_3$ : A theoretical study. <i>Journal of Molecular Structure</i> , 2015, 1081, 437-442.	1.8	5
3303	Mechanistic Understanding of the Divergent Reactivity of Cyclopropenes in Rh(III)-Catalyzed C $\hat{A}$ H Activation/Cycloaddition Reactions of <i>N</i> -Phenoxyacetamide and <i>N</i> -Pivaloxybenzamide. <i>Journal of Organic Chemistry</i> , 2015, 80, 8113-8121.	1.7	67
3304	Half-sandwich $\text{Ru}(\hat{I}^6\text{-C}_6\text{H}_6)$ complexes with chiral aroylthioureas for enhanced asymmetric transfer hydrogenation of ketones $\hat{A}$ experimental and theoretical studies. <i>Catalysis Science and Technology</i> , 2015, 5, 4790-4799.	2.1	28
3305	Icosahedral metallocarborane/carborane species derived from 1,1 $\hat{A}$ -bis(o-carborane). <i>Dalton Transactions</i> , 2015, 44, 5628-5637.	1.6	34
3306	Catalytic CO Oxidation on Single Pt-Atom Doped Aluminum Oxide Clusters: Electronegativity-Ladder Effect. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15414-15420.	1.5	40
3307	Theoretical study on the activity of hydrogen atom of imidazolium ring in ionic liquids. <i>Computational and Theoretical Chemistry</i> , 2015, 1067, 7-12.	1.1	2
3308	Mechanistic insights into the dehalogenation reaction of fluoroacetate/fluoroacetic acid. <i>Journal of Chemical Physics</i> , 2015, 142, 194301.	1.2	7
3309	Gold: Oxidative Addition to Au(I). <i>Springer Theses</i> , 2015, , 129-193.	0.0	0
3310	A Theoretical Investigation of 1-Butanol Unimolecular Decomposition. <i>Lecture Notes in Computer Science</i> , 2015, , 384-393.	1.0	1
3311	In silico study on the mechanism of formation of hydrazine and nitrogen in the reactions of excess hydroxylamine with 2,4-dinitrophenyl diethyl phosphate. <i>New Journal of Chemistry</i> , 2015, 39, 3558-3563.	1.4	1

#	ARTICLE	IF	CITATIONS
3312	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. <i>RSC Advances</i> , 2015, 5, 58464-58477.	1.7	53
3313	Mechanism and stereoselectivity of the Rh(III)-catalyzed cyclopropanation of diazooxindole: a density functional theory study. <i>RSC Advances</i> , 2015, 5, 57781-57791.	1.7	31
3314	Theoretical Investigations toward the Asymmetric Insertion Reaction of Diazoester with Aldehyde Catalyzed by N-Protonated Chiral Oxazaborolidine: Mechanisms and Stereoselectivity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8422-8431.	1.1	25
3315	Pyridine N-Oxide vs Pyridine Substrates for Rh(III)-Catalyzed Oxidative C-H Bond Functionalization. <i>Journal of the American Chemical Society</i> , 2015, 137, 9843-9854.	6.6	89
3316	Decomposition reaction rate of BCl <sub>3</sub> -CH <sub>4</sub> -H <sub>2</sub> in the gas phase. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	4
3317	Proton-Assisted Mechanism of NO Reduction on a Dinuclear Ruthenium Complex. <i>Inorganic Chemistry</i> , 2015, 54, 7181-7191.	1.9	19
3318	Investigation on the photodriven catalytic coupling reaction mechanism of p-aminothiophenol on the silver cluster. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550019.	1.8	3
3319	[DBU] and H <sub>2</sub> as effective catalyst form for 2,3-dihydropyrido[2,3-d]pyrimidin-4(1H)-ones: A DFT Study. <i>Journal of Computational Chemistry</i> , 2015, 36, 1295-1303.	1.5	14
3320	An example of a stepwise mechanism for the catalyst-free 1,3-dipolar cycloaddition between a nitrile oxide and an electron rich alkene. <i>Tetrahedron Letters</i> , 2015, 56, 4857-4863.	0.7	29
3321	Theoretical Investigation on Mechanistic and Kinetic Transformation of 2,2,4,4,5-Pentabromodiphenyl Ether. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6404-6411.	1.1	20
3322	Mechanistic Understanding of the Aryl-Dependent Ring Formations in Rh(III)-Catalyzed C-H Activation/Cycloaddition of Benzamides and Methylene cyclopropanes by DFT Calculations. <i>Organometallics</i> , 2015, 34, 3012-3020.	1.1	68
3323	C-doped boron nitride fullerene as a novel catalyst for acetylene hydrochlorination: a DFT study. <i>RSC Advances</i> , 2015, 5, 56348-56355.	1.7	41
3324	Mechanistic insights into the synergistic catalysis by Au(I), Ga(III), and counterions in the Nakamura reaction. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 7412-7420.	1.5	28
3325	Gas-phase reaction of CeVO <sub>5</sub> cluster ions with C <sub>2</sub> H <sub>4</sub> : the reactivity of cluster bonded peroxides. <i>Dalton Transactions</i> , 2015, 44, 3128-3135.	1.6	9
3326	Water-catalysis in the gas phase reaction of dithioformic acid with hydroxyl radical: global reaction route mapping of oxidative pathways for hydrogen abstraction. <i>RSC Advances</i> , 2015, 5, 50989-50998.	1.7	6
3327	Theoretical studies of cobalt(I)-catalyzed hydroacylation of vinylsilanes and alkyl aldehydes. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 431-436.	0.9	6
3328	Atmospheric oxidation of methyl and ethyl tert-butyl ethers initiated by hydroxyl radicals. A quantum chemistry study. <i>Fuel</i> , 2015, 159, 269-279.	3.4	11
3329	Enzymatic hydroxylation of an unactivated methylene C-H bond guided by molecular dynamics simulations. <i>Nature Chemistry</i> , 2015, 7, 653-660.	6.6	100

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3330	VUV Photofragmentation of CH <sub>2</sub> I <sub>2</sub> : The [CH <sub>2</sub> I] <sup>+</sup> Iso-diodomethane Intermediate in the I-Loss Channel from [CH <sub>2</sub> I <sub>2</sub> ] <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2015, 119, 3704-3709.	1.1	12
3331	Syntheses of Tricyanofluoroborates M[BF(CN) <sub>3</sub> ] (M = Na, K): (CH <sub>3</sub> ) <sub>3</sub> SiCl Catalysis, Countercation Effect, and Reaction Intermediates. <i>Inorganic Chemistry</i> , 2015, 54, 3403-3412.	1.9	31
3332	Infrared Matrix Isolation Study of the Thermal and Photochemical Reactions of Ozone with Trimethylgallium. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2834-2844.	1.1	3
3333	Theoretical Investigation on the Reaction between OH Radical and 4,4-Dimethyl-1-pentene in the Presence of O <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2015, 119, 4065-4072.	1.1	9
3334	Rate coefficients for the reaction of OH radicals with cis-3-hexene: an experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8714-8722.	1.3	6
3335	Theoretical investigation of the hydrogen shift reactions in peroxy radicals derived from the atmospheric decomposition of 3-methyl-3-buten-1-ol (MBO331). <i>Chemical Physics Letters</i> , 2015, 619, 236-240.	1.2	19
3336	The origin of regio- and stereoselectivity in the 1,3-dipolar cycloaddition of nitrile oxides with C <sub>1</sub> -substituted 7-oxabenzonorbornadienes, a DFT study. <i>RSC Advances</i> , 2015, 5, 38489-38498.	1.7	14
3337	Theoretical study on the thermal decomposition and isomerization of 3-Me-1-heptyl radical. <i>Computational and Theoretical Chemistry</i> , 2015, 1063, 10-18.	1.1	2
3338	The Unexpected Mechanism Underlying the High-Valent Mono-oxo-rhenium(V) Hydride Catalyzed Hydrosilylation of C≡N Functionalities: Insights from a DFT Study. <i>ChemPhysChem</i> , 2015, 16, 1052-1060.	1.0	5
3339	3H-Pyrroles from ketoximes and acetylene: synthesis, stability and quantum-chemical insight. <i>Tetrahedron</i> , 2015, 71, 3273-3281.	1.0	25
3340	Theoretical investigation on SnCl <sub>4</sub> -catalyzed tandem dimerization/oxy-2-azonia-Cope rearrangements between <sup>1,2</sup> , <sup>1,3</sup> -unsaturated ketones and imines. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	1
3341	Quantum chemical study of the isomerization of 24-methylenecycloartanol, a potential marker of olive oil refining. <i>Journal of Molecular Modeling</i> , 2015, 21, 111.	0.8	1
3342	Mechanism of CO preferential oxidation catalyzed by Cu n Pt (n=12): a DFT study. <i>Research on Chemical Intermediates</i> , 2015, 41, 10049-10066.	1.3	4
3343	Synthesis of radiolabelled aryl azides from diazonium salts: experimental and computational results permit the identification of the preferred mechanism. <i>Chemical Communications</i> , 2015, 51, 8954-8957.	2.2	18
3344	A DFT Study of Inter- and Intramolecular Aryne Ene Reactions. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2826-2834.	1.2	28
3345	Understanding Bond Formation in Polar One-Step Reactions. Topological Analyses of the Reaction between Nitrones and Lithium Ynolates. <i>Journal of Organic Chemistry</i> , 2015, 80, 4076-4083.	1.7	32
3346	Mechanistic Studies of Copper(I)-Catalyzed 1,3-Halogen Migration. <i>Journal of the American Chemical Society</i> , 2015, 137, 5346-5354.	6.6	49
3347	A quantum mechanical study of the mechanism and stereoselectivity of the N-heterocyclic carbene catalyzed [4 + 2] annulation reaction of enals with azodicarboxylates. <i>Organic Chemistry Frontiers</i> , 2015, 2, 874-884.	2.3	48

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3348	Synthesis of arylboronates by boron-induced ipso-deantimonation of triarylstibanes with boron trihalides and its application in one-pot two-step transmetalation/cross-coupling reactions. <i>Journal of Organometallic Chemistry</i> , 2015, 788, 9-16.	0.8	7
3349	The mechanism of dehydration in chromophore maturation of wild-type green fluorescent protein: A theoretical study. <i>Chemical Physics Letters</i> , 2015, 631-632, 42-46.	1.2	9
3350	Free-radical copolymerisation of acrylamides, acrylates, and $\hat{1}\pm$ -olefins. <i>Molecular Physics</i> , 2015, 113, 1809-1822.	0.8	2
3351	Theoretical study of catalytic oxidation of CO on free Pd <sub>x</sub> O <sub>2</sub> <sup>+</sup> (x) Tj ETQq1 1.0.784314 rgBT /Ov	1.7	5
3352	Catalytic reduction of NO by CO on Rh <sub>4</sub> <sup>+</sup> clusters: a density functional theory study. <i>Catalysis Science and Technology</i> , 2015, 5, 3203-3215.	2.1	12
3353	Mechanism and regioselectivity of 1,3-dipolar cycloaddition reactions of bicyclic monoterpenes with aryl and heteroaryl nitrile oxides: a DFT study. <i>Canadian Journal of Chemistry</i> , 2015, 93, 749-753.	0.6	7
3354	Influence of the N <sup>-</sup> N Coligand: C <sup>-</sup> C Coupling Instead of Formation of Imidazol-2-yl Complexes at {Mo( $\hat{1}$ <sup>3</sup> -allyl)(CO) <sub>2</sub> } Fragments. <i>Theoretical and Experimental Studies. Inorganic Chemistry</i> , 2015, 54, 2580-2590.	1.9	8
3355	Mechanisms of Reactions of Sulfur Hydride Hydroxide: Tautomerism, Condensations, and C-Sulfonylation and O-Sulfonylation of 2,4-Pentanedione. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3500-3517.	1.1	7
3356	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10715-10725.	1.3	20
3357	Direct Detection of a Triplet Vinylnitrene, 1,4-Naphthoquinone-2-yl nitrene, in Solution and Cryogenic Matrices. <i>Journal of the American Chemical Society</i> , 2015, 137, 4207-4214.	6.6	29
3358	Ethanol Dehydration in HZSM-5 Studied by Density Functional Theory: Evidence for a Concerted Process. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3604-3614.	1.1	44
3359	A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4214-4223.	1.1	28
3360	Theoretical insight into the C <sup>-</sup> H and C <sup>-</sup> C scission mechanism of ethane on a tetrahedral Pt <sub>4</sub> subnanocluster. <i>RSC Advances</i> , 2015, 5, 40978-40988.	1.7	4
3361	A density functional theory study of the Cu <sup>+</sup> ·(CO) <sub>n</sub> (n = 1-3) complexes. <i>Journal of Coordination Chemistry</i> , 2015, 68, 1528-1543.	0.8	8
3362	Theoretical study on the mechanism of self-cleavage reaction of the glmS ribozyme. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	1
3363	Isomerisation of nido-[C <sub>2</sub> B <sub>10</sub> H <sub>12</sub> ] <sup>2-</sup> dianions: unprecedented rearrangements and new structural motifs in carborane cluster chemistry. <i>Chemical Science</i> , 2015, 6, 3117-3128.	3.7	24
3364	Mechanism and Kinetics of Low-Temperature Oxidation of a Biodiesel Surrogate: Methyl Propanoate Radicals with Oxygen Molecule. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3689-3703.	1.1	24
3365	Feasibility of Intramolecular Proton Transfers in Terpene Biosynthesis - Guiding Principles. <i>Journal of the American Chemical Society</i> , 2015, 137, 4134-4140.	6.6	31



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3366	Highly Chemoselective and Versatile Method for Direct Conversion of Carboxylic Acids to Ketones Utilizing Zinc Ate Complexes. <i>Chemistry - an Asian Journal</i> , 2015, 10, 1286-1290.	1.7	9
3367	Density Functional Theory Study of Rh(III)-Catalyzed C-H Activations and Intermolecular Annulations between Benzamide Derivatives and Allenes. <i>Inorganic Chemistry</i> , 2015, 54, 3958-3969.	1.9	25
3368	Gold-Catalysed Synthesis of Exocyclic Vinylogous Amides and $\beta$ -Amino Ketones: A Detailed Study on the 5 $\rightarrow$ exo/6 $\rightarrow$ endo Selectivity, Methodology and Scope. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3251-3265.	1.2	23
3369	Influence of chlorine coordination number on the catalytic mechanism of ruthenium chloride catalysts in the acetylene hydrochlorination reaction: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7720-7730.	1.3	35
3370	How rhodium (III) complexes catalyze alkenylation of C(sp <sup>3</sup> )-H bond of 8-methylquinolines. <i>Journal of Organometallic Chemistry</i> , 2015, 787, 1-7.	0.8	6
3371	A density functional theory analysis of the molecular hydrogen dissociation on Al <sub>n</sub> Pt (n = 1-12) clusters. <i>Journal of Structural Chemistry</i> , 2015, 56, 608-618.	0.3	2
3372	Advanced NMR Techniques: Defining Carbohydrate Structures and Ligand-Receptor Interactions. , 2015, , 121-146.		0
3373	Strong chemisorption of CO on M@B <sub>n</sub> (M = Co, Ir, Rh, Ru, Ta, Nb, Tj) ETQq1 1 0.784314 rgBT /Ov 82524-82530.	1.7	9
3374	Density Functional Theory Study of Cyanoetheneselenol: A Molecule of Astrobiological Interest. <i>Origins of Life and Evolution of Biospheres</i> , 2015, 45, 455-468.	0.8	0
3376	Atmospheric chemistry of alkyl iodides: theoretical studies on the mechanisms and kinetics of CH <sub>3</sub> I/C <sub>2</sub> H <sub>5</sub> I + NO <sub>3</sub> reactions. <i>RSC Advances</i> , 2015, 5, 88087-88095.	1.7	13
3377	Bingel-Hirsch Reaction on Sc <sub>2</sub> @C <sub>66</sub> : A Highly Regioselective Bond Neighboring to Unsaturated Linear Triquinanes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 26196-26201.	1.5	8
3378	A quantum chemical study of unexpected reaction of $\beta$ -chloroacyl chlorides with 1,2-dichloroethylene in the presence of aluminum chloride. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 116-122.	1.1	1
3379	Ethylene adsorption and transformation on zeolite Ga <sup>+</sup> /ZSM-5. <i>Russian Chemical Bulletin</i> , 2015, 64, 278-283.	0.4	2
3380	Trimerization of Alkynes in the Presence of a Hydrotris(pyrazolyl)borate Iridium Catalyst and the Effect of Substituent Groups on the Reaction Mechanism: A Computational Study. <i>Organometallics</i> , 2015, 34, 4965-4974.	1.1	18
3381	Hydrogen abstraction mechanisms and reaction rates of toluene+NO <sub>3</sub> . <i>Journal of Molecular Modeling</i> , 2015, 21, 207.	0.8	4
3382	Mechanism for the Reaction of a Tungsten-Germolyne Complex with $\beta$ , $\beta$ -Unsaturated Ketones: A DFT Study. <i>Journal of Chemical Sciences</i> , 2015, 127, 1477-1483.	0.7	2
3383	Heuristics-Guided Exploration of Reaction Mechanisms. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5712-5722.	2.3	127
3384	Mechanistic study on the cellulose dissolution in ionic liquids by density functional theory. <i>Chinese Journal of Chemical Engineering</i> , 2015, 23, 1894-1906.	1.7	34

#	ARTICLE	IF	CITATIONS
3385	Molecular pathways of SOCl <sub>2</sub> hydrolysis within mono- and diaqua complexes. A quantum chemical study. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 56-65.	1.1	1
3386	Dual Gold Catalysis: Stepwise Catalyst Transfer via Dinuclear Clusters. <i>Journal of the American Chemical Society</i> , 2015, 137, 10668-10676.	6.6	88
3387	Structure and spectroscopic properties of neutral and cationic tetratomic [C,H,N,Zn] isomers: A theoretical study. <i>Journal of Chemical Physics</i> , 2015, 142, 184301.	1.2	8
3388	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. <i>RSC Advances</i> , 2015, 5, 37119-37129.	1.7	23
3389	Competing Mechanisms, Substituent Effects, and Regioselectivities of Nickel-Catalyzed [2 + 2 + 2] Cycloaddition between Carbonyne and Alkynes: A DFT Study. <i>Journal of Organic Chemistry</i> , 2015, 80, 9108-9117.	1.7	16
3390	Thermal and Photolytic Transformation of NHC-B,N-Heterocycles: Controlled Generation of Blue Fluorescent 1,3-Azaborinine Derivatives and 1 <i>H</i> -imidazo[1,2- <i>a</i> ]indoles by External Stimuli. <i>Chemistry - A European Journal</i> , 2015, 21, 13961-13970.	1.7	31
3391	Theoretical investigation of the mechanism and kinetics of the CH <sub>3</sub> NH <sub>2</sub> + O(3P) reaction. <i>Progress in Reaction Kinetics and Mechanism</i> , 2015, 40, 249-260.	1.1	1
3392	Computational study on mechanisms of the anticancer drug: Cisplatin and novel polynuclear platinum(II) interaction with sulfur-donor biomolecules and DNA purine bases. <i>Computational and Theoretical Chemistry</i> , 2015, 1074, 36-49.	1.1	9
3393	Understanding the participation of 3-nitropyridine in polar Diels-Alder reactions. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2015, 1072, 37-42.	1.1	13
3394	A DFT study of the mechanism of Brønsted acid catalysed Povarov reactions. <i>Tetrahedron</i> , 2015, 71, 9339-9345.	1.0	18
3395	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. <i>RSC Advances</i> , 2015, 5, 84797-84809.	1.7	21
3396	The Kinetics of the Reaction C <sub>2</sub> H <sub>5</sub> <sup>+</sup> + H <sub>2</sub> → C <sub>2</sub> H <sub>6</sub> <sup>+</sup> + H over an Extended Temperature Range (213–623 K): Experiment and Modeling. <i>Zeitschrift Fur Physikalische Chemie</i> , 2015, 229, 1475-1501.		
3397	Theoretical Investigation of the Methanol Decomposition by Fe <sup>+</sup> and Fe(C <sub>2</sub> H <sub>4</sub> ) <sup>+</sup> : A σ-Type Ligand Effect. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10204-10211.	1.1	4
3398	Catalytic oxidation of CO by N <sub>2</sub> O on neutral Y <sub>2</sub> MO <sub>5</sub> (M = Y, Al) clusters: a density functional theory study. <i>RSC Advances</i> , 2015, 5, 76651-76659.	1.7	12
3399	Unusual Benzyl Migration Reactivity in NHC-Bearing Group 4 Metal Chelates: Synthesis, Characterization, and Mechanistic Investigations. <i>Organometallics</i> , 2015, 34, 4854-4863.	1.1	25
3400	Computational study on the mechanism and enantioselectivity of Rh <sub>2</sub> (S-PTAD) <sub>4</sub> catalyzed asymmetric [4+3] cycloaddition between vinylcarbenoids and dienes. <i>RSC Advances</i> , 2015, 5, 83459-83470.	1.7	8
3401	Imidazolium Sulfonates as Environmental-Friendly Catalytic Systems for the Synthesis of Biologically Active 2-Amino-4 <i>H</i> -chromenes: Mechanistic Insights. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12042-12049.	1.2	17
3402	Influence of the double bond on the hydrogen abstraction reactions of methyl esters with hydrogen radical: an ab initio and chemical kinetic study. <i>RSC Advances</i> , 2015, 5, 68314-68325.	1.7	23

#	ARTICLE	IF	CITATIONS
3403	Theoretical studies of nickel-catalyzed ring-opening hydroacylation of methylenecyclopropanes and benzaldehydes. <i>Journal of Molecular Modeling</i> , 2015, 21, 203.	0.8	1
3404	Insights into the Unexpected Chemoselectivity for the N-Heterocyclic Carbene-Catalyzed Annulation Reaction of Allenals with Chalcones. <i>Journal of Organic Chemistry</i> , 2015, 80, 8619-8630.	1.7	37
3405	Quantum-Chemical Calculation of Carbododecahedron Formation in Carbon Plasma. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9133-9139.	1.1	8
3406	Reactions of Azine Anions with Nitrogen and Oxygen Atoms: Implications for Titan's Upper Atmosphere and Interstellar Chemistry. <i>Journal of the American Chemical Society</i> , 2015, 137, 10700-10709.	6.6	23
3407	Catalytic mechanisms of Au <sub>11</sub> and Au <sub>11</sub> -nPt <sub>n</sub> (n=1-2) clusters: a DFT investigation on the oxidation of CO by O <sub>2</sub> . <i>Journal of Molecular Modeling</i> , 2015, 21, 230.	0.8	10
3408	1,3-Dipolar cycloaddition of nitrones to transition metal-bound isocyanides: DFT and HSAB principle theoretical model together with an analysis of vibrational spectra. <i>Journal of Organometallic Chemistry</i> , 2015, 797, 8-12.	0.8	14
3409	Gas-Phase Reactivity of Cesium-Containing Species by Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9373-9384.	1.1	6
3410	Mechanistic Studies on Stereoselective Organocatalytic Direct $\hat{I}^2$ -C-H Activation in an Aliphatic Chain by Chiral N-Heterocyclic Carbenes. <i>ACS Catalysis</i> , 2015, 5, 5794-5802.	5.5	37
3411	Study of the competitive mechanisms of cyclohexane dehydrogenation by gas-phase Ni <sub>2</sub> + cationic dimer: one-face dehydrogenation versus flip dehydrogenation. <i>Journal of Molecular Modeling</i> , 2015, 21, 152.	0.8	4
3412	Multicomponent Reaction of <i>Z</i> -Chlorooximes, Isocyanides, and Hydroxylamines as Hypernucleophilic Traps. A One-Pot Route to Aminodioximes and Their Transformation into 5-Amino-1,2,4-oxadiazoles by Mitsunobu-Beckmann Rearrangement. <i>Journal of Organic Chemistry</i> , 2015, 80, 9652-9661.	1.7	21
3413	The reactivity of stoichiometric tungsten oxide clusters towards carbon monoxide: the effects of cluster sizes and charge states. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11499-11508.	1.3	7
3414	Kinetic and mechanistic investigations of the thermal decomposition of methyl-substituted cycloalkyl radicals. <i>RSC Advances</i> , 2015, 5, 28044-28053.	1.7	1
3415	Hydrolysis reaction of 2,4-dichlorophenoxyacetic acid. A kinetic and computational study. <i>Chemical Physics Letters</i> , 2015, 639, 57-62.	1.2	4
3416	Radical Mechanism of Isocyanide-Alkyne Cycloaddition by Multicatalysis of Ag <sub>2</sub> CO <sub>3</sub> , Solvent, and Substrate. <i>ACS Catalysis</i> , 2015, 5, 6177-6184.	5.5	54
3417	The effect of (H <sub>2</sub> O) <sub>n</sub> (n=1-2) or H <sub>2</sub> S on the hydrogen abstraction reaction of H <sub>2</sub> S by OH radicals in the atmosphere. <i>Computational and Theoretical Chemistry</i> , 2015, 1069, 77-85.	1.1	25
3418	Hydrogenation of biomass-derived levulinic acid to $\hat{I}^3$ -valerolactone catalyzed by PNP-Ir pincer complexes: A computational study. <i>Journal of Organometallic Chemistry</i> , 2015, 797, 165-170.	0.8	13
3419	Exploring the mechanism of isomerisation and water-migration in the water-complexes of amino-acid <i>L</i> -proline: electrostatic potential and vibrational analysis. <i>RSC Advances</i> , 2015, 5, 82587-82604.	1.7	7
3420	A theoretical investigation into thiophenic derivative cracking mechanism over acidic and cation-exchanged beta zeolites. <i>Computational and Theoretical Chemistry</i> , 2015, 1074, 112-124.	1.1	3

#	ARTICLE	IF	CITATIONS
3421	Photoelectron Imaging Spectroscopy of AuC <sub>3</sub> H <sup>+</sup> Anions: Four Isomers. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11265-11270.	1.1	11
3422	Effect of Steric Congestion on the Stepwise Character and Synchronicity of a 1,3-Dipolar Reaction of a Nitrile Ylide and an Olefin. <i>Journal of Chemical Research</i> , 2015, 39, 640-644.	0.6	7
3423	Origin of Stereodivergence in Cooperative Asymmetric Catalysis with Simultaneous Involvement of Two Chiral Catalysts. <i>Journal of the American Chemical Society</i> , 2015, 137, 15712-15722.	6.6	99
3424	Mechanistic and stereoselectivity study for the reaction of trifluoropyruvates with arylpropenes catalyzed by a cationic Lewis acid rhodium complex. <i>RSC Advances</i> , 2015, 5, 100147-100158.	1.7	15
3425	Regio- and Stereoselective 1,3-Dipolar Cycloaddition of Cyclic Azomethine Imines to Platinum(IV)-Bound Nitriles Giving 1,2,4-Triazoline Species. <i>Inorganic Chemistry</i> , 2015, 54, 11018-11030.	1.9	12
3426	Theoretical Study on the Catalytic Reduction Mechanism of NO by CO on Tetrahedral Rh <sub>4</sub> Subnanocluster. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11548-11564.	1.1	13
3427	Theoretical study of the decomposition mechanism of a series of group III triazides X(N <sub>3</sub> ) <sub>3</sub> (X = B, Al, Ga). <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1.0 68-76.		0
3428	A New Series of Antibacterial Nitrosopyrimidines: Synthesis and Structure-Activity Relationship. <i>Archiv Der Pharmazie</i> , 2015, 348, 68-80.	2.1	7
3429	Mechanism of the Gaseous Hydrolysis Reaction of SO <sub>2</sub> : Effects of NH <sub>3</sub> versus H <sub>2</sub> O. <i>Journal of Physical Chemistry A</i> , 2015, 119, 102-111.	1.1	61
3430	Photolysis of acetophenone derivatives with cyclopropyl substituents. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 137-146.	0.9	1
3431	Adsorption and Dissociation of H <sub>2</sub> on B <sub>n</sub> and MgB <sub>n</sub> (n = 7) Clusters: A DFT Investigation. <i>Journal of Cluster Science</i> , 2015, 26, 983-999.	1.7	9
3432	Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1628-1635.	1.1	12
3433	Synthesis of the ABC fragment of calyciphylline A-type Daphniphyllum alkaloids. <i>Tetrahedron</i> , 2015, 71, 3642-3651.	1.0	31
3434	Theoretical investigation on atmospheric reaction of atomic O(3P) with acrylonitrile. <i>Computational and Theoretical Chemistry</i> , 2015, 1052, 17-25.	1.1	3
3435	DFT and theoretical kinetics studies on the reaction of nitrate radical with $\alpha$ -pinene and $\beta$ -pinene. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 123-128.	1.1	5
3436	Reaction sampling and reactivity prediction using the stochastic surface walking method. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2757-2769.	1.3	66
3437	Computational investigation of hydrogen storage on scandium-acetylene system. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 420-428.	3.8	29
3438	Pyrolysis of ethanol: A shock-tube/TOF-MS and modeling study. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 465-472.	2.4	37

#	ARTICLE	IF	CITATIONS
3439	Phototautomerization on the Singlet and Triplet Surface in <i>o</i> -Hydroxyacetophenone Derivatives in Polar Solvents. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2668-2676.	1.2	9
3440	A computational study on the hydrogenation of CO <sub>2</sub> catalyzed by a tetraphos-ligated cobalt complex: monohydride vs. dihydride. <i>Catalysis Science and Technology</i> , 2015, 5, 1006-1013.	2.1	23
3441	Divergent Reactivity of Homologue <i>ortho</i> -Allenylbenzaldehydes Controlled by the Tether Length: Chromone versus Chromene Formation. <i>Chemistry - A European Journal</i> , 2015, 21, 1533-1541.	1.7	15
3442	Theoretical study on the mechanism of reaction of novel iminoether-containing Pt(II) anticancer drugs with biological targets. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 24-34.	1.1	9
3443	Theoretical study of the corannulene ozonolysis and evaluation of the various reaction paths. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 72-78.	1.1	7
3444	Mechanism and kinetics of low-temperature oxidation of a biodiesel surrogate methyl acetate radicals with molecular oxygen. <i>Structural Chemistry</i> , 2015, 26, 431-444.	1.0	13
3445	Polar Diels-Alder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study. <i>Journal of Molecular Structure</i> , 2015, 1079, 47-53.	1.8	26
3446	Theoretical study on the reaction mechanisms of the aldol-condensation of 5-hydroxymethylfurfural with acetone catalyzed by MgO and MgO <sup>+</sup> . <i>Catalysis Today</i> , 2015, 245, 100-107.	2.2	15
3447	A low content Au-based catalyst for hydrochlorination of C <sub>2</sub> H <sub>2</sub> and its industrial scale-up for future PVC processes. <i>Green Chemistry</i> , 2015, 17, 356-364.	4.6	104
3448	A mechanistic study of the decomposition and reactivity of the C <sub>4</sub> F <sub>9</sub> OC <sub>2</sub> H <sub>4</sub> radical derived from HFE-7200 between 200 and 400 K. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 301-308.	1.1	1
3449	Dynamic behavior of rearranging carbocations – implications for terpene biosynthesis. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 377-390.	1.3	79
3450	DFT study on the regio- and stereo-selectivity of the Diels-Alder reaction between a cycloprop-2-ene carboxylate and some cyclic 1,3-dienes. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 193-204.	1.1	3
3451	Theoretical Mechanism Study on the Reaction of FOO Radical with NO. <i>Journal of Chemistry</i> , 2016, 2016, 1-6.	0.9	1
3452	Protonation Sites, Tandem Mass Spectrometry and Computational Calculations of <i>o</i> -Carbonyl Carbazolequinone Derivatives. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1071.	1.8	3
3453	New Vistas on the Anionic Polymerization of Styrene in Non-Polar Solvents by Means of Density Functional Theory. <i>Polymers</i> , 2016, 8, 371.	2.0	7
3454	Theoretical Study on Gas Phase Reactions of OH Hydrogen-Abstraction from Formyl Fluoride with Different Catalysts. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 325-334.	0.6	2
3455	Theoretical Studies on Mechanism and Rate Constant of Gas Phase Hydrolysis of Glyoxal Catalyzed by Sulfuric Acid. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 335-343.	0.6	9
3456	Theoretical Study on Mechanism and Kinetics of Reaction of O(3P) with Propane. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 430-436.	0.6	5

#	ARTICLE	IF	CITATIONS
3457	To bridge or not to bridge: The role of sulfuric acid in the Beckmann rearrangement. <i>Chemical Physics Letters</i> , 2016, 659, 100-104.	1.2	5
3458	Methane Activation Mediated by a Series of Cerium–Vanadium Bimetallic Oxide Cluster Cations: Tuning Reactivity by Doping. <i>ChemPhysChem</i> , 2016, 17, 1112-1118.	1.0	6
3459	Investigation of agostic interaction through NBO analysis and its impact on $\beta^2$ -hydride elimination and dehydrogenation: a DFT approach. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	10
3460	Perfluorinated [8]Circulene and Its Nonplanar Fragments: Synthesis, Structural Analysis, and Properties. <i>Chemistry - A European Journal</i> , 2016, 22, 9198-9208.	1.7	27
3461	Interplay between aromaticity and strain in double group transfer reactions to 1,2-benzyne. <i>Journal of Computational Chemistry</i> , 2016, 37, 1265-1273.	1.5	20
3462	A mechanistic insight into the effect of piperidine as an organocatalyst on the [3 + 2] cycloaddition reaction of benzalacetone with phenyl azide from a computational study. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 7324-7333.	1.5	5
3463	Reactivity and Selectivity of Bowl-Shaped Polycyclic Aromatic Hydrocarbons: Relationship to $C_{60}$ . <i>Chemistry - A European Journal</i> , 2016, 22, 1368-1378.	1.7	31
3464	Mechanism of Ylide Transfer to $\alpha$ -Carbonyl Compounds: Density Functional Calculations. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 830-839.	1.2	3
3465	Understanding the Reactivity of Planar Polycyclic Aromatic Hydrocarbons: Towards the Graphene Limit. <i>Chemistry - A European Journal</i> , 2016, 22, 10572-10580.	1.7	27
3466	Factors Controlling the Reactivity and Selectivity of the Diels–Alder Reactions Involving 1,2-Azaborines. <i>Journal of Organic Chemistry</i> , 2016, 81, 6554-6562.	1.7	18
3467	A computational study on the N-heterocyclic carbene-catalyzed $C_{sp^2} \rightarrow C_{sp^3}$ bond activation/[4+2] cycloaddition cascade reaction of cyclobutenones with imines: a new application of the conservation principle of molecular orbital symmetry. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19933-19943.	1.3	36
3468	Insights into the Cascade Reaction of CO and Heteroallenes Mediated by Dinitrogen Hafnocene Complexes: The Indirect Effect of Nitride's Nucleophilicity. <i>Chemistry - A European Journal</i> , 2016, 22, 4743-4747.	1.7	1
3469	Multiple CO Oxidation Promoted by $Au_2$ Dimers in $Au_2TiO_4$ Cluster Anions. <i>Chemistry - A European Journal</i> , 2016, 22, 9024-9029.	1.7	21
3470	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12417-12419.	1.2	1
3471	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4977-4979.	2.1	0
3472	The redox mechanism of $Np^{VI}$ with hydrazine: a DFT study. <i>RSC Advances</i> , 2016, 6, 109045-109053.	1.7	10
3473	Reactions of Manganese and Rhenium Vinylidene Complexes with Hydrophosphoryl Compounds. <i>Organometallics</i> , 2016, 35, 3903-3913.	1.1	6
3474	Mechanism of thermal decomposition of allyltrichlorosilane with formation of three labile intermediates: dichlorosilylene, allyl radical, and atomic chlorine. <i>Russian Chemical Bulletin</i> , 2016, 65, 1216-1224.	0.4	2

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3475	Communication: "Position" does matter: The photofragmentation of the nitroimidazole isomers. <i>Journal of Chemical Physics</i> , 2016, 145, 191102.	1.2	25
3476	The excited-state structure, vibrations, lifetimes, and nonradiative dynamics of jet-cooled 1-methylcytosine. <i>Journal of Chemical Physics</i> , 2016, 145, 134307.	1.2	16
3477	Insights into the Competing Mechanisms and Origin of Enantioselectivity for N-Heterocyclic Carbene-Catalyzed Reaction of Aldehyde with Enamide. <i>Scientific Reports</i> , 2016, 6, 38200.	1.6	19
3478	Mechanism and kinetic properties for the gas-phase ozonolysis of Î²-ionone. <i>RSC Advances</i> , 2016, 6, 114256-114263.	1.7	1
3479	Hydrocarbons and clusters of group 13 elements, high energy production, and low CO <sub>2</sub> release, an energetic analysis. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 23196-23203.	3.8	1
3480	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9679-9681.	1.1	3
3481	Celebrating Our 120th Anniversary. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27731-27733.	1.5	0
3482	Role of water clusters in the reaction of the simplest Criegee intermediate CH <sub>2</sub> OO with water vapour. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	22
3483	Theoretical study on the mechanism of the gas phase reaction of methoxybenzene with ozone. <i>RSC Advances</i> , 2016, 6, 113561-113569.	1.7	17
3484	Reactions of substituted benzene anions with N and O atoms: Chemistry in Titan's upper atmosphere and the interstellar medium. <i>Journal of Chemical Physics</i> , 2016, 144, 214304.	1.2	13
3485	Theoretical study of the gaseous hydrolysis of NO <sub>2</sub> in the presence of NH <sub>3</sub> as a source of atmospheric HONO. <i>Environmental Chemistry</i> , 2016, 13, 611.	0.7	21
3486	The role of the second order Jahn-Teller effect in the thermal reactions of ethylene. <i>Russian Journal of Physical Chemistry B</i> , 2016, 10, 884-889.	0.2	0
3487	Theoretical study of the mechanism of stable phosphorus ylides derived from 2-aminothiophenol in the presence of different dialkyl acetylenedicarboxylates. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016, 191, 1063-1068.	0.8	3
3488	Roles of the active species involved in the photocatalytic oxidation of benzyl alcohol into benzaldehyde on TiO <sub>2</sub> under UV light: Experimental and DFT studies. <i>Journal of Molecular Catalysis A</i> , 2016, 420, 82-87.	4.8	29
3489	Oxidation of SO <sub>2</sub> to SO <sub>3</sub> by Cerium Oxide Cluster Cations Ce <sub>2</sub> O <sub>4</sub> <sup>+</sup> and Ce <sub>3</sub> O <sub>6</sub> <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2016, 120, 3843-3848.	1.1	20
3490	Mesoporous niobiosilicate NbMCF modified with alkali metals in the synthesis of chromene derivatives. <i>Catalysis Today</i> , 2016, 277, 133-142.	2.2	17
3491	Operando Molecular Spectroscopy During Ethylene Polymerization by Supported CrO <sub>x</sub> /SiO <sub>2</sub> Catalysts: Active Sites, Reaction Intermediates, and Structure-Activity Relationship. <i>Topics in Catalysis</i> , 2016, 59, 725-739.	1.3	51
3492	The mechanism and kinetic studies for Cl-initiated oxidation of allyl acetate in troposphere. <i>Computational and Theoretical Chemistry</i> , 2016, 1087, 48-56.	1.1	7

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3493	Curly arrows meet electron density transfers in chemical reaction mechanisms: from electron localization function (ELF) analysis to valence-shell electron-pair repulsion (VSEPR) inspired interpretation. <i>Chemical Communications</i> , 2016, 52, 8183-8195.	2.2	66
3494	Asymmetric aza-Morita-Baylis-Hillman reactions of chiral N-phosphonyl imines with acrylates via GAP chemistry/technology. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 6024-6035.	1.5	7
3495	Cations or Radicals? Inherent Reactivity of Biosynthetic Intermediates in the B-Ring Formation of Rotenoid Natural Products. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2372-2379.	1.1	1
3496	Theoretical studies on the hydrolysis mechanism of acetamiprid. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	9
3497	Captodative substitution induced acceleration effect towards 4π electrocyclic ring-opening of substituted cyclobutenes. <i>RSC Advances</i> , 2016, 6, 25503-25510.	1.7	6
3498	Methane activation by metal-free Lewis acid centers only – a computational design and mechanism study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11539-11549.	1.3	8
3499	The mechanisms for N-heterocyclic olefin-catalyzed formation of cyclic carbonate from CO <sub>2</sub> and propargylic alcohols. <i>Journal of Molecular Modeling</i> , 2016, 22, 94.	0.8	11
3500	Cooperative Asymmetric Catalysis by N-Heterocyclic Carbenes and Brønsted Acid in β-Lactam Formation: Insights into Mechanism and Stereoselectivity. <i>ACS Catalysis</i> , 2016, 6, 3118-3126.	5.5	58
3501	The catalytic mechanism of CO oxidation in AlAu <sub>6</sub> clusters determined by density functional theory. <i>Journal of Structural Chemistry</i> , 2016, 57, 54-64.	0.3	1
3502	Mechanisms of the Water-Gas Shift Reaction Catalyzed by Ruthenium Carbonyl Complexes. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2408-2419.	1.1	21
3503	Mechanistic Insights into Radical-Mediated Oxidation of Tryptophan from ab Initio Quantum Chemistry Calculations and QM/MM Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2926-2939.	1.1	6
3504	Atmospheric chemistry of ethers, esters, and alcohols on the lifetimes, temperature dependence, and kinetic isotope effect: an example of CF <sub>3</sub> CX <sub>2</sub> CX <sub>2</sub> OX with OX reactions (X = H, D). <i>RSC Advances</i> , 2016, 6, 36096-36108.	1.7	12
3505	Kudi: A free open-source python library for the analysis of properties along reaction paths. <i>Journal of Molecular Modeling</i> , 2016, 22, 110.	0.8	6
3506	Synthesis and Hydrolysis of Uranyl, Neptunyl, and Plutonyl Gas-Phase Complexes Exhibiting Discrete Actinide-Carbon Bonds. <i>Organometallics</i> , 2016, 35, 1228-1240.	1.1	30
3507	OH-initiated tropospheric photooxidation of allyl acetate: a theoretical study. <i>Canadian Journal of Chemistry</i> , 2016, 94, 648-657.	0.6	2
3508	Mechanistic and energetic study of the atmospheric reaction of hydrosulfinyl and mercapto radicals. <i>Computational and Theoretical Chemistry</i> , 2016, 1086, 25-35.	1.1	4
3509	Quantum Monte Carlo Study of the Reactions of CH with Acrolein: Major and Minor Channels. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3602-3612.	1.1	21
3510	Water-catalyzed decomposition of the simplest Criegee intermediate CH <sub>2</sub> OO. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	27



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3511	Understanding the mechanisms, regioselectivities and enantioselectivities of the DMAP-catalyzed [2+4] cycloaddition of $\beta^3$ -methyl allenolate and phenyl(phenyldiazenyl)methanone. <i>RSC Advances</i> , 2016, 6, 84177-84186.	1.7	7
3512	Theoretical study on activation mechanism of fluorine substitution reactions of Keggin-MAL <sub>12</sub> in aqueous solutions. <i>Journal of Coordination Chemistry</i> , 2016, 69, 2864-2871.	0.8	1
3513	Catalysts for Isocyanate-Free Polyurea Synthesis: Mechanism and Application. <i>ACS Catalysis</i> , 2016, 6, 6883-6891.	5.5	48
3514	Insights into $\text{N}^{\text{H}}$ -Heterocyclic Carbene-Catalyzed [4+2] Annulation Reaction of Enals with Nitroalkenes: Mechanisms, Origin of Chemo- and Stereoselectivity, and Role of Catalyst. <i>Chemistry - an Asian Journal</i> , 2016, 11, 3046-3054.	1.7	32
3515	Mechanistic Insights into Water-Catalyzed Formation of Levoglucosenone from Anhydrosugar Intermediates by Means of High-Level Theoretical Procedures. <i>Australian Journal of Chemistry</i> , 2016, 69, 943.	0.5	15
3516	Thermal Methane Conversion to Syngas Mediated by Rh <sub>1</sub> -Doped Aluminum Oxide Cluster Cations RhAl <sub>3</sub> O <sub>4</sub> <sup>+</sup> . <i>Journal of the American Chemical Society</i> , 2016, 138, 12854-12860.	6.6	47
3517	A DFT study of the mechanism and the regioselectivity of [3 + 2] cycloaddition reactions of nitrile oxides with $\beta^2$ -acetylenic aldehyde. <i>Molecular Physics</i> , 2016, 114, 3193-3200.	0.8	4
3518	A density functional theory study on the performance of graphene and N-doped graphene supported Au <sub>3</sub> cluster catalyst for acetylene hydrochlorination. <i>Canadian Journal of Chemistry</i> , 2016, 94, 842-847.	0.6	10
3519	Theoretical study on the mechanism of palladium-catalyzed sp <sup>2</sup> CH bond activation using cyano as a directing group. <i>Journal of Organometallic Chemistry</i> , 2016, 824, 88-98.	0.8	6
3520	Further Insight into the Mechanism of the Novel Multicomponent Reactions Involving Isoquinoline and Dimethyl Acetylenedicarboxylate in the Presence of 3-Methylindole: Theoretical and Experimental Approach. <i>International Journal of Chemical Kinetics</i> , 2016, 48, 770-778.	1.0	4
3521	Computational insight into the cooperative role of non-covalent interactions in the aza-Henry reaction catalyzed by quinine derivatives: mechanism and enantioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 9588-9597.	1.5	11
3522	Effect of Lewis acids on the stereoregularity of N,N-dimethyl acrylamide: A computational approach. <i>European Polymer Journal</i> , 2016, 83, 67-76.	2.6	3
3523	Computational investigation into the gas-phase ozonolysis of the conjugated monoterpene $\beta^2$ -phellandrene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27991-28002.	1.3	14
3524	Hydrogen shift reactions in four methyl-buten-ol (MBO) peroxy radicals and their impact on the atmosphere. <i>Atmospheric Environment</i> , 2016, 147, 79-87.	1.9	15
3525	Theoretical investigation on activation of ethene by the HNbN <sup>-</sup> anion in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2016, 1096, 74-79.	1.1	1
3526	Nucleophilicity of Oximes Based upon Addition to a Nitriliumcloso-Decaborate Cluster. <i>Organometallics</i> , 2016, 35, 3612-3623.	1.1	52
3527	Hydrolysis mechanism of anticancer drug lobaplatin in aqueous medium under neutral and acidic conditions: A DFT study. <i>Chemical Physics Letters</i> , 2016, 663, 115-122.	1.2	16
3528	Theoretical Study of the Catalytic Hydrogenation of Alkenes by a Disilaferracyclic Complex: Can the Fe-Si $\sigma$ -Bond-Assisted Activation of H-H Bonds Allow Development of a Catalysis of Iron?. <i>Journal of Organic Chemistry</i> , 2016, 81, 10900-10911.	1.7	18

#	ARTICLE	IF	CITATIONS
3529	A theoretical study on the hetero-Diels-Alder reaction of phosphorous substituted diaza- and oxaza-alkenes with olefins derivatives. RSC Advances, 2016, 6, 89440-89449.	1.7	4
3530	Theoretical investigation of the reaction of ethanol with ground-state Co <sup>+</sup> (3F). Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	0
3531	Decarboxylation Facilitated by Carbocation Formation and Rearrangement during Steam Distillation of Vetiver Oil. Journal of Natural Products, 2016, 79, 2744-2748.	1.5	4
3532	Origin of the Different Reactivity of the Triatomic Anions HMoN <sup>+</sup> and ZrNH <sup>+</sup> toward Alkane: Compositions of the Active Orbitals. Journal of Physical Chemistry A, 2016, 120, 7786-7791.	1.1	4
3533	Theoretical kinetics study of thymine tautomerism and interaction of Na <sup>+</sup> with its tautomers. Molecular Physics, 2016, 114, 3356-3374.	0.8	4
3534	A mechanistic study on guanidine-catalyzed chemical fixation of CO <sub>2</sub> with 2-aminobenzonitrile to quinazoline-2,4(1H,3H)-dione. Organic Chemistry Frontiers, 2016, 3, 823-835.	2.3	29
3535	Special catalytic effects of intermediate-water for rapid shock initiation of Î <sup>2</sup> -HMX. RSC Advances, 2016, 6, 93103-93110.	1.7	12
3536	Theoretical study on the influence of water for the tautomerization of 3-hydroxy-2(1H)-pyridinethione in the solution. Chemical Physics Letters, 2016, 660, 22-26.	1.2	4
3537	Understanding metastable phase transformation during crystallization of RDX, HMX and CL-20: experimental and DFT studies. Physical Chemistry Chemical Physics, 2016, 18, 23554-23571.	1.3	53
3538	Mechanistic insight on (E)-methyl 3-(2-aminophenyl)acrylate cyclization reaction by multicatalysis of solvent and substrate. Journal of Computational Chemistry, 2016, 37, 2386-2394.	1.5	6
3539	A DFT Study on the Binuclear CuAAC Reaction: Mechanism in Light of New Experiments. Organometallics, 2016, 35, 2589-2599.	1.1	49
3540	Addition and abstraction reaction mechanism of 2,4,5-trimethylphenol with OH radical - A first principle study. Computational and Theoretical Chemistry, 2016, 1092, 90-107.	1.1	10
3541	Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions. Journal of the American Chemical Society, 2016, 138, 11368-11377.	6.6	85
3542	A DFT study of the mechanism of NHC catalysed annulation reactions involving Î±,Î²-unsaturated acyl azoliums and Î <sup>2</sup> -naphthol. Organic and Biomolecular Chemistry, 2016, 14, 8338-8345.	1.5	11
3543	Photoreactions with a Twist: Atropisomerism-Driven Divergent Reactivity of Enones with UV and Visible Light. Chemistry - A European Journal, 2016, 22, 11339-11348.	1.7	16
3544	Investigating the mechanism of the selective hydrogenation reaction of cinnamaldehyde catalyzed by Pt <sub>n</sub> clusters. Journal of Molecular Modeling, 2016, 22, 186.	0.8	3
3545	Mechanistic insights from theory on the reduction of CO <sub>2</sub> , N <sub>2</sub> O, and SO <sub>2</sub> molecules using tripodal diimine-enolate substituted magnesium( <i>scp</i> ) dimers. Dalton Transactions, 2016, 45, 14789-14800.	1.6	7
3546	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

#	ARTICLE	IF	CITATIONS
3547	Exploration of Unimolecular Gas-Phase Detoxication Pathways of Sarin and Soman: A Computational Study from the Perspective of Reaction Energetics and Kinetics. <i>Chemical Research in Toxicology</i> , 2016, 29, 1439-1457.	1.7	11
3548	Selective hydrogenation of cinnamaldehyde catalyzed by Co-doped Pt clusters: a density functional theoretical study. <i>RSC Advances</i> , 2016, 6, 88277-88286.	1.7	9
3549	An identification of the C=C bonding spin adduct in the spin trapping of N-methyl benzohydroxamic acid radical by 5,5-dimethyl-1-pyrroline N-oxide. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	8
3550	Ozonolysis mechanism of heterocyclic organic sulfides: A computational study. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 88-93.	1.1	4
3551	Diazomethane addition to sumanene as a subfullerene structure: A theoretical mechanistic study. <i>Computational and Theoretical Chemistry</i> , 2016, 1093, 40-47.	1.1	2
3552	Dynamic NMR and Quantum-Chemical Study of the Stereochemistry and Stability of the Chiral MoO <sub>2</sub> (acac) <sub>2</sub> Complex in Solution. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6677-6687.	1.1	6
3553	Cyclization of N-arylcyclopropanecarboxamides into N-arylpyrrolidinones under electron ionization and in the condensed phase. <i>Rapid Communications in Mass Spectrometry</i> , 2016, 30, 2416-2422.	0.7	0
3554	Photolysis of Carbonyl Diisocyanate: Generation of Isocyanatocarbonyl Nitrene and Diazomethanone. <i>Chemistry - an Asian Journal</i> , 2016, 11, 2953-2959.	1.7	18
3555	A theoretical study of DABCO and PPh <sub>3</sub> catalyzed annulations of allenolates with azodicarboxylate. <i>RSC Advances</i> , 2016, 6, 82260-82269.	1.7	12
3556	Carbon Dioxide Capture and Release by Anions with Solvent-Dependent Behaviour: A Theoretical Study. <i>Chemistry - A European Journal</i> , 2016, 22, 14056-14063.	1.7	12
3557	Theoretical study on the oligomerization mechanisms of bihydroxysilicone. <i>Journal of Molecular Modeling</i> , 2016, 22, 211.	0.8	3
3558	Mechanistic and kinetic study on the reaction of thiophene with hydroxyl radical. <i>Computational and Theoretical Chemistry</i> , 2016, 1092, 74-81.	1.1	8
3559	Regioselectivity of Sc <sub>2</sub> C <sub>2</sub> @C <sub>3v</sub> (8)-C <sub>82</sub> : Role of the Sumanene-Type Hexagon in Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2016, 81, 8169-8174.	1.7	11
3560	Mechanism of Ligand-Controlled Regioselectivity-Switchable Copper-Catalyzed Alkylboration of Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 14611-14617.	1.7	36
3561	Computational study of H-abstraction reactions from CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> Cl/CH <sub>3</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>2</sub> Cl by Cl atom and OH radical and fate of alkoxy radicals. <i>Environmental Science and Pollution Research</i> , 2016, 23, 23467-23484.	2.7	20
3562	Using Molecular Architecture to Control the Reactivity of a Triplet Vinylnitrene. <i>Journal of the American Chemical Society</i> , 2016, 138, 14905-14914.	6.6	28
3563	Mechanism of formation of ketones by palladium-catalysed desulfitative reaction: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2016, 1095, 29-35.	1.1	0
3564	Substitution effects on interaction forces in Na <sup>+</sup> -C <sub>4</sub> H <sub>4</sub> O complexes. Computational study. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 234-244.	1.1	0

#	ARTICLE	IF	CITATIONS
3565	A Theoretical Study on the Mechanism and Kinetics of the Reaction of Methylthiyl Radical with Ozone. Bulletin of the Chemical Society of Japan, 2016, 89, 681-691.	2.0	1
3566	Trimerization of Acetylene Catalyzed by Ir(PH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> PH <sub>2</sub> )Cl(cod): A Computational Study. Bulletin of the Chemical Society of Japan, 2016, 89, 584-594.	2.0	1
3567	Multi-Pathway Consequent Chemoselectivities of CpRuCl(PPh <sub>3</sub> ) <sub>2</sub> /Me-Catalysed Norbornadiene Alkyne Cycloadditions. Chemistry - A European Journal, 2016, 22, 15396-15403.	1.7	6
3568	Understanding the Oxidative Addition of C=C Bonds to Group 13 Compounds. Chemistry - A European Journal, 2016, 22, 13669-13676.	1.7	25
3569	First principles model calculations of the biosynthetic pathway in selinadiene synthase. Bioorganic and Medicinal Chemistry, 2016, 24, 4867-4870.	1.4	11
3570	Theoretical investigations towards the [4+2] cycloaddition of ketenes with 1-azadienes catalyzed by N-heterocyclic carbenes: mechanism and stereoselectivity. Tetrahedron, 2016, 72, 5295-5300.	1.0	16
3571	Metal-Catalyzed Cyclization Reactions of 2,3,4-Trieneols: A Joint Experimental-Computational Study. Chemistry - A European Journal, 2016, 22, 11667-11676.	1.7	7
3572	First Experimental and Theoretical Kinetic Study of the Reaction of 4-Hydroxy-4-methyl 2-pentanone as a Function of Temperature. International Journal of Chemical Kinetics, 2016, 48, 584-600.	1.0	6
3573	Theoretical investigations toward TMEDA-catalyzed [2 + 4] annulation of allenolate with 1-aza-1,3-diene: mechanism, regioselectivity, and role of the catalyst. RSC Advances, 2016, 6, 70723-70731.	1.7	20
3574	Theoretical Study of Mechanism and Kinetics of the Reaction of NO <sub>2</sub> with s-Triazine. Propellants, Explosives, Pyrotechnics, 2016, 41, 987-993.	1.0	0
3575	Mechanism of Boron-Catalyzed N-Alkylation of Amines with Carboxylic Acids. Journal of Organic Chemistry, 2016, 81, 6235-6243.	1.7	27
3576	How the mechanism of a [3 + 2] cycloaddition reaction involving a stabilized N-lithiated azomethine ylide toward a C-deficient alkene is changed to stepwise by solvent polarity? What is the origin of its regio- and endo stereospecificity? A DFT study using NBO, QTAIM, and NCI analyses. RSC Advances, 2016, 6, 75299-75314.	1.7	20
3577	Theoretical studies on the spin trapping of the 2-chloro-5-hydroxy-1,4-benzoquinone radical by 5,5-dimethyl-1-pyrroline N-oxide (DMPO): the identification of the C=O bonding spin adduct. RSC Advances, 2016, 6, 48099-48108.	1.7	10
3578	DFT exploration of mechanistic pathways of an aza-Morita-Baylis-Hillman reaction. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
3579	Dehydrogenation of lithium hydrazinidoborane: Insight from computational analysis. International Journal of Hydrogen Energy, 2016, 41, 18953-18962.	3.8	7
3580	Density Functional Study of Oxygen Insertion into Niobium-Phosphorus Bonds: Novel Mechanism for Liberating P <sub>3</sub> Synthons. Organometallics, 2016, 35, 3624-3634.	1.1	6
3581	A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols. Inorganic Chemistry, 2016, 55, 11372-11382.	1.9	16
3582	Deeper Insight into the Factors Controlling H <sub>2</sub> Activation by Geminal Aminoborane-Based Frustrated Lewis Pairs. Chemistry - A European Journal, 2016, 22, 18801-18809.	1.7	52

#	ARTICLE	IF	CITATIONS
3583	Mechanism for phenanthridines synthesis by nitrogenation of 2-acetylbiphenyls in acidic solution: a DFT study. <i>Journal of Molecular Modeling</i> , 2016, 22, 280.	0.8	3
3584	Deeper Insight into the Diels-Alder Reaction through the Activation Strain Model. <i>Chemistry - an Asian Journal</i> , 2016, 11, 3297-3304.	1.7	47
3585	Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with $\beta$ -amino amide ligands. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 11125-11136.	1.5	7
3586	Adsorption and decarbonylation of furfural over H-ZSM-5 zeolite: a DFT study. <i>RSC Advances</i> , 2016, 6, 105888-105894.	1.7	37
3587	Early events in the photochemistry of 5-diazo Meldrum's acid: formation of a product manifold in $\pi$ -N bound and pre-dissociated intersection seam regions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30785-30793.	1.3	11
3588	Global reaction route mapping of water-catalysed gas phase oxidation of glyoxylic acid with hydroxyl radical. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3
3589	A nine-atom rhodium-aluminum oxide cluster oxidizes five carbon monoxide molecules. <i>Nature Communications</i> , 2016, 7, 11404.	5.8	36
3590	A comparative computational study of N-heterocyclic olefin and N-heterocyclic carbene mediated carboxylative cyclization of propargyl alcohols with CO <sub>2</sub> . <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10875-10885.	1.5	19
3591	Quantum chemical study of mechanisms of organic reactions: V. Addition of ethane-1,2-dithiol to 4-hydroxy-4-methylpent-2-ynenitrile. <i>Russian Journal of Organic Chemistry</i> , 2016, 52, 1267-1276.	0.3	2
3592	A DFT study of [3 + 2] cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 70, 296-304.	1.3	17
3593	The Stability of $\beta$ -Hydroperoxyalkyl Radicals. <i>Chemistry - A European Journal</i> , 2016, 22, 18092-18100.	1.7	24
3594	The catalytic effect of the $\text{NH}_3$ base on the chemical events in the caryolene-forming carbocation cascade. <i>Journal of Computational Chemistry</i> , 2016, 37, 1068-1081.	1.5	8
3595	Photoenolization of $\alpha$ -Methylvalerophenone Ester Derivative. <i>Photochemistry and Photobiology</i> , 2016, 92, 388-398.	1.3	6
3596	Insights into Stereoselective Aminomethylation Reaction of $\beta,\beta$ -Unsaturated Aldehyde with N,O-Acetal via N-Heterocyclic Carbene and Brønsted Acid/Base Cooperative Organocatalysis. <i>Journal of Organic Chemistry</i> , 2016, 81, 5370-5380.	1.7	59
3597	A new insight of degradation reaction mechanism on desflurane radical with a catalyst of NO: A theoretical perspective. <i>Chemical Physics Letters</i> , 2016, 658, 168-175.	1.2	3
3598	Phosphorane lifetime and stereo-electronic effects along the alkaline hydrolysis of phosphate esters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 18255-18267.	1.3	16
3599	A DFT study of solvent effects on the kinetics and mechanism of the [3,3] hetero-Cope rearrangement of 1-butene thiobenzoate. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016, 41, 153-158.	1.1	3
3600	Why is a proton transformed into a hydride by [NiFe] hydrogenases? An intrinsic reactivity analysis based on conceptual DFT. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15369-15374.	1.3	12

#	ARTICLE	IF	CITATIONS
3601	Impact of the water dimer on the atmospheric reactivity of carbonyl oxides. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17698-17712.	1.3	78
3602	Divergent ynamide reactivity in the presence of azides – an experimental and computational study. <i>Chemical Science</i> , 2016, 7, 6032-6040.	3.7	32
3603	DFT investigations on AuVO <sub>4</sub> as a barrier-free catalyst for oxidation of CO with O <sub>2</sub> . <i>Chemical Physics</i> , 2016, 475, 69-76.	1.3	15
3604	The possibility of sensing and inactivating the hazardous air pollutant species via adsorption and their [2 + 3] cycloaddition reactions with C <sub>20</sub> fullerene. <i>Sensors and Actuators B: Chemical</i> , 2016, 237, 591-596.	4.0	18
3605	New Insights on the Mechanism of Cyclization in Chromophore Maturation of Wild-Type Green Fluorescence Protein: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5386-5394.	1.2	5
3606	A theoretical investigation on hydrolysis mechanism of biologically relevant Pt(II)/Pd(II) complexes with $\sigma$ -donor and $\pi$ -acceptor carrier ligand. <i>Chemical Physics Letters</i> , 2016, 657, 148-155.	1.2	4
3607	Investigation of the possibility of functionalization of C <sub>20</sub> fullerene by benzene via Diels-Alder reaction. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2016, 84, 55-59.	1.3	15
3608	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. <i>Biochemistry</i> , 2016, 55, 3315-3328.	1.2	6
3609	When To Let Go – Diradical Intermediates from Zwitterionic Transition State Structures?. <i>Journal of Organic Chemistry</i> , 2016, 81, 5295-5302.	1.7	12
3610	Consecutive H <sub>2</sub> Oxidation Mediated by Au <sub>2</sub> VO <sub>4</sub> <sup>+</sup> Clusters. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10452-10459.	1.5	11
3611	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO <sub>2</sub> ] <sup>+</sup> (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. <i>Journal of the American Chemical Society</i> , 2016, 138, 7973-7981.	6.6	90
3612	Substituent effect and ligand exchange control the reactivity in ruthenium(II)-catalyzed hydroacylation of isoprenes and aldehydes – A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650019.	1.8	3
3613	Understanding the carbenoid-type reactivity of nitrile ylides in [3+2] cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	23
3614	Kinetics investigation of the hydrogen abstraction reaction between CH <sub>3</sub> SS and CN radicals. <i>Journal of Molecular Modeling</i> , 2016, 22, 36.	0.8	1
3615	A DFT study on NHC-catalyzed intramolecular aldehyde-ketone crossed-benzoin reaction: mechanism, regioselectivity, stereoselectivity, and role of NHC. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 6577-6590.	1.5	38
3616	The Effect of Position Replacement of Functional Groups on the Stepwise character of 1,3-Dipolar Reaction of a Nitrile Oxide and an Alkene. <i>Helvetica Chimica Acta</i> , 2016, 99, 273-280.	1.0	17
3617	Understanding the stereoselectivity in Brønsted acid catalysed Povarov reactions generating cis/trans CF <sub>3</sub> -substituted tetrahydroquinolines: a DFT study. <i>RSC Advances</i> , 2016, 6, 17064-17073.	1.7	17
3618	A Recyclable Organocatalyst for Asymmetric Michael Addition. <i>Catalysis Letters</i> , 2016, 146, 587-595.	1.4	4

#	ARTICLE	IF	CITATIONS
3619	Ruthenium(II)-PNN pincer complex catalyzed dehydrogenation of benzyl alcohol to ester: A DFT study. <i>Journal of Molecular Structure</i> , 2016, 1110, 24-31.	1.8	5
3620	Type-I dyotropic rearrangement for 1,2-disubstituted cyclohexanes: substitution effect on activation energy. <i>RSC Advances</i> , 2016, 6, 10549-10556.	1.7	6
3621	A theoretical study on intermolecular [2+2] radical cation cycloaddition reactions and the competition between concerted and stepwise mechanisms. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 163-172.	1.1	3
3622	Theoretical Studies on Palladium-Mediated Enantioselective C-H Iodination. <i>Journal of Organic Chemistry</i> , 2016, 81, 1006-1020.	1.7	18
3623	Ab initio and direct dynamics study on the hydrogen abstraction reaction $C_2H_3 + CH_3CHO$ . <i>Computational and Theoretical Chemistry</i> , 2016, 1075, 63-69.	1.1	3
3624	Density Functional and Kinetic Monte Carlo Study of Cu-Catalyzed Cross-Dehydrogenative Coupling Reaction of Thiazoles with THF. <i>Journal of Organic Chemistry</i> , 2016, 81, 1806-1812.	1.7	4
3625	A theoretical study on the anticancer drug Au(I) N-heterocyclic carbene complexes $[(R_2Im)_2Au]^+$ ( $R = Me$ ). <i>Tj ETQq0 0 0 rgBT /Overlock</i> 2016, 135, 1.	0.5	4
3626	A gas-phase ab initio study of the hydrolysis of HCN. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3
3627	DFT Study on the Mechanism and Stereoselectivity of NHC-Catalyzed Synthesis of Substituted Trifluoromethyl Dihydropyranones with Contiguous Stereocenters. <i>Journal of Organic Chemistry</i> , 2016, 81, 868-877.	1.7	28
3628	Mechanistic Insights into the Initiation Step of the Base Promoted Direct C-H Arylation of Benzene in the Presence of Additive. <i>Journal of Organic Chemistry</i> , 2016, 81, 632-639.	1.7	38
3629	DFT perspective toward [3 + 2] annulation reaction of enals with $\alpha$ -ketoamides through NHC and Brønsted acid cooperative catalysis: mechanism, stereoselectivity, and role of NHC. <i>Organic Chemistry Frontiers</i> , 2016, 3, 190-203.	2.3	74
3630	Comprehensive theoretical study of the phenyl azide addition onto armchair (5, 5) single wall carbon nanotube. <i>Computational and Theoretical Chemistry</i> , 2016, 1075, 38-46.	1.1	2
3631	Mechanistic and kinetic study on the reaction of ozone and trans-2-chlorovinyl dichloroarsine. <i>Chemosphere</i> , 2016, 150, 329-340.	4.2	2
3632	Dehydrogenation of propylene mediated by $CeVO_4^+$ : An interesting example for the chemistry of binary Ce-V transition-metal oxide cluster cations. <i>International Journal of Mass Spectrometry</i> , 2016, 401, 39-45.	0.7	5
3633	The molecular mechanism of palladium-catalysed cyanoesterification of methyl cyanofornate onto norbornene. <i>Dalton Transactions</i> , 2016, 45, 7786-7793.	1.6	9
3634	Intramolecular charge transfer in aminobenzonitriles and tetrafluoro counterparts: fluorescence explained by competition between low-lying excited states and radiationless deactivation. Part I: A mechanistic overview of the parent system ABN. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6861-6874.	1.3	20
3635	Solid state and dynamic solution structures of O-carbamidine amidoximes gives further insight into the mechanism of zinc(II)-mediated generation of 1,2,4-oxadiazoles. <i>Journal of Molecular Structure</i> , 2016, 1111, 142-150.	1.8	44
3636	Experimental and Theoretical Study of the Effectiveness and Stability of Gold(I) Catalysts Used in the Synthesis of Cyclic Acetals. <i>Organometallics</i> , 2016, 35, 732-740.	1.1	8

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3637	Formation mechanisms of 3,4-dinitrofurazan via nitration reaction of furazan. <i>Chemical Physics Letters</i> , 2016, 647, 85-88.	1.2	5
3638	Stereo-, Regio-, and Chemoselective [3 + 2]-Cycloaddition of (2 <i>E</i> ,4 <i>E</i> )-Ethyl 5-(Phenylsulfonyl)penta-2,4-dienoate with Various Azomethine Ylides, Nitrones, and Nitrile Oxides: Synthesis of Pyrrolidine, Isoxazolidine, and Isoxazoline Derivatives and a Computational Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 2340-2354.	1.7	16
3639	Revisiting oxime–nitron tautomerism. Evidence of nitron tautomer participation in oxime nucleophilic addition reactions. <i>RSC Advances</i> , 2016, 6, 22161-22173.	1.7	29
3640	Gas-Phase Reactions of Methoxyphenols with NO <sub>3</sub> Radicals: Kinetics, Products, and Mechanisms. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1213-1221.	1.1	25
3641	Regioselectivity of Stoichiometric Metathesis of Vinylsilanes with Second-Generation Grubbs Catalyst: A Combined DFT and Experimental Study. <i>Organometallics</i> , 2016, 35, 621-628.	1.1	12
3642	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO <sub>2</sub> . <i>Molecular Physics</i> , 2016, 114, 1374-1391.	0.8	20
3643	DFT study on the CuBr-catalyzed synthesis of highly substituted furans: effects of solvent DMF, substrate MeOH, trace H <sub>2</sub> O and the metallic valence state of Cu. <i>RSC Advances</i> , 2016, 6, 20294-20305.	1.7	11
3644	A DFT study on PBu <sub>3</sub> -catalyzed intramolecular cyclizations of N-allylic substituted $\hat{\iota}$ -amino nitriles for the formation of functionalized pyrrolidines: mechanisms, selectivities, and the role of catalysts. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 3130-3141.	1.5	32
3645	Insights into the Mechanistic Role of Diphenylphosphine Selenide, Diphenylphosphine, and Primary Amines in the Formation of CdSe Monomers. <i>Journal of Physical Chemistry A</i> , 2016, 120, 918-931.	1.1	7
3646	The role of CuCl on the mechanism of dibenzo-p-dioxin formation from poly-chlorophenol precursors: A computational study. <i>Chemosphere</i> , 2016, 145, 77-82.	4.2	4
3647	Pd-Catalyzed $\hat{\iota}$ -Arylation of Sulfones in a Three-Component Synthesis of 3-[2-(Phenyl/methylsulfonyl)ethyl]indoles. <i>ACS Catalysis</i> , 2016, 6, 1691-1700.	5.5	17
3648	An experimental and theoretical approach on the kinetics and mechanism for the formation of a four-membered (S, S) chelated Pt( $\sigma$ -C) complex. <i>RSC Advances</i> , 2016, 6, 18288-18299.	1.7	7
3649	A new model for C–C bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of [3+2] cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes. <i>Tetrahedron</i> , 2016, 72, 1524-1532.	1.0	62
3650	Understanding the Mechanism of the Lewis Acid Promoted [3 + 2] Cycloaddition of Propargylic Alcohol and $\hat{\iota}$ -Oxo Ketene Dithioacetals. <i>Journal of Organic Chemistry</i> , 2016, 81, 1989-1997.	1.7	13
3651	Origins of the ANRORC reactivity in nitroimidazole derivatives. <i>RSC Advances</i> , 2016, 6, 25215-25221.	1.7	2
3652	Mechanisms and reactivity differences for the cobalt-catalyzed enantioselective intramolecular hydroacylation of ketones and alkenes: insights from density functional calculations. <i>Journal of Molecular Modeling</i> , 2016, 22, 60.	0.8	6
3653	Dynamic/Thermochemical Balance Drives Unusual Alkyl/F Exchange Reactions in Siloxides and Analogs. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1644-1651.	1.1	1
3654	Cycloaddition Reactions of Indanedione ketene with Electron-Rich Dienophiles: An Experimental and a Theoretical Study. <i>Journal of Organic Chemistry</i> , 2016, 81, 2383-2398.	1.7	5



#	ARTICLE	IF	CITATIONS
3655	Comparison of Thiyl, Alkoxy, and Alkyl Radical Addition to Double Bonds: The Unusual Contrasting Behavior of Sulfur and Oxygen Radical Chemistry. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1750-1755.	1.1	21
3656	Functionalization of the sumanene by nitrous oxide: A mechanistic study. <i>Computational and Theoretical Chemistry</i> , 2016, 1082, 49-57.	1.1	7
3657	Oxidation of NO <sub>2</sub> <sup>•</sup> by small oxygen species HO <sub>2</sub> <sup>•</sup> and O <sub>2</sub> <sup>•-</sup> : the role of negative charge, electronic spin and water solvation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9524-9536.	1.3	4
3658	Theoretical and kinetic study of the hydrogen atom abstraction reactions of unsaturated C6 methyl esters with hydroxyl radical. <i>Chemical Physics Letters</i> , 2016, 650, 119-125.	1.2	18
3659	Mechanism of Rh <sub>2</sub> (II)-Catalyzed Indole Formation: The Catalyst Does Not Control Product Selectivity. <i>Journal of the American Chemical Society</i> , 2016, 138, 487-490.	6.6	53
3660	Palladium-Silver Cooperativity in an Aryl Amination Reaction through C-H Functionalization. <i>ACS Catalysis</i> , 2016, 6, 696-708.	5.5	68
3661	<i>Ab initio</i> and direct dynamics study on the C <sub>2</sub> H <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> OH reaction. <i>Molecular Physics</i> , 2016, 114, 315-324.	0.8	6
3662	Revealing Stepwise Mechanisms in Dipolar Cycloaddition Reactions: Computational Study of the Reaction between Nitrones and Isocyanates. <i>Journal of Organic Chemistry</i> , 2016, 81, 673-680.	1.7	25
3663	Mechanism of the Visible Light-Mediated Gold-Catalyzed Oxyarylation Reaction of Alkenes. <i>ACS Catalysis</i> , 2016, 6, 798-808.	5.5	91
3664	Copper-Catalyzed Regioselective C-H Sulfonylation of 8-Aminoquinolines. <i>Journal of Organic Chemistry</i> , 2016, 81, 946-955.	1.7	97
3665	Theoretical study of the catalytic oxidation mechanism of 5-hydroxymethylfurfural to 2,5-diformylfuran by PMo-containing Keggin heteropolyacid. <i>Catalysis Science and Technology</i> , 2016, 6, 3776-3787.	2.1	29
3666	Pd <sup>II</sup> -mediated integration of isocyanides and azide ions might proceed via formal 1,3-dipolar cycloaddition between RNC ligands and uncomplexed azide. <i>New Journal of Chemistry</i> , 2016, 40, 521-527.	1.4	16
3667	Density functional theory study of the regio- and stereoselectivity of 1,3-dipolar cycloaddition reactions between 2-ethylthio-4-phenyl-1-azetidin and some substituted nitrile oxides. <i>Structural Chemistry</i> , 2016, 27, 1041-1047.	1.0	4
3668	The effect of the metal fragment on the aromaticity and synchronicity of the gold( <i>scp</i> )-catalysed divinylcyclopropane-cycloheptadiene rearrangement. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11677-11682.	1.3	5
3669	An efficient route to regioselective functionalization of benzo[b]thiophenes via palladium-catalyzed decarboxylative Heck coupling reactions: insights from experiment and computation. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 895-904.	1.5	17
3670	The Reaction between Bromine and the Water Dimer and the Highly Exothermic Reverse Reaction. <i>Journal of Computational Chemistry</i> , 2016, 37, 177-182.	1.5	3
3671	Insights into the mechanism of binding of the gold(III) dithiocarbamate derivatives to cysteine or DNA purine bases. <i>Structural Chemistry</i> , 2016, 27, 651-662.	1.0	5
3672	An experimental and theoretical kinetic study of the reaction of OH radicals with tetrahydrofuran. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 143-150.	2.4	31

#	ARTICLE	IF	CITATIONS
3673	Insights into the Thermal Eliminations and Photoeliminations of B,N-Heterocycles: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 753-761.	1.1	9
3674	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with ketenes. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1618-1627.	1.5	33
3675	The decomposition of benzenesulfonyl azide: a matrix isolation and computational study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3792-3799.	1.3	20
3676	Chiral discrimination of $\hat{1}\pm$ -hydroxy acids and N-Ts- $\hat{1}\pm$ -amino acids induced by tetraaza macrocyclic chiral solvating agents by using $^1\text{H}$ NMR spectroscopy. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1642-1650.	1.5	17
3677	Mechanistic study of hemicucurbit[6]uril formation by step-growth oligomerization and end-to-end cyclization. <i>Chemical Physics Letters</i> , 2017, 669, 92-98.	1.2	3
3678	Computational investigation of $\hat{1}\text{C}-\text{C}$ bond strengths in fluorinated ethylenes. <i>Journal of Fluorine Chemistry</i> , 2017, 194, 33-39.	0.9	4
3679	Theoretical investigation on the decomposition reaction mechanisms and kinetics of methyl vinyl ether initialized by OH radical. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	2
3680	Reaction mechanisms and kinetics of the elimination processes of 2-chloroethylsilane and derivatives: A DFT study using CTST, RRKM, and BET theories. <i>Chemical Physics</i> , 2017, 485-486, 140-148.	0.9	3
3681	Terminal Alkyne-Induced Decomposition of a Phosphine-Free Ruthenium Alkylidene Catalyst. <i>ChemCatChem</i> , 2017, 9, 2284-2291.	1.8	5
3682	Mechanisms for nickel(0)/N-heterocyclic carbene-catalyzed intramolecular alkene hydroacylation: insights from a DFT study. <i>Journal of Molecular Modeling</i> , 2017, 23, 11.	0.8	6
3683	Organic Lewis Pairs Based on Phosphine and Electrophilic Silane for the Direct and Controlled Polymerization of Methyl Methacrylate: Experimental and Theoretical Investigations. <i>Macromolecules</i> , 2017, 50, 762-774.	2.2	39
3684	Mechanisms and stereoselectivities of the DABCO-catalyzed Rauhut-Currier reaction of $\hat{1}\pm, \hat{1}^2$ -unsaturated ketones and aryl acrylates: a computational investigation. <i>RSC Advances</i> , 2017, 7, 2890-2896.	1.7	5
3685	Atmospheric fate of diketones and OH radical kinetics, reaction force, ETS-NOCV analysis. <i>Molecular Physics</i> , 2017, 115, 839-859.	0.8	9
3686	Theoretical prediction on the synthesis of 2,3-dihydropyridines through Co(III)-catalysed reaction of unsaturated oximes with alkenes. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25353.	1.0	1
3687	$\hat{1}\text{f}$ -CAM Mechanisms for the Hydrogenation of Alkenes by $\hat{1}\text{cis}$ - and $\hat{1}\text{trans}$ -Disilametallacyclic Carbonyl Complexes (M = Fe, Ru, Os): Experimental and Theoretical Studies. <i>Bulletin of the Chemical Society of Japan</i> , 2017, 90, 613-626.	2.0	9
3688	Rationalization of the mechanism of in situ Pd(0) formation for cross-coupling reactions from novel unsymmetrical pincer palladacycles using DFT calculations. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 71-81.	0.8	10
3689	QM/MM (ABEEM) Study on the Ligand Substitution Processes of Ruthenium(III) Complex NAMI-A. <i>Chinese Journal of Chemistry</i> , 2017, 35, 354-362.	2.6	1
3690	A theoretical study on the reaction mechanism and kinetics of allyl alcohol ( $\text{CH}_2=\text{CHCH}_2\text{OH}$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 895-911.	0.8	16

#	ARTICLE	IF	CITATIONS
3691	Theoretical investigation toward organophosphine-catalyzed [3+3] annulation of Morita-Baylis-Hillman carbonates with azomethine imines: Mechanism, origin of stereoselectivity, and role of catalyst. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25367.	1.0	18
3692	Base-Promoted Transmetalation Reactions of Protic N-Heterocyclic Carbenes and Acyclic Diamino Carbenes from Mn <sup>I</sup> to Au <sup>I</sup> : A Mechanistic Study. <i>Organometallics</i> , 2017, 36, 1035-1041.	1.1	16
3693	Dissociation of methane on Ni <sub>4</sub> cluster-A DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1106, 7-14.	1.1	21
3694	Theoretical prediction of the synthesis of 2,3-dihydropyridines through Ir(III)-catalysed reaction of unsaturated oximes with alkenes. <i>RSC Advances</i> , 2017, 7, 5649-5659.	1.7	0
3695	Singlet Photoreactivity of 3-Methyl-2-phenyl-2H-azirine. <i>Australian Journal of Chemistry</i> , 2017, 70, 413.	0.5	10
3696	Mechanism of extractive/oxidative desulfurization using the ionic liquid imidazole acetate: a computational study. <i>Journal of Molecular Modeling</i> , 2017, 23, 54.	0.8	4
3697	Rapid Hydrogen Shift Reactions in Acyl Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1470-1479.	1.1	28
3698	One Lump or Two? A Plurality of Pathways in Gold(III)-Catalyzed Cyclization Transforming Propargyl Acetates to a Carene-like Bicyclo[4.1.0]heptane. <i>Organometallics</i> , 2017, 36, 920-926.	1.1	6
3699	Theoretical exploration of mechanism of carbapenam formation in catalytic Kinugasa reaction. <i>Tetrahedron</i> , 2017, 73, 1673-1681.	1.0	14
3700	Performance of Dimethyl Sulfoxide and Brønsted Acid Catalysts in Fructose Conversion to 5-Hydroxymethylfurfural. <i>ACS Catalysis</i> , 2017, 7, 2199-2212.	5.5	100
3701	Jones oxidation of glycerol catalysed by small gold clusters. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6620-6625.	1.3	16
3702	Unexpected regioselectivity observed in the bromination and epoxidation reactions of p-benzoquinone-fused norbornadiene: An experimental and computational study. <i>Tetrahedron</i> , 2017, 73, 1640-1649.	1.0	13
3703	A combined high-temperature experimental and theoretical kinetic study of the reaction of dimethyl carbonate with OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7147-7157.	1.3	15
3704	Theoretical Study on Ruthenium-Catalyzed Hydrocarbamoylative Cyclization of 1,6-Diyne with Dimethylformamide. <i>Organometallics</i> , 2017, 36, 1154-1163.	1.1	6
3705	Sulphuric acid-catalysed formation of hemiacetal from glyoxal and ethanol. <i>Chemical Physics Letters</i> , 2017, 675, 27-34.	1.2	5
3706	On adduct formation and reactivity in the OCS + OH reaction: A combined theoretical and experimental study. <i>Chemical Physics Letters</i> , 2017, 675, 111-117.	1.2	2
3707	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. <i>Tetrahedron</i> , 2017, 73, 1718-1724.	1.0	65
3708	Theoretical studies of some bimolecular reactions during the decomposition of CH <sub>3</sub> NO <sub>2</sub> : reactions between NO <sub>2</sub> and nine intermediates. <i>Journal of Molecular Modeling</i> , 2017, 23, 62.	0.8	1

#	ARTICLE	IF	CITATIONS
3709	Cyanoform and Its Isomers. Relative Stabilities, Spectroscopic Features, and Rearrangements by Coupled Cluster and MCSCF-Based Methods. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1319-1327.	1.1	4
3710	A quantum chemical study on $\dot{\text{E}}^{\text{TM}}\text{Cl}$ -initiated atmospheric degradation of acrylonitrile. <i>RSC Advances</i> , 2017, 7, 20574-20581.	1.7	3
3711	Cope Rearrangement in Bicyclo[5.1.0]octa-2,5-diene and its Mono- and Di-Hetero Analogues: A DFT Study. <i>Australian Journal of Chemistry</i> , 2017, 70, 683.	0.5	0
3712	Structure and Spectroscopic Properties of [Mg,C,N,O] Isomers: Plausible Astronomical Molecules. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 158-167.	1.2	15
3713	Copper(I)-Catalyzed 1,3-Dipolar Cycloaddition of Ketonitrones to Dialkylcyanamides: A Step toward Sustainable Generation of 2,3-Dihydro-1,2,4-oxadiazoles. <i>ACS Omega</i> , 2017, 2, 1380-1391.	1.6	32
3714	The atmospheric oxidation of $\text{CH}_3\text{OOH}$ by the OH radical: the effect of water vapor. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12331-12342.	1.3	28
3715	Hydrolysis mechanism of (N, N) chelated cytotoxic Pt/Pd(II)-dichloro complexes: A theoretical approach. <i>Chemical Physics Letters</i> , 2017, 678, 241-249.	1.2	5
3716	1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium Complexes with Arylnitrile $\text{N-Oxides}$ . <i>Journal of Organic Chemistry</i> , 2017, 82, 5096-5101.	1.7	7
3717	Mechanisms of Carbonyl Activation by BINOL $\text{N-Triflylphosphoramides}$ : Enantioselective Nazarov Cyclizations. <i>ACS Catalysis</i> , 2017, 7, 3466-3476.	5.5	25
3718	Effect of Lewis acid bulkiness on the stereoselectivity of Diels-Alder reactions between acyclic dienes and $\text{E}^{\text{TM}}$ -enals. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1390-1399.	2.3	29
3719	Mechanism for ruthenium hydride-catalyzed regioselective hydroacylation of enones and aldehydes to give 1,3-diketones: Insights from density functional calculations. <i>Molecular Catalysis</i> , 2017, 433, 55-61.	1.0	3
3720	Density functional theory study of mechanism of epoxy-carboxylic acid curing reaction. <i>Journal of Computational Chemistry</i> , 2017, 38, 1093-1102.	1.5	30
3721	New trace of secondary organic aerosol from oxidation of acetonitrile with radical hydroxyl. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 72-81.	1.1	5
3722	Hypercoordinate Iodine Catalysts in Enantioselective Transformation: The Role of Catalyst Folding in Stereoselectivity. <i>ACS Catalysis</i> , 2017, 7, 4189-4196.	5.5	40
3723	Navigating Past a Fork in the Road: Carbocation- $\pi$ Interactions Can Manipulate Dynamic Behavior of Reactions Facing Post-Transition-State Bifurcations. <i>Journal of the American Chemical Society</i> , 2017, 139, 7485-7493.	6.6	51
3724	A DFT study of the ring-opening polymerization mechanism of $\epsilon$ -lactide and $\epsilon$ -caprolactone using aluminium salen-type initiators: Towards an understanding of their reactivities in homo- and copolymerization. <i>Molecular Catalysis</i> , 2017, 436, 145-156.	1.0	24
3725	Surface-Catalyzed Reaction between the Gases Hydrogen Chloride and Isoprene. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 122-129.	1.2	2
3726	Mechanism of Nickel-Catalyzed Suzuki-Miyaura Coupling of Amides. <i>Chemistry - an Asian Journal</i> , 2017, 12, 1765-1772.	1.7	25

#	ARTICLE	IF	CITATIONS
3727	Understanding the Reactivity of Ion-Encapsulated Fullerenes. <i>Chemistry - A European Journal</i> , 2017, 23, 11030-11036.	1.7	33
3728	Toward understanding regioselectivity and molecular mechanism in the synthesis of CF <sub>2</sub> H-containing 2-pyrazolines: A molecular electron-density theory study. <i>Journal of Fluorine Chemistry</i> , 2017, 199, 77-91.	0.9	13
3729	H <sub>2</sub> Oxidation Mediated by Au <sub>1</sub> -Doped Vanadium Oxide Cluster Cation AuV <sub>2</sub> O <sub>5</sub> <sup>+</sup> : A Comparative Study with AuCe <sub>2</sub> O <sub>4</sub> <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2017, 121, 4069-4075.	1.1	5
3730	Introducing topology to assess the synchronicity of organic reactions. Dual reactivity of oximes with alkenes as a case study. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1541-1554.	2.3	22
3731	Mechanistic and kinetic study on the reaction of methylperoxy radical with atomic iodine. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 512-520.	1.3	2
3732	The Effect of the cis-donor in pincer ligands on hydrogenolysis of Pd-OH: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 165-170.	0.8	4
3733	Theoretical Studies for Switching Regioselectivity in Ruthenium Hydride-Catalyzed Alkyne Hydroacylation. <i>ChemistrySelect</i> , 2017, 2, 2858-2865.	0.7	1
3734	Experimental and Computational Studies of the Reactions of N and O Atoms with Small Heterocyclic Anions. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3655-3661.	1.1	9
3735	A DFT study on the reaction mechanism between tetrachloro-o-benzoquinone and H <sub>2</sub> O <sub>2</sub> and an alternative reaction approach to produce the hydroxyl radical. <i>RSC Advances</i> , 2017, 7, 22919-22926.	1.7	11
3736	A Mechanistic Insight into the Ligand-Controlled Asymmetric Arylation of Aliphatic $\hat{\pm}$ -Amino Anion Equivalents: Origin of Regio- and Enantioselectivities. <i>Inorganic Chemistry</i> , 2017, 56, 5984-5992.	1.9	6
3737	Steric interactions controlling the <i>syn</i> diastereofacial selectivity in the [3+2] cycloaddition reaction between acetonitrile oxide and 7-oxanorborn-5-en-2-ones: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3710.	0.9	23
3738	Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2804-2822.	2.3	40
3739	Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10070-10086.	7.2	1,060
3740	Inactivation possibility of pyrene by C <sub>20</sub> fullerene via cycloaddition reactions: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2017, 1112, 37-45.	1.1	13
3741	Hydrolysis theory based on density functional studies for cytotoxic Pt(II) and Pd(II) complexes with benzimidazole derivative. <i>Chemical Physics Letters</i> , 2017, 678, 250-258.	1.2	5
3742	The possibility of using C <sub>20</sub> fullerene and graphene as semiconductor segments for detection, and destruction of cyanogen-chloride chemical agent. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 80-84.	1.3	16
3743	The mechanism of oxidation in chromophore maturation of wild-type green fluorescent protein: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12942-12952.	1.3	9
3744	Detailed kinetic mechanism for CH <sub>3</sub> OO + NO reaction - An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 14-23.	1.1	18

#	ARTICLE	IF	CITATIONS
3745	Mechanisms and stereoselectivities of phosphine-catalyzed Rauhut-Currier reaction between N-phenylmaleimide and 2-benzoyl acrylate: A computational investigation. <i>Molecular Catalysis</i> , 2017, 432, 292-298.	1.0	9
3746	Mechanistic Insight into the Molecular TiO <sub>2</sub> -Mediated Gas Phase Detoxication of DMMP: A Theoretical Approach. <i>Chemical Research in Toxicology</i> , 2017, 30, 1177-1187.	1.7	9
3747	Understanding the reaction mechanism of the Lewis acid (MgBr <sub>2</sub> )-catalysed [3+2] cycloaddition reaction between C-methoxycarbonyl nitrene and 2-propen-1-ol: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	9
3748	Mechanistic Insight into the Enhancement of Reactivity of C <sub>60</sub> <sup>+</sup> in Comparison with Neutral C <sub>60</sub> and EMFs towards Different Fundamental Reactions: A DFT Approach. <i>ChemistrySelect</i> , 2017, 2, 4039-4053.	0.7	3
3749	A DFT computational study on the molecular mechanism of reaction between pyridinium salts and $\pi$ -deficient ethylenes: Why furan derivatives are formed instead of feasible cyclopropane derivatives and [3 + 2] cycloadducts?. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 87-100.	1.1	6
3750	Insights on the Reactivity of Terminal Phosphanido Metal Complexes toward Activated Alkynes from Theoretical Computations. <i>Inorganic Chemistry</i> , 2017, 56, 6652-6661.	1.9	2
3751	Theoretical insights into the selectivity of 1,6-enyne cycloisomerization on gold clusters: Orbital interaction role. <i>Computational and Theoretical Chemistry</i> , 2017, 1113, 94-100.	1.1	1
3752	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrenes with strained allenes. <i>RSC Advances</i> , 2017, 7, 26879-26887.	1.7	19
3753	Understanding the reactivity of bis(propargyl) aromatic esters towards GAP: a theoretical exploration. <i>New Journal of Chemistry</i> , 2017, 41, 7886-7892.	1.4	6
3754	Das Distortion/Interaction-Activation-Strain-Modell zur Analyse von Reaktionsgeschwindigkeiten. <i>Angewandte Chemie</i> , 2017, 129, 10204-10221.	1.6	209
3755	Epoxy and Oxidoannulene Oxidation Mechanisms of Fused-Pentagon Chlorofullerenes: Oxides Linked by a Pirouette-Type Transition State. <i>Journal of Organic Chemistry</i> , 2017, 82, 6541-6549.	1.7	2
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#	ARTICLE	IF	CITATIONS
3763	Pyrolysis of n-butane investigated using synchrotron threshold photoelectron photoion coincidence spectroscopy. <i>RSC Advances</i> , 2017, 7, 28746-28753.	1.7	7
3764	Mechanisms of DABCO- and DMAP-catalyzed [2+4] cycloaddition reactions of methylallenoate with methyleneindolonone: A DFT study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25408.	1.0	4
3765	Computational insights into the S <sub>3</sub> transfer reaction: A special case of double group transfer reaction featuring bicyclically delocalized aromatic transition state geometries. <i>Journal of Computational Chemistry</i> , 2017, 38, 1966-1973.	1.5	3
3766	Computational study on the mechanism and kinetics of Cl-initiated oxidation of ethyl acrylate. <i>Structural Chemistry</i> , 2017, 28, 1831-1842.	1.0	7
3767	Migration and desorption of hydrogen atom and molecule on/from graphene. <i>Carbon</i> , 2017, 121, 248-256.	5.4	19
3768	Effective Catalytic Performance of Plasma-Enhanced W <sub>2</sub> N/AC as Catalysts for Acetylene Hydrochlorination. <i>Topics in Catalysis</i> , 2017, 60, 1016-1023.	1.3	6
3769	On the feasibility of reactions through the fullerene wall: a theoretical study of NH <sub>x</sub> @C <sub>60</sub> . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17199-17209.	1.3	4
3770	Regio- and Stereoselectivity in 1,3-Dipolar Cycloadditions: Activation Strain Analyses for Reactions of Hydrazoic Acid with Substituted Alkenes. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 4313-4318.	1.2	5
3771	Understanding the influence of hydrogen pressure on the enantioselectivity of hydrogenation: A combined theory-experiment approach. <i>Journal of Organometallic Chemistry</i> , 2017, 836-837, 90-99.	0.8	3
3772	Computational study on the mechanism and kinetics for the reaction between HCHO and HO <sub>2</sub> . <i>Molecular Simulation</i> , 2017, 43, 900-907.	0.9	3
3773	A Theoretical Study on Methane C-H Bond Activation by Bare [FeO] <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2017, 121, 3501-3514.	1.1	16
3774	Influence of the Transition-Metal Fragment on the Reactivity of Metallaanthracenes. <i>Chemistry - A European Journal</i> , 2017, 23, 6634-6642.	1.7	26
3775	A theoretical insight into the formation mechanisms of C/N-ribonucleosides with pyrimidine and ribose. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10413-10426.	1.3	4
3776	Studies on hydrolysis mechanism of anticancer ruthenium drug ImH[trans-Ru(Im) <sub>2</sub> Cl <sub>4</sub> ] via ABEEM/rf polarizable force field combined with QM and MD-FEP. <i>Chemical Research in Chinese Universities</i> , 2017, 33, 239-247.	1.3	3
3777	Experimental and Theoretical Studies on the Mechanism of the C-S Bond Activation of Pd <sup>II</sup> Thiolate/Thioether Complexes. <i>Organometallics</i> , 2017, 36, 1303-1321.	1.1	8
3778	Theoretical investigation of water-gas shift reaction catalyzed by water-soluble Rh(III)-EDTA complex. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	0
3779	Effect of Substituent on the Mechanism and Chemoselectivity of the Gold(I)-Catalyzed Propargyl Ester Tandem Cyclization. <i>Organometallics</i> , 2017, 36, 1164-1172.	1.1	22
3780	Enantioselective Diels-Alder-lactamization organocascades employing a furan-based diene. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 3179-3183.	1.5	17

#	ARTICLE	IF	CITATIONS
3781	Mechanism and Kinetics of the Reaction of Nitrosamines with OH Radical: A Theoretical Study. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 339-353.	1.0	14
3782	Mechanism of Water Oxidation Catalyzed by a Mononuclear Manganese Complex. <i>ChemSusChem</i> , 2017, 10, 903-911.	3.6	40
3783	A revised mechanism for the $\alpha$ -ketoacid hydroxylamine amide forming ligations. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 416-425.	1.5	8
3784	Reaction mechanism of cyanoethynyl radical (C <sub>3</sub> N) with ethylene (C <sub>2</sub> H <sub>4</sub> ) to form C <sub>5</sub> H <sub>3</sub> N and H: a theoretical investigation. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	2
3785	Thermochemical and Kinetics of CH <sub>3</sub> SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 419-428.	1.1	10
3786	Reaction of NO <sub>3</sub> radical with benzyl alcohol - A DFT study. <i>Computational and Theoretical Chemistry</i> , 2017, 1102, 51-59.	1.1	9
3787	Theoretical Study of the Gaseous Hydrolysis of NO <sub>2</sub> in the Presence of Amines. <i>Journal of Physical Chemistry A</i> , 2017, 121, 226-237.	1.1	22
3788	Anomerization reaction of bare and microhydrated <i>d</i> -erythrose via explicitly correlated coupled cluster approach. Two water molecules are optimal. <i>Journal of Computational Chemistry</i> , 2017, 38, 288-303.	1.5	4
3789	Diversity of reactivity modes upon interplay between Au( <i>iii</i> )-bound isocyanides and cyclic nitrones: a theoretical consideration. <i>Dalton Transactions</i> , 2017, 46, 786-802.	1.6	4
3790	Understanding the Effect of $\alpha$ -Cationic Phosphines and Group 15 Analogues on $\beta$ -Acid Catalysis. <i>Organometallics</i> , 2017, 36, 460-466.	1.1	26
3791	Theoretical Study of the Reaction Mechanism and Kinetics of HO <sub>2</sub> with XCHO (X = F, Cl). <i>International Journal of Chemical Kinetics</i> , 2017, 49, 130-139.	1.0	13
3792	The Variediene-Forming Carbocation Cyclization/Rearrangement Cascade. <i>Australian Journal of Chemistry</i> , 2017, 70, 362.	0.5	18
3793	Liberation of three dihydrogens from two ethene molecules as mediated by the tantalum nitride anion cluster Ta <sub>3</sub> N <sub>2</sub> <sup>+</sup> at room temperature. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3136-3142.	1.3	9
3794	The role of arsenic in the hydrolysis and DNA metalation processes in an arsenous acid-platinum( <i>ii</i> ) anticancer complex. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1328-1334.	1.3	12
3795	A theoretical investigation on bio-transformation of third generation anti-cancer drug Heptaplatin and its interaction with DNA purine bases. <i>Chemical Physics Letters</i> , 2017, 690, 105-115.	1.2	3
3796	Mechanistic Insight into the Cu-Catalyzed C-S Cross-Coupling of Thioacetate with Aryl Halides: A Joint Experimental-Computational Study. <i>Journal of Organic Chemistry</i> , 2017, 82, 11464-11473.	1.7	33
3797	Synthesis of hyperbranched low molecular weight polyethylene oils by an iminopyridine nickel( <i>sc</i> ) catalyst. <i>Polymer Chemistry</i> , 2017, 8, 6443-6454.	1.9	37
3798	Theoretical design and mechanistic study of the metal-free reduction of CO <sub>2</sub> to CO. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28313-28322.	1.3	6



#	ARTICLE	IF	CITATIONS
3799	Catalytic coupling reaction mechanism of 4-nitrobenzenethiol on silver clusters: a density functional theoretical study. <i>Journal of Molecular Modeling</i> , 2017, 23, 321.	0.8	1
3800	Tetrazol-5-ylidene Gold(III) Complexes from Sequential [2 + 3] Cycloaddition of Azide to Metal-Bound Isocyanides and N4 Alkylation. <i>Organometallics</i> , 2017, 36, 3974-3980.	1.1	18
3801	DFT and AFIR Study on the Mechanism and the Origin of Enantioselectivity in Iron-Catalyzed Cross-Coupling Reactions. <i>Journal of the American Chemical Society</i> , 2017, 139, 16117-16125.	6.6	74
3802	Mechanistic investigation on N-oxyl C <sup>+</sup> -O relay via non-Brook rearrangement: reaction conditions promote synthesis of furo[3,2-c]pyridinones. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 9127-9138.	1.5	4
3803	Quantum modeling of the reaction between ozone and hydrogen cyanide. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750063.	1.8	0
3804	Understanding the mechanism of the decomposition reaction of nitroethyl benzoate through the Molecular Electron Density Theory. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	13
3805	Theoretical Study on DBU-Catalyzed Insertion of Isatins into Aryl Difluoronitromethyl Ketones: A Case for Predicting Chemoselectivity Using Electrophilic Parr Function. <i>ACS Omega</i> , 2017, 2, 7029-7038.	1.6	16
3806	Theoretical Studies of Allene Synthesis through Cadmium Iodide-Mediated Allenylation of Terminal Alkynes. <i>Asian Journal of Organic Chemistry</i> , 2017, 6, 1778-1782.	1.3	8
3807	Competition between HO <sub>2</sub> and H <sub>2</sub> O <sub>2</sub> Reactions with CH <sub>2</sub> OO <i>anti</i> -CH <sub>3</sub> CHO in the Oligomer Formation: A Theoretical Perspective. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6981-6991.	1.1	21
3808	The atmospheric oxidation mechanism and kinetics of 1,3,5-trimethylbenzene initiated by OH radicals "a theoretical study. <i>New Journal of Chemistry</i> , 2017, 41, 10259-10271.	1.4	19
3809	Reactions between microhydrated superoxide anions and formic acid. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 23176-23186.	1.3	3
3810	Computational study on the mechanism and kinetics for reaction of CH <sub>3</sub> SH + H with water vapor. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 235-240.	1.1	4
3811	Ab initio dynamics of unimolecular decomposition of $\beta$ -propiolactone and $\beta$ -propiolactam. <i>Chemical Physics Letters</i> , 2017, 686, 55-59.	1.2	6
3812	Asymmetric Dual Chiral Catalysis using Iridium Phosphoramidites and Diarylprolinol Silyl Ethers: Insights into Stereodivergence. <i>ACS Catalysis</i> , 2017, 7, 6675-6685.	5.5	23
3813	Theoretical study on the reaction of Cp* (pentamethylcyclopentadienyl)(Cl)Zr(diene) with isonitriles. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 177-187.	1.1	1
3814	Synthesis, characterisation and in vitro cytotoxicity of mixed ligand Pt(II) oxadiazoline complexes with hexamethylenetetramine and 7-nitro-1,3,5-triazaadamantane. <i>Dalton Transactions</i> , 2017, 46, 12226-12238.	1.6	6
3815	Quantum chemical studies of mechanisms of organic reactions: VI. Reaction of ethane-1,2-dithiol with vinylidene chloride. <i>Russian Journal of Organic Chemistry</i> , 2017, 53, 986-994.	0.3	8
3816	Insights into the Reaction Mechanism of Criegee Intermediate CH <sub>2</sub> OO with Methane and Implications for the Formation of Methanol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7236-7245.	1.1	31

#	ARTICLE	IF	CITATIONS
3817	Mechanism for the S <sub>N</sub> Ar reaction of atrazine with endogenous thiols: experimental and theoretical study. <i>New Journal of Chemistry</i> , 2017, 41, 12671-12677.	1.4	12
3818	Mechanistic and kinetic study on the reaction of methylperoxyl radical with atomic hydrogen. <i>Chemical Physics Letters</i> , 2017, 687, 276-283.	1.2	0
3819	Effects of base strength on the copper-catalyzed cycloisomerization of propargylic acetates to form indolizines: A DFT study. <i>Tetrahedron</i> , 2017, 73, 6092-6100.	1.0	11
3820	A computational mechanistic study on the chemo-, regio- and stereoselectivity of cycloaddition reactions leading to $\hat{1}^3$ -dihydropyran and tetrahydrocarbazol compounds. <i>Computational and Theoretical Chemistry</i> , 2017, 1118, 153-165.	1.1	2
3821	Concerted double proton-transfer electron-transfer between catechol and superoxide radical anion. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26179-26190.	1.3	30
3822	Organocatalyzed oxidation of benzyl alcohols by a tetrazole-amino-saccharin: A combined experimental and theoretical (DFT) study. <i>Molecular Catalysis</i> , 2017, 442, 57-65.	1.0	16
3823	Theoretical insights into the reaction of Cp*(Cl)Hf(diene) with isonitriles. <i>RSC Advances</i> , 2017, 7, 44979-44989.	1.7	2
3824	Computational design of bio-inspired carnosine-based HOBr antioxidants. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 905-913.	1.3	8
3825	Planarizing cytosine: The S1 state structure, vibrations, and nonradiative dynamics of jet-cooled 5,6-trimethylenecytosine. <i>Journal of Chemical Physics</i> , 2017, 146, 244308.	1.2	8
3826	Mechanistic investigation of the atmospheric reaction of NH <sub>2</sub> with NO <sub>2</sub> and study of the catalytic effects of water molecule on kinetic path. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750053.	1.8	2
3827	Mechanisms and stereoselectivities of NHC-catalyzed [4 + 2] cycloaddition reaction between phenylacetic acid and o-quinone methide: A computational investigation. <i>Molecular Catalysis</i> , 2017, 441, 199-208.	1.0	7
3828	A molecular electron density theory study of [3+2] cycloaddition reactions of chiral azomethine ylides with $\hat{1}^2$ -nitrostyrene. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	21
3829	Influence of Base Strength on the Proton Transfer Reaction by Density Functional Theory. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 3947-3956.	1.2	15
3830	Theoretical Investigations on the Mechanism and Kinetics of OH Radical Initiated Reactions of Monochloroacetic Acid. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6028-6035.	1.1	8
3831	Promotion catalytic role of ethanol on Brønsted acid for the sequential dehydration-etherification of fructose to 5-ethoxymethylfurfural. <i>Journal of Catalysis</i> , 2017, 352, 586-598.	3.1	40
3832	Theoretical study on photochemistry of Irgacure 907. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2017, 347, 78-85.	2.0	11
3833	Pericyclic or Pseudopericyclic? The Case of an Allylic Transposition in the Synthesis of a Saccharin Derivative. <i>Journal of Chemical Education</i> , 2017, 94, 988-993.	1.1	7
3834	A DFT study of hydrogen and methane activation by B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> /P(t-Bu) <sub>3</sub> and Al(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> /P(t-Bu) <sub>3</sub> frustrated Lewis pairs. <i>Journal of Molecular Modeling</i> , 2017, 23, 234.	0.8	13

#	ARTICLE	IF	CITATIONS
3835	Mechanistic investigation inspired by water-gas reaction for hydrobromic acid-catalyzed Friedel-Crafts type reaction of 1-naphthol and formaldehyde. <i>Journal of Computational Chemistry</i> , 2017, 38, 2268-2275.	1.5	4
3836	Insight into the Mechanism of Reverse Water-gas Shift Reaction and Ethanol Formation Catalyzed by Mo <sub>6</sub> S <sub>8</sub> -TM Clusters. <i>Molecular Catalysis</i> , 2017, 439, 155-162.	1.0	16
3837	Experimental and theoretical investigations of the kinetics and mechanism of the Cl <sup>+</sup> -4-hydroxy-4-methyl-2-pentanone reaction. <i>Atmospheric Environment</i> , 2017, 166, 315-326.	1.9	12
3838	A theoretical study on [2+2] cycloaddition reactions under visible light irradiation induced by energy transfer. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 47-54.	1.1	2
3839	New Theoretical Insights into the Contributions of Poly(methylbenzene) and Alkene Cycles to the Methanol to Propene Process in H-FAU Zeolite. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16216-16237.	1.5	10
3840	Approach Matters: The Kinetics of Interfacial Inverse Electron Demand Diels-Alder Reactions. <i>Chemistry - A European Journal</i> , 2017, 23, 13015-13022.	1.7	11
3841	Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes. <i>Journal of Organic Chemistry</i> , 2017, 82, 8668-8675.	1.7	59
3842	ETS-NOCV Decomposition of the Reaction Force: The HCN/CNH Isomerization Reaction Assisted by Water. <i>Journal of Computational Chemistry</i> , 2017, 38, 2076-2087.	1.5	19
3843	DFT studies on the mechanism of Ag <sub>2</sub> CO <sub>3</sub> -catalyzed hydroazidation of unactivated terminal alkynes with TMSN <sub>3</sub> : An insight into the silver(I) activation mode. <i>Journal of Computational Chemistry</i> , 2017, 38, 2289-2297.	1.5	8
3844	Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. <i>New Journal of Chemistry</i> , 2017, 41, 9674-9687.	1.4	7
3845	Prebiotic molecules formation through the gas-phase reaction between HNO and CH <sub>2</sub> CHOH <sub>2</sub> <sup>+</sup> . <i>Astronomy and Astrophysics</i> , 2017, 603, A139.	2.1	8
3846	Insights into chemoselective fluorination reaction of alkynals via N-heterocyclic carbene and Brønsted base cooperative catalysis. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	11
3847	A theoretical study on the mechanism of xylobiose during pyrolysis process. <i>Computational and Theoretical Chemistry</i> , 2017, 1117, 130-140.	1.1	25
3848	A computational insight into cyclopropanone activated dehydration reaction of alcohols. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 77, 106-114.	1.3	2
3849	Mechanistic Investigation of Thermal and Photoreactions between Boron and Silane. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6531-6537.	1.1	4
3850	Synthesis, Optical Properties, and DNA Interaction of New Diquats Based on Triazolopyridines and Triazoloquinolines. <i>Chemistry - A European Journal</i> , 2017, 23, 12825-12832.	1.7	8
3851	Synthesis of the octahydronaphthalene core of nahuic acid A via a B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -catalyzed intramolecular Diels-Alder (IMDA) reaction. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7430-7438.	1.5	3
3852	Transition Metal-Catalysed Intramolecular Carbenoid C-H Insertion for Pyrrolidine Formation by Decomposition of $\alpha$ -Diazoesters. <i>Advanced Synthesis and Catalysis</i> , 2017, 359, 3654-3664.	2.1	16

#	ARTICLE	IF	CITATIONS
3853	Laser flash photolysis of nanocrystalline $\hat{\pm}$ -azido-p-methoxy-acetophenone. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7380-7386.	1.5	6
3855	Understanding the reactivity and regioselectivity of [3+2] cycloaddition reactions between substituted nitrile oxides and methyl acrylate. A molecular electron density theory study. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25451.	1.0	27
3856	DFT study of chromium tricarbonyl complexes of coronene and kekulene. <i>Moscow University Chemistry Bulletin</i> , 2017, 72, 201-211.	0.2	3
3857	Allylic Azide Rearrangements Investigated by Density Functional Theory Calculations. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 1419-1426.	1.0	7
3858	Theoretical study of the Cl-initiated atmospheric oxidation of methyl isopropenyl ketone. <i>RSC Advances</i> , 2017, 7, 52801-52811.	1.7	6
3859	Computational insights for the hydride transfer and distinctive roles of key residues in cholesterol oxidase. <i>Scientific Reports</i> , 2017, 7, 17265.	1.6	16
3860	Reaction mechanism of the cation radicals of thymine and thymine derivatives in aqueous solution: A theoretical study. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750070.	1.8	0
3861	The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9698-9707.	1.1	15
3862	Substituent Effects on the Reactivity of Cyclic Tertiary Sulfamidates. <i>Journal of Organic Chemistry</i> , 2017, 82, 13250-13255.	1.7	10
3863	Exploring the Mechanism and Stereoselectivity in Chiral Cinchona-Catalyzed Heterodimerization of Ketenes. <i>Journal of Organic Chemistry</i> , 2017, 82, 13449-13458.	1.7	10
3864	Quantum chemical study of the structures and dynamic behavior of tricarbonyl complexes of Group 6 metals (Cr, Mo, W) with polyaromatic hydrocarbons using the density functional theory. <i>Russian Chemical Bulletin</i> , 2017, 66, 1163-1176.	0.4	4
3865	The key role of Au-substrate interactions in catalytic gold subnanoclusters. <i>Nature Communications</i> , 2017, 8, 1657.	5.8	35
3866	A theoretical investigation on the mechanism and kinetics of the gas-phase reaction of naphthalene with OH radical. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	9
3867	Computational Study on $\hat{\pm}$ <sup>3</sup> -C=C-H Functionalization of $\hat{\pm}$ , $\hat{\pm}$ <sup>2</sup> -Unsaturated Ester Catalyzed by N-Heterocyclic Carbene: Mechanisms, Origin of Stereoselectivity, and Role of Catalyst. <i>Journal of Organic Chemistry</i> , 2017, 82, 13043-13050.	1.7	55
3868	Theoretical Studies of the Glycosidation of 2-O-Substituted 5-Fluorouracil: N-Regioselective Synthesis with the Phase-Transfer-Catalysis Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8866-8883.	1.1	4
3869	Mechanisms of metal-catalyzed cycloisomerizations of <i>o</i> -propargylbiaryls and <i>o</i> -allenylbiaryls to phenanthrenes: a DFT study. <i>Catalysis Science and Technology</i> , 2017, 7, 6026-6041.	2.1	9
3870	Active sites formation and their transformations during ethylene polymerization by the Phillips CrOx/SiO <sub>2</sub> catalyst. <i>Journal of Catalysis</i> , 2017, 352, 314-328.	3.1	33
3871	Insight into the Formation of Anhydrosugars in Glucose Pyrolysis: A Joint Computational and Experimental Investigation. <i>Energy &amp; Fuels</i> , 2017, 31, 8291-8299.	2.5	22

#	ARTICLE	IF	CITATIONS
3872	Computational study on NHC-catalyzed enantioselective and chemoselective fluorination of aliphatic aldehydes. <i>Organic Chemistry Frontiers</i> , 2017, 4, 1987-1998.	2.3	47
3873	A computational study on the mechanism of ynamide-mediated amide bond formation from carboxylic acids and amines. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 6367-6374.	1.5	18
3874	Multiple Mechanisms for the Thermal Decomposition of Metallaisoxazolin-5-ones from Computational Investigations. <i>Journal of Organic Chemistry</i> , 2017, 82, 8438-8443.	1.7	1
3875	Factors Governing the Diels-Alder Reactivity of (2,7)Pyrenophanes. <i>Journal of Organic Chemistry</i> , 2017, 82, 8157-8164.	1.7	8
3876	Theoretical insights into C-C bond formation through isonitrile insertion into a Cp*Ti complex. <i>RSC Advances</i> , 2017, 7, 34816-34829.	1.7	2
3877	Combined Theoretical and Experimental Studies of Nickel-Catalyzed Cross-Coupling of Methoxyarenes with Arylboronic Esters via C-O Bond Cleavage. <i>Journal of the American Chemical Society</i> , 2017, 139, 10347-10358.	6.6	87
3878	Combined Experimental and Computational Study on Ruthenium(II)-Catalyzed Reactions of Dienes with Aldehydes and N,N-Dimethylformamide. <i>Journal of Organic Chemistry</i> , 2017, 82, 7964-7973.	1.7	8
3879	Theoretical investigations on the methylation of N-H bond using CO <sub>2</sub> and hydrosilane catalyzed by Zinc II complexes: Mechanism and ligand effect. <i>Journal of CO<sub>2</sub> Utilization</i> , 2017, 20, 178-189.	3.3	11
3880	A theoretical study on synthesis mechanisms of $\alpha,\beta$ -unsaturated carbon $\beta$ -amino ester catalyzed by PPh <sub>3</sub> . <i>Structural Chemistry</i> , 2017, 28, 1959-1968.	1.0	4
3881	Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products. <i>Environmental Science and Pollution Research</i> , 2017, 24, 18458-18469.	2.7	25
3882	Theoretical insights into the reaction mechanism between tetrachloro-o-benzoquinone and N-methyl benzohydroxamic acid. <i>RSC Advances</i> , 2017, 7, 32419-32426.	1.7	7
3883	Theoretical basis of 2,4-methyl migration, an intramolecular rearrangement, during isomerization of alkyladamantyl cations. <i>Petroleum Chemistry</i> , 2017, 57, 374-379.	0.4	1
3884	Solvolysis of organophosphorus pesticide parathion with simple and $\alpha$ nucleophiles: a theoretical study. <i>Journal of Chemical Sciences</i> , 2017, 129, 1301-1317.	0.7	7
3885	Mechanism of thermal decomposition of HFO-1234yf by DFT study. <i>International Journal of Refrigeration</i> , 2017, 74, 399-411.	1.8	47
3886	Exploring Partners for the Domino $\alpha$ -Arylation/Michael Addition Reaction Leading to Tetrahydroisoquinolines. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 799-805.	1.2	8
3887	Mechanism of the Copper/TEMPO-Catalyzed Aerobic Oxidation of Alcohols. <i>Chemistry - A European Journal</i> , 2017, 23, 1368-1378.	1.7	45
3888	Theoretical Insights into the Synthesis of 2,3-Dihydropyridines from Unsaturated Oximes by Rh <sup>III</sup> -Catalyzed C-H Activation - A DFT Study. <i>European Journal of Organic Chemistry</i> , 2017, 2017, 397-408.	1.2	1
3889	Mechanism of CuAAC reaction: In acetic acid and aprotic conditions. <i>Journal of Molecular Catalysis A</i> , 2017, 426, 150-157.	4.8	12

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3890	Theoretical study on the reaction mechanisms and stereoselectivities of DABCO-catalyzed Rauhut-currier/cyclization reaction of methyl acrylate with 2-benzoyl-3-phenylacrylonitrile. International Journal of Quantum Chemistry, 2017, 117, e25325.	1.0	4
3891	Density Functional Determination of the Energetics of the Formation of <i>trans</i> -Stilbene Catalyzed by Sulfenate Anions. ChemCatChem, 2017, 9, 278-281.	1.8	7
3892	Phenanthro[9,10- <i>a</i> ]corannulene by one-step annulative $\pi$ -extension of corannulene. Canadian Journal of Chemistry, 2017, 95, 329-333.	0.6	44
3893	Putative biosynthetic cycloadditions en route to the diterpenoid (+)-chatancin. Tetrahedron, 2017, 73, 4227-4232.	1.0	6
3894	Electrophilic activation of CO <sub>2</sub> in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	11
3895	Nucleophilic aromatic substitution in chlorinated aromatic systems with a glutathione thiolate model. Journal of Physical Organic Chemistry, 2017, 30, e3640.	0.9	2
3896	DFT mechanistic study of reactions of $\text{D}_1\text{6H}_6$ and 1,3,5-Ad <sub>3</sub> C <sub>6</sub> H <sub>3</sub> with CBr <sub>3</sub> . The first example of hydride transfer from aromatic C-H bond to electrophile. Journal of Molecular Catalysis A, 2017, 426, 610-617.	4.8	5
3897	Cryptic post-transition state bifurcations that reduce the efficiency of lactone-forming Rh-carbenoid C-H insertions. Chemical Science, 2017, 8, 1442-1449.	3.7	69
3898	Spin Transfer in Polymer Degradation of Abnormal Linkage. Journal of Electronic Materials, 2017, 46, 3933-3937.	1.0	2
3899	A DFT study of the mechanism and selectivities of the [3+2] cycloaddition reaction between 3-(benzylideneamino)oxindole and <i>trans</i> -nitrostyrene. Journal of Physical Organic Chemistry, 2017, 30, e3637.	0.9	22
3900	Selective sensing of ozone and the chemically active gaseous species of the troposphere by using the C <sub>20</sub> fullerene and graphene segment. Talanta, 2017, 162, 505-510.	2.9	69
3901	Computational model for the acylation step of the $\beta$ -lactam ring: Potential application for l,d-transpeptidase 2 in mycobacterium tuberculosis. Journal of Molecular Structure, 2017, 1128, 94-102.	1.8	41
3902	A Hemilabile and Cooperative N-Donor-Functionalized 1,2,3-Triazol-5-ylidene Ligand for Alkyne Hydrothiolation Reactions. Chemistry - A European Journal, 2017, 23, 1393-1401.	1.7	46
3903	Role of Lewis acid additives in a palladium catalyzed directed C-H functionalization reaction of benzohydroxamic acid to isoxazolone. Organic and Biomolecular Chemistry, 2017, 15, 246-255.	1.5	10
3904	Theoretical studies on the hydrogen abstraction reactions of methyl esters with HO <sub>2</sub> radical and the following $\beta$ -scission reactions. Journal of Physical Organic Chemistry, 2017, 30, e3668.	0.9	10
3905	Reaction mechanism of the preferential oxidation of the CO reaction in an H <sub>2</sub> stream over Cu-Ni bimetallic catalysts: A computational study. Journal of Structural Chemistry, 2017, 58, 1611-1624.	0.3	0
3906	Catalytic Aromatic Borylation via in situ-Generated Borenium Species. Heterocycles, 2017, 95, 158.	0.4	23
3907	Synthesis, characterization, and activity of a covalently anchored heterogeneous perylene diimide photocatalyst. Chinese Journal of Catalysis, 2017, 38, 2094-2101.	6.9	24

#	ARTICLE	IF	CITATIONS
3908	Quantum mechanical and multichannel RRKM studies of the reaction N <sub>2</sub> O + O (3P). <i>Arabian Journal of Chemistry</i> , 2017, 10, S3559-S3568.	2.3	0
3909	A theoretical investigation of decomposition and reactivity of the atmospheric C <sub>3</sub> F <sub>7</sub> OCH <sub>2</sub> O radical. <i>Arabian Journal of Chemistry</i> , 2017, 10, S1604-S1612.	2.3	4
3910	BET & ELF Quantum Topological Analysis of Neutral 2-Aza-Cope Rearrangement of $\hat{\beta}$ -Alkenyl Nitrones. <i>Molecules</i> , 2017, 22, 1371.	1.7	4
3911	Understanding the Heteroatom Effect on the Ullmann Copper-Catalyzed Cross-Coupling of X-Arylation (X = NH, O, S) Mechanism. <i>Catalysts</i> , 2017, 7, 388.	1.6	12
3912	Solvent Effects on the Mechanistic of Ketene and Halogenated Ketene Cycloadditions with Cyclopentadiene: A DFT Study. <i>Oriental Journal of Chemistry</i> , 2017, 33, 1265-1275.	0.1	0
3913	Synthesis, Crystal Structure and DFT Studies of 1,3-Dimethyl-5-propionylpyrimidine-2,4,6(1H,3H,5H)-trione. <i>Crystals</i> , 2017, 7, 31.	1.0	6
3914	On Searching for a Stepwise Channel for the Mechanism of a 1,3-Dipolar Cycloaddition between a Thiocarbonyl <i>S</i> -Oxide and C <sub>20</sub> Fullerene using Born-Oppenheimer <i>ab Initio</i> QM/MM Molecular Dynamics. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017, 42, 282-288.	1.1	0
3915	Applicability of DFT model in reactive distillation. <i>Physical Sciences Reviews</i> , 2017, 2, .	0.8	0
3916	Metal-Mediated Addition of N-Nucleophiles to Isocyanides: Mechanistic Aspects. <i>Molecules</i> , 2017, 22, 1141.	1.7	6
3917	Theoretical Study of ClOO + NO Reaction: Mechanism and Kinetics. <i>Molecules</i> , 2017, 22, 2121.	1.7	2
3918	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. <i>Molecules</i> , 2017, 22, 750.	1.7	76
3919	Rationalizing the Regioselectivity of the Diels-Alder Biscycloaddition of Fullerenes. <i>Journal of Organic Chemistry</i> , 2018, 83, 3285-3292.	1.7	11
3920	Demystifying the Mechanism of Regio- and Isolelective Epoxide Polymerization Using the Vandenberg Catalyst. <i>Macromolecules</i> , 2018, 51, 1777-1786.	2.2	26
3921	Insights into the isothioureia-catalyzed asymmetric [4 + 2] annulation of phenylacetic acid with alkylidene pyrazolone. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2301-2311.	1.5	31
3922	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold-Thiolate Linkers Innocent?. <i>Journal of the American Chemical Society</i> , 2018, 140, 4354-4362.	6.6	66
3923	Detailed kinetic modeling of thermal decomposition of guaiacol – A model compound for biomass lignin. <i>Biomass and Bioenergy</i> , 2018, 112, 45-60.	2.9	21
3924	A theoretical mechanistic study for C-H and C-C bond activations of cyclohexane catalyzed by NiAl + in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2018, 1129, 48-56.	1.1	3
3925	Predicting Productive Binding Modes for Substrates and Carbocation Intermediates in Terpene Synthases – Bornyl Diphosphate Synthase As a Representative Case. <i>ACS Catalysis</i> , 2018, 8, 3322-3330.	5.5	34

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3926	Disilaruthena- and Ferracyclic Complexes Containing Isocyanide Ligands as Effective Catalysts for Hydrogenation of Unfunctionalized Sterically Hindered Alkenes. <i>Journal of the American Chemical Society</i> , 2018, 140, 4119-4134.	6.6	38
3927	Catalysis of the acetylene hydrochlorination reaction by Si-doped Au clusters: a DFT study. <i>Journal of Molecular Modeling</i> , 2018, 24, 61.	0.8	12
3928	A molecular electron density theory study of the [3+2] cycloaddition reaction between an azomethine imine and electron deficient ethylenes. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3830.	0.9	22
3929	Bridging the Gap between Pentacene and Perfluoropentacene: Synthesis and Characterization of 2,3,9,10-Tetrafluoropentacene in the Neutral, Cationic, and Dicationic States. <i>Journal of Organic Chemistry</i> , 2018, 83, 3149-3158.	1.7	24
3930	Theoretical study on the mechanism and enantioselectivity of NHC-catalyzed intramolecular S <sub>N</sub> 2 nucleophilic substitution: what are the roles of NHC and DBU?. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1493-1501.	2.3	26
3931	Mechanism investigation on the reactions of ClF <sub>3</sub> O and <i>n</i> -decane by combining density functional theory and spontaneous emission spectroscopy. <i>RSC Advances</i> , 2018, 8, 8836-8841.	1.7	1
3932	Enantiocontrol by assembled attractive interactions in copper-catalyzed asymmetric direct alkynylation of $\alpha$ -ketoesters with terminal alkynes: OH <sup>-</sup> -CH <sup>-</sup> O two-point hydrogen bonding combined with dispersive attractions. <i>Chemical Science</i> , 2018, 9, 3484-3493.	3.7	43
3933	A Maze of Dyotropic Rearrangements and Triple Shifts: Carbocation Rearrangements Connecting Stemarene, Stemodene, Betaerdene, Aphidicolene, and Scopadulanol. <i>Journal of Organic Chemistry</i> , 2018, 83, 3780-3793.	1.7	16
3934	Biosynthesis and Conformational Properties of the Irregular Sesquiterpenoids Isothapsadiene and $\beta$ -Isothapsenol. <i>Journal of Organic Chemistry</i> , 2018, 83, 5724-5730.	1.7	2
3935	Mechanistic insights into the ligand-controlled regioselectivity in Cu-catalyzed terminal alkynes alkylation. <i>Journal of Organometallic Chemistry</i> , 2018, 871, 48-55.	0.8	9
3936	Dioxygenation of metal(II) $\epsilon$ -cysteinato complexes in CDO biomimetic models: Can ruthenium and osmium reach iron performances?. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25525.	1.0	2
3937	Methane Dissociation on Bimetallic AuNi <sub>3</sub> , Au <sub>2</sub> Ni <sub>2</sub> and Au <sub>3</sub> Ni Clusters: A DFT Study. <i>ChemistrySelect</i> , 2018, 3, 3133-3140.	0.7	7
3938	Theoretical investigation on the C-H activation of an enaminone and its coupling reaction with diphenylacetylene to a naphthalene catalyzed by Rh(III) complexes. <i>Molecular Catalysis</i> , 2018, 452, 100-107.	1.0	6
3939	Wavelength-dependent photochemistry of 2-azidovinylbenzene and 2-phenyl-2H-azirine. <i>Journal of Molecular Structure</i> , 2018, 1172, 94-101.	1.8	10
3940	Insights into 2- and 4(5)-Nitroimidazole Decomposition into Relevant Ions and Molecules Induced by VUV Ionization. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4031-4041.	1.1	27
3941	Comprehensive Mechanistic Insight into Cooperative Lewis Acid/Cp*Co(III)-Catalyzed C-H/N-H Activation for the Synthesis of Isoquinolin-3-ones. <i>Inorganic Chemistry</i> , 2018, 57, 2804-2814.	1.9	26
3942	Theoretical Study of Sesterfisherol Biosynthesis: Computational Prediction of Key Amino Acid Residue in Terpene Synthase. <i>Scientific Reports</i> , 2018, 8, 2473.	1.6	39
3943	Computational study on the mechanisms and kinetics of the CH <sub>2</sub> =CHCH <sub>2</sub> I with OH reaction. <i>Structural Chemistry</i> , 2018, 29, 1045-1055.	1.0	3



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3944	Infrared Dynamics of Iron Carbonyl Diene Complexes. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3497-3505.	1.1	3
3945	A DFT study on N-heterocyclic carbene catalyzed [4+2] annulation reaction with in situ generated heterocyclic ortho-quinodimethane: Mechanism, origin of enantioselectivity and role of catalyst. <i>Tetrahedron</i> , 2018, 74, 1009-1015.	1.0	9
3946	Computational insights into reduction of the Phillips CrOx/SiO2 catalyst by ethylene and CO. <i>Journal of Catalysis</i> , 2018, 359, 261-271.	3.1	21
3947	High Catalytic Activity of Vanadium Complexes in Alkane Oxidations with Hydrogen Peroxide: An Effect of 8-Hydroxyquinoline Derivatives as Noninnocent Ligands. <i>Inorganic Chemistry</i> , 2018, 57, 1824-1839.	1.9	51
3948	Mechanistic insights into N-heterocyclic carbene (NHC)-catalyzed N-acylation of N-sulfonylcarboxamides with aldehydes. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3811.	0.9	5
3949	Mechanistic insight into the ruthenium-catalyzed cycloaddition of diynes with 2,3-diphenyl-2H-azirines: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2018, 1127, 16-21.	1.1	5
3950	[3+2] cycloaddition reaction between CF3-substituted thiocarbonyl ylides and thioketones: Exploration of regioselectivity and mechanistic aspects using Molecular Electron Density Theory. <i>Journal of Fluorine Chemistry</i> , 2018, 209, 14-22.	0.9	10
3951	Rhodium Catalyzed Asymmetric Hydroamination of Internal Alkynes with Indoline: Mechanism, Origin of Enantioselectivity, and Role of Additives. <i>Journal of Organic Chemistry</i> , 2018, 83, 2627-2639.	1.7	12
3952	Efficient Transition State Optimization of Periodic Structures through Automated Relaxed Potential Energy Surface Scans. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 981-990.	2.3	47
3953	Hydrolytic Stability of Boronate Ester-Linked Covalent Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2018, 1, 1700015.	1.3	57
3954	Atmospheric Reaction of Cl with 4-Hydroxy-2-pentanone (4H2P): A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2135-2143.	1.1	6
3955	DFT Studies on the Water-Assisted Synergistic Proton Dissociation Mechanism for the Spontaneous Hydrolysis Reaction of Al <sup>3+</sup> in Aqueous Solution. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 269-277.	1.2	16
3956	Ab initio kinetics of the HOSO <sub>2</sub> + SO <sub>3</sub> + HO <sub>2</sub> reaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6677-6687.	1.3	15
3957	Reactivity of amino acid anions with nitrogen and oxygen atoms. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4990-4996.	1.3	10
3958	Kinetic and mechanistic study on gas phase reactions of ozone with a series of cis-3-hexenyl esters. <i>RSC Advances</i> , 2018, 8, 4230-4238.	1.7	8
3959	Theoretical study on mechanism of reaction between tert-butyl isocyanide and dimethyl acetylenedicarboxylate in presence of ethanethiol or thiophenol. <i>Research on Chemical Intermediates</i> , 2018, 44, 2653-2665.	1.3	3
3960	Baldwin-Type Rules for Metal-Controlled Intramolecular Migratory Insertions. A Computational Study of Ni, Pd, and Pt Case. <i>Organometallics</i> , 2018, 37, 390-395.	1.1	13
3961	Fe <sub>2</sub> O <sub>3</sub> Cation Mediated Propane Oxidation by Dioxygen in the Gas Phase. <i>Chemistry - A European Journal</i> , 2018, 24, 5920-5926.	1.7	5

#	ARTICLE	IF	CITATIONS
3962	Sulphur dioxide cooperation in hydrolysis reactions of vanadium oxide and hydroxide cluster dianions. <i>New Journal of Chemistry</i> , 2018, 42, 4008-4016.	1.4	7
3963	A computational investigation of the sulphuric acid-catalysed 1,4-hydrogen transfer in higher Criegee intermediates. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25599.	1.0	6
3964	C=C bond formation in the intramolecular Diels-Alder reaction of triene amides. <i>Heliyon</i> , 2018, 4, e00504.	1.4	9
3965	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C=N-Dialkyl Nitrones with Ethylene Derivatives. <i>Journal of Organic Chemistry</i> , 2018, 83, 2182-2197.	1.7	102
3966	Reactivity of hydropersulfides toward the hydroxyl radical unraveled: disulfide bond cleavage, hydrogen atom transfer, and proton-coupled electron transfer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4793-4804.	1.3	9
3967	DFT study on $\hat{\pm}$ -regioselectivity of photo-organocatalytic functionalization of aldehydes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 355, 9-15.	2.0	0
3968	Accurate density functional theory (DFT) protocol for screening and designing chain transfer and branching agents for LDPE systems. <i>Molecular Systems Design and Engineering</i> , 2018, 3, 228-242.	1.7	4
3969	Substituent Effect on the Stability and $^{14}\text{N}$ NQR Parameters of Linkage Isomers of Nitriles in a Rhodium Half-Sandwich Metallocycle: A Theoretical Study. <i>Journal of the Chinese Chemical Society</i> , 2018, 65, 416-423.	0.8	2
3970	Theoretical study on the mechanisms and kinetics of the $\hat{I}^2$ -elimination of 2,2-dihaloethyltrihalosilanes ( $\text{X}=\text{F}, \text{Cl}, \text{Br}$ ) compounds: a DFT study along with a natural bond orbital analysis. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2018, 124, 27-44.	0.8	13
3971	A combined experimental and theoretical study of the thermal [3+2] cycloaddition of carbonyl ylides with activated alkenes. <i>Journal of Molecular Structure</i> , 2018, 1157, 276-287.	1.8	9
3972	Theoretical Study of the Metal-Controlled Dehydrogenation Mechanism of $\text{Mn}_2\text{H}_3\text{BH}_3$ ( $\text{M} = \text{Li}, \text{Na}, \text{K}$ ): A New Family of Hydrogen Storage Material. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1344-1349.	1.1	4
3973	A new mechanism for internal nucleophilic substitution reactions. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 1101-1112.	1.5	1
3974	Reaction mechanisms of 3-amino-4-nitro-furoxan formation by 3-amide-4-nitro-furoxan and sodium hypochlorite in water and benzene solvents. <i>Computational and Theoretical Chemistry</i> , 2018, 1125, 69-76.	1.1	3
3975	Stereocontrol through Synergistic Catalysis in the Enantioselective $\hat{\pm}$ -Alkenylation of Aldehyde: A Computational Study. <i>Journal of Organic Chemistry</i> , 2018, 83, 1304-1311.	1.7	1
3976	A theoretical study on La-activated bicyclo-oligomerization of acetylene to form naphthalene in gas phase using density functional theory (DFT). <i>Structural Chemistry</i> , 2018, 29, 171-178.	1.0	3
3977	Ethanol synthesis catalyzed by single Ni atom supported on Mo <sub>6</sub> S <sub>8</sub> support. <i>Applied Catalysis A: General</i> , 2018, 553, 52-64.	2.2	15
3978	A molecular electron density theory study of the chemo- and regioselective [3+2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. <i>Chemical Physics</i> , 2018, 501, 128-137.	0.9	11
3979	Theoretical insight into the regioselective ring-expansions of bicyclic aziridinium ions. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 796-806.	1.5	16

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3980	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 33.	0.8	6
3981	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1107-1120.	1.2	69
3982	Investigating the reaction pathways of chemical functionalization of C <sub>20</sub> fullerene by nitrile oxide and azide; A computational study. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850003.	1.8	0
3983	How Does the Catalyst Affect the Reaction Pathway? DFT Analysis of the Mechanism and Selectivity in the 1,6-Diyne Ester Cycloisomerization. <i>Organometallics</i> , 2018, 37, 261-270.	1.1	8
3984	Mechanism for acetic acid-catalyzed ester aminolysis. <i>Chinese Chemical Letters</i> , 2018, 29, 1233-1236.	4.8	2
3985	The Dissociation Mechanism of Poly(1-vinyl-4-ethylbenzylstyrene (PAMS) Dimers Induced by Spin Polarization. <i>ChemistrySelect</i> , 2018, 3, 2553-2557.	0.7	1
3986	Comparison of atmospheric reactions of NH <sub>3</sub> and NH <sub>2</sub> with hydroxyl radical on the singlet, doublet and triplet potential energy surfaces, kinetic and mechanistic study. <i>Chemical Physics</i> , 2018, 507, 51-69.	0.9	8
3987	Selective Conversion of Methane by Rh <sub>1</sub> -Doped Aluminum Oxide Cluster Anions RhAl <sub>2</sub> O <sub>4</sub> : A Comparison with the Reactivity of PtAl <sub>2</sub> O <sub>4</sub> . <i>Journal of Physical Chemistry A</i> , 2018, 122, 3950-3955.	1.1	20
3988	Computational study on GaCl <sub>3</sub> -mediated reactions of donor-acceptor cyclopropanes with aromatic aldehydes: mechanism and role of GaCl <sub>3</sub> and aldehydes. <i>Organic Chemistry Frontiers</i> , 2018, 5, 1702-1712.	2.3	8
3989	Modeling Organic Reactions – General Approaches, Caveats, and Concerns. , 2018, , 1-29.		3
3990	Do dihydroxymagnesium carboxylates form Grignard-type reagents? A theoretical investigation on decarboxylative fragmentation. <i>Journal of Molecular Modeling</i> , 2018, 24, 106.	0.8	1
3991	Novel nitrogen-doped Au-embedded graphene single-atom catalysts for acetylene hydrochlorination: A density functional theory study. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 83-89.	1.1	19
3992	Mechanisms of phosphine-catalyzed [4+3] annulation of allenolates with C, N-cyclic azomethine imines; A DFT investigation. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25626.	1.0	7
3993	Ni(COD) <sub>2</sub> -Catalyzed <i>ipso</i> -Silylation of 2-Methoxynaphthalene: A Density Functional Theory Study. <i>Organometallics</i> , 2018, 37, 1141-1149.	1.1	26
3994	Energy transfer or electron transfer? DFT study on the mechanism of [2+2] cycloadditions induced by visible light photocatalysts. <i>Tetrahedron Letters</i> , 2018, 59, 1651-1660.	0.7	6
3995	Exploring the Chemoselective Dehydrogenative Silylation and Hydrogenation of Divinylsiloxane with Hydrosilane from DFT Computation. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1993-1999.	1.2	2
3996	Low temperature kinetics and theoretical studies of the reaction CN + CH <sub>3</sub> NH <sub>2</sub> : a potential source of cyanamide and methyl cyanamide in the interstellar medium. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5478-5489.	1.3	33
3997	Mechanism and selectivity of rhodium-catalyzed C-H bond arylation of indoles. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25526.	1.0	7

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3998	Unraveling the Nature of the Catalytic Power of Fluoroacetate Dehalogenase. <i>ChemCatChem</i> , 2018, 10, 1052-1063.	1.8	14
3999	Hydrolysis of a neonicotinoid: a theoretical study on the reaction mechanism of dinotefuran. <i>Structural Chemistry</i> , 2018, 29, 315-325.	1.0	9
4000	<sc>DFT</sc> study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25497.	1.0	41
4001	First principles computational study on hydrolysis of hazardous chemicals phosphorus trichloride and oxychloride (PCl <sub>3</sub> and POCl <sub>3</sub> ) catalyzed by molecular water clusters. <i>Journal of Hazardous Materials</i> , 2018, 341, 457-463.	6.5	13
4002	Mechanisms and stereoselectivities of phosphine-catalyzed domino reaction of $\beta$ -benzyl allenolate with 5-phenylmethylene thiazolone: a computational investigation. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	1
4003	Explaining the singlet complexes detected for the reaction $Zr(3F) + CH_3CH_3$ through a non-spin flip scheme. <i>Journal of Molecular Modeling</i> , 2018, 24, 12.	0.8	3
4004	Mechanistic Insights into Solvent and Ligand Dependency in Cu(I)-Catalyzed Allylic Alkylation with <i>gem</i> -Diborylalkanes. <i>Journal of Organic Chemistry</i> , 2018, 83, 561-570.	1.7	14
4005	Tandem Cope-rearrangement and [2+2] cycloaddition of cis-1,2-diethynylcyclopropane and its mono-hetero analogues: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 142-148.	1.1	2
4006	Organocatalytic Enantioselective Higher-Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1246-1250.	7.2	42
4007	Gold-Catalyzed Divergent Ring-Closing Modes of Indole-Tethered Amino Allenynes. <i>Chemistry - A European Journal</i> , 2018, 24, 1448-1454.	1.7	6
4008	Theoretical study with DFT on the mechanism of visible light-driven $\beta$ -functionalization of aldehydes. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 154-160.	1.1	1
4009	Theoretical study on DABCO-catalyzed ring expansion of cyclopropyl ketone: Mechanism, chemoselectivity, and role of catalyst. <i>Computational and Theoretical Chemistry</i> , 2018, 1123, 20-25.	1.1	12
4010	Performance of edges on carbon for the catalytic hydroxylation of benzene to phenol. <i>Catalysis Science and Technology</i> , 2018, 8, 176-186.	2.1	13
4011	Consecutive Oxidation of Three H <sub>2</sub> Molecules by a Gold-Vanadium Oxide Cluster Cation AuVO <sub>4</sub> <sup>+</sup> . <i>Topics in Catalysis</i> , 2018, 61, 28-34.	1.3	6
4012	Theoretical Study of Solvent Effect on the Kinetics and Thermochemistry of the Reaction of a (NHC)Cu(boryl) Complex with Ethylene. <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 2628-2633.	0.1	1
4013	Density Functional Theory Study on the Mechanisms of Platinum- and Gold-Catalyzed Cycloisomerizations of Biaryl Propargyl Alcohol and Indolyl Allenol to Phenanthrene and Carbazole. <i>ChemistrySelect</i> , 2018, 3, 12093-12107.	0.7	5
4014	Crystal structure, spectroscopic studies and theoretical studies of thiobarbituric acid derivatives: understanding the hydrogen-bonding patterns. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1703-1714.	0.2	4
4015	Understanding the mechanism and stereoselectivity of NHC-catalyzed [3 + 2] cycloaddition of 3-bromoaldehydes and isatin <i>N</i> -Boc ketimines. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 9251-9258.	1.5	14

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4016	Tropospheric oxidation of methyl hydrotrioxide (CH <sub>3</sub> OOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417.	1.3	7
4017	Detailed kinetics of tetrafluoroethene ozonolysis. Physical Chemistry Chemical Physics, 2018, 20, 28059-28067.	1.3	4
4018	The non-covalently bound SO <sub>2</sub> system, including an interpretation of the differences between SO <sub>2</sub> and O <sub>2</sub> . Physical Chemistry Chemical Physics, 2018, 20, 28840-28847.	1.3	5
4019	A Computational Approach for Hydrolysis of the Third-Generation Anticancer Drug: Trans-Platinum(II) Complex of 3-Aminoflavone. Journal of Structural Chemistry, 2018, 59, 1791-1796.	0.3	4
4020	Influence of the charge on the reactivity of azafullerenes. Physical Chemistry Chemical Physics, 2018, 20, 28011-28018.	1.3	11
4021	H <sub>2</sub> dissociation by Au <sup>1</sup> -doped closed-shell titanium oxide cluster anions. Chinese Journal of Chemical Physics, 2018, 31, 457-462.	0.6	4
4022	11. Applicability of DFT model in reactive distillation. , 2018, , 283-308.		0
4023	The mechanism of pyrolysis of 2-azidoethanol: A theoretical study. Computational and Theoretical Chemistry, 2018, 1146, 10-14.	1.1	2
4024	Reaction between Indazole and Pd-Bound Isocyanides—A Theoretical Mechanistic Study. Molecules, 2018, 23, 2942.	1.7	3
4025	Mechanisms of the Ethynyl Radical Reaction with Molecular Oxygen. Journal of Physical Chemistry A, 2018, 122, 9498-9511.	1.1	4
4026	New Insight into the Chloroacetanilide Herbicide Degradation Mechanism through a Nucleophilic Attack of Hydrogen Sulfide. International Journal of Molecular Sciences, 2018, 19, 2864.	1.8	18
4027	Towards a comprehensive understanding of the Si(100)-2 $\times$ 1 surface termination through hydrogen passivation using methylamine and methanol: a theoretical approach. Journal of Molecular Modeling, 2018, 24, 286.	0.8	0
4028	Catalytic hydrolyses of trifluoroacetyl fluoride by water. Chemical Physics Letters, 2018, 713, 137-144.	1.2	2
4029	Influence of the Lewis Acid/Base Pairs on the Reactivity of Geminal CH <sub>2</sub> Frustrated Lewis Pairs. Chemistry - A European Journal, 2018, 24, 17823-17831.	1.7	34
4030	A Theoretical Investigation on the Regioselectivity of the Diels-Alder Cycloaddition of 9-(Methoxymethyl) Anthracene And Citraconic Anhydride. Journal of Structural Chemistry, 2018, 59, 1810-1817.	0.3	1
4031	Quantum Chemical Study of Mechanisms of Organic Reactions: VII. Reaction of Ethane-1,2-dithiol with 1,3-Dichloropropene in the System Hydrazine Hydrate-KOH. Russian Journal of Organic Chemistry, 2018, 54, 1446-1452.	0.3	5
4032	Theoretical Study on the Mechanism of Rearrangement Reactions of Bicyclic Derivatives of Cyclopropane to Monocyclic Derivatives under the Catalysis of Pt-Salt. ACS Omega, 2018, 3, 16165-16174.	1.6	3
4033	Mechanistic insight on water and substrate catalyzed the synthesis of 3-(1-hydroxyindol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one: Driving by noncovalent interactions. Journal of Computational Chemistry, 2018, 39, 2316-2323.		15

#	ARTICLE	IF	CITATIONS
4034	On the electron flow sequence driving the hydrometallation of acetylene by lithium hydride. <i>Journal of Molecular Modeling</i> , 2018, 24, 305.	0.8	5
4035	A theoretical investigation of the reaction between the amidogen, NH, and the ethyl, C <sub>2</sub> H <sub>5</sub> , radicals: a possible gas-phase formation route of interstellar and planetary ethanimine. <i>Molecular Astrophysics</i> , 2018, 13, 30-37.	1.7	24
4036	Post-transition state bifurcations induce dynamical detours in Pummerer-like reactions. <i>Chemical Science</i> , 2018, 9, 8937-8945.	3.7	45
4037	Mechanistic insight into water exchange and aqua/fluoride ligand substitution reactions on aqueous species of Al, Ga and In. <i>Journal of Coordination Chemistry</i> , 2018, 71, 3847-3859.	0.8	1
4038	Direct hydroxylation of benzene to phenol mediated by nanosized vanadium oxide cluster ions at room temperature. <i>Journal of Chemical Physics</i> , 2018, 149, 074308.	1.2	3
4039	Mechanistic insights into N- $\beta$ -Bromosuccinimide-promoted synthesis of imidazo[1,2- <i>a</i> ]pyridine in water: Reactivity mediated by substrates and solvent. <i>Journal of Computational Chemistry</i> , 2018, 39, 2324-2332.	1.5	2
4040	Supported structure-controlled graphitic carbon nitride catalyst for dehydrochlorination of 1,2-dichloroethane. <i>Catalysis Science and Technology</i> , 2018, 8, 5334-5343.	2.1	11
4041	Theoretical Study of the Copper-Catalyzed Hydroarylation of (Trifluoromethyl)alkyne with Phenylboronic Acid. <i>Journal of Organic Chemistry</i> , 2018, 83, 12775-12783.	1.7	11
4042	Iron-catalyzed olefin synthesis by direct coupling of alkenes with alcohols: A DFT investigation. <i>Computational and Theoretical Chemistry</i> , 2018, 1143, 36-42.	1.1	0
4043	Temperature-Dependent Kinetics of the Reaction of a Criegee Intermediate with Propionaldehyde: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8433-8445.	1.1	14
4044	QM/MM Investigations on the Bioluminescent Decomposition of Coelenterazine Dioxetanone in Obelin. <i>Chemical Research in Chinese Universities</i> , 2018, 34, 758-766.	1.3	13
4045	Cavity Ring-Down Absorption Spectroscopy: Optical Characterization of ICI Product in Photodissociation of CH <sub>2</sub> ICI at 248 nm. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8344-8353.	1.1	2
4046	Computational study on the mechanism and kinetics of NO <sub>3</sub> -initiated atmosphere oxidation of vinyl acetate. <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 18-25.	1.1	11
4047	Atmospheric Fate of Criegee Intermediate Formed During Ozonolysis of Styrene in the Presence of H <sub>2</sub> O and NH <sub>3</sub> : The Crucial Role of Stereochemistry. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8377-8389.	1.1	13
4048	DFT study of double 1,3-dipolar cycloaddition of nitrilimines with allenates. <i>Monatshefte für Chemie</i> , 2018, 149, 2183-2193.	0.9	11
4049	Reaction probability and defluorination mechanisms of a potent greenhouse gas SF <sub>5</sub> CF <sub>3</sub> attacked by CH <sub>3</sub> radical: a theoretical study. <i>Molecular Physics</i> , 2018, 116, 2226-2238.	0.8	1
4050	Theoretical Investigations on the Reactivity of Hydrogen Peroxide toward 2,3,7,8-Tetrachlorodibenzo-p-dioxin. <i>Molecules</i> , 2018, 23, 2826.	1.7	3
4051	Theoretical Investigations on the Reactivity of Methylidyne Radical toward 2,3,7,8-Tetrachlorodibenzo-p-Dioxin: A DFT and Molecular Dynamics Study. <i>Molecules</i> , 2018, 23, 2685.	1.7	1

#	ARTICLE	IF	CITATIONS
4052	The Energetic Viability of $\hat{1}$ -Piperidine Dimerization in Lysine-derived Alkaloid Biosynthesis. <i>Metabolites</i> , 2018, 8, 48.	1.3	11
4053	Exploring the Conversion of Macrocyclic 2,2'-Biaryl Bis(thioureas) into Cyclic Monothioureas: An Experimental and Computational Investigation. <i>Journal of Organic Chemistry</i> , 2018, 83, 14022-14035.	1.7	3
4054	Computational Insight Into Vitamin K1 $\gamma$ -Hydroxylation by Cytochrome P450 4F2. <i>Frontiers in Pharmacology</i> , 2018, 9, 1065.	1.6	8
4055	Theoretical investigation of the mechanism for the reductive dehalogenation of methyl halides mediated by the CoI-based compounds cobalamin and cobaloxime. <i>Journal of Molecular Modeling</i> , 2018, 24, 316.	0.8	8
4056	Theoretical and Kinetic Properties of OH Radical-Initiated Oxidation of Galaxolide in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9151-9159.	1.1	6
4057	The catalytic role of water in the binding site of L,d-transpeptidase 2 within acylation mechanism: A QM/MM (ONIOM) modelling. <i>Tuberculosis</i> , 2018, 113, 222-230.	0.8	13
4058	Ligation state of nickel during C O bond activation with monodentate phosphines. <i>Tetrahedron</i> , 2018, 74, 6717-6725.	1.0	17
4059	Synthesis of Tripeptide Derivatives with Three Stereogenic Centers and Chiral Recognition Probed by Tetraaza Macrocyclic Chiral Solvating Agents Derived from <i>D</i> -Phenylalanine and (1 <i>S</i> ,2 <i>S</i> )-(+)-1,2-Diaminocyclohexane via $^1\text{H}$ NMR Spectroscopy. <i>Journal of Organic Chemistry</i> , 2018, 83, 13874-13887.	1.7	17
4060	Theoretical Insights into the Interaction Mechanisms between Nitric Acid and Nitrous Oxide Initiated by an Excess Electron. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7312-7319.	1.1	6
4061	Two chiral catalysts in action: insights into cooperativity and stereoselectivity in proline and cinchona-thiourea dual organocatalysis. <i>Chemical Science</i> , 2018, 9, 8738-8747.	3.7	30
4062	Mechanisms and stereoselectivities of phosphine-catalyzed (3+3) cycloaddition reaction between azomethine imine and ynone: A computational study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25729.	1.0	1
4063	Theoretical investigation of gold(I)-catalyzed intramolecular SEAr in isoxazole derivatives: Mechanisms, origin of regioselectivity, and role of hydrogen acceptor. <i>Molecular Catalysis</i> , 2018, 460, 27-35.	1.0	11
4064	Density functional theory studies on the external OH-induced barrierless proton dissociation mechanism for the forced hydrolysis reaction of $\text{Al}^{3+}(\text{aq})$ . <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25682.	1.0	4
4065	Unexpected Reaction Pathways Leading to Thiodiglycol During the Degradation of Long-Chain Sulfur Mustards. <i>Journal of Organic Chemistry</i> , 2018, 83, 12432-12439.	1.7	3
4066	Where and How Does an Organic Molecule Having a C-X Bond Release $\text{X}^{-}$ Anion Like an Inorganic Compound? A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7598-7613.	1.1	2
4067	Low Temperature Oxidation Kinetics of Biodiesel Molecules: Rate Rules for Concerted $\text{HO}_2$ Elimination from Alkyl Ester Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8259-8273.	1.1	14
4068	Theoretical Study of the $\text{C}_2\text{H}_5 + \text{HO}_2$ Reaction: Mechanism and Kinetics. <i>Molecules</i> , 2018, 23, 1919.	1.7	2
4069	Mechanistic insight into the ruthenium-catalyzed cycloaddition of enynes with alkynes: A theoretical study. <i>Journal of Organometallic Chemistry</i> , 2018, 875, 46-51.	0.8	7

#	ARTICLE	IF	CITATIONS
4070	A DFT mechanistic study of the ODH of n-hexane over isolated H <sub>3</sub> VO <sub>4</sub> . <i>Molecular Catalysis</i> , 2018, 452, 83-92.	1.0	4
4071	Mechanistic Study of the Reactions of Methyl Peroxy Radical with Methanol or Hydroxyl Methyl Radical. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5078-5088.	1.1	17
4072	Transient metal-centered states mediate isomerization of a photochromic ruthenium-sulfoxide complex. <i>Nature Communications</i> , 2018, 9, 1989.	5.8	29
4073	Mechanism for Co(dppp)-catalyzed regioselective intermolecular hydroacylation of 1,3-dienes and benzaldehydes: Insights from density functional calculations. <i>Journal of Organometallic Chemistry</i> , 2018, 868, 102-111.	0.8	7
4074	Reaction Kinetics of Hydrogen Atom Abstraction from C <sub>4</sub> -C <sub>6</sub> Alkenes by the Hydrogen Atom and Methyl Radical. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5202-5210.	1.1	15
4075	Hydrogenation of Multiple Bonds by Geminal Aminoborane-Based Frustrated Lewis Pairs. <i>Chemistry - A European Journal</i> , 2018, 24, 8833-8840.	1.7	32
4076	Palladium Catalysis in the Intramolecular Carbene C-H Insertion of $\alpha$ -Diazomethyl(methoxycarbonyl)acetamides to Form $\beta$ -Lactams. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 4446-4455.	1.2	14
4077	Double Hydrogen-Atom Exchange Reactions of HX (X = F, Cl, Br, I) with HO <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2018, 122, 5251-5260.	1.1	6
4078	The DFT study of Si-doped Pd <sub>6</sub> Si clusters for selective acetylene hydrogenation reaction. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 129-137.	1.3	10
4079	Puckering transitions in cyclohexane: Revisited. <i>Chemical Physics Letters</i> , 2018, 702, 82-89.	1.2	9
4080	Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 478, 3042-3048.	1.6	5
4081	Solvent effects on cycloaddition reactions of potent spin-trapping probe N-tert-butylmethanimine N-oxide: A DFT study. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1850027.	1.8	2
4082	Theoretical investigation on the gas phase decomposition of ethyl acetate by Ni <sup>+</sup> . <i>Structural Chemistry</i> , 2018, 29, 1449-1456.	1.0	3
4083	Solvent effect on isomerization reaction of [( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )(CO) <sub>2</sub> Re C(C <sub>2</sub> H <sub>5</sub> O) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> )] carbene complex to [( $\eta$ -5-C <sub>5</sub> H <sub>5</sub> )(CO)(COC <sub>2</sub> H <sub>5</sub> O) <sub>2</sub> Re C(C <sub>6</sub> H <sub>5</sub> )] carbyne complex: A computational investigation. <i>Journal of Molecular Liquids</i> , 2018, 265, 164-171.	2.3	14
4084	A Theoretical Investigation of the Reaction H+SiS <sub>2</sub> and Implications for the Chemistry of Silicon in the Interstellar Medium. <i>Lecture Notes in Computer Science</i> , 2018, , 719-729.	1.0	2
4085	A Theoretical Investigation of the Reaction N(2D) <sup>+</sup> +C <sub>6</sub> H <sub>6</sub> and Implications for the Upper Atmosphere of Titan. <i>Lecture Notes in Computer Science</i> , 2018, , 763-772.	1.0	10
4086	Copper-catalyzed cyclopropanation reaction of but-2-ene. <i>Journal of Molecular Modeling</i> , 2018, 24, 195.	0.8	9
4087	The Effect of Polymer Structures on Complete Degradation: A First-Principles Study. <i>ChemistryOpen</i> , 2018, 7, 463-466.	0.9	5



#	ARTICLE	IF	CITATIONS
4088	Theoretical study on the elimination kinetics in the gas phase of allyl methyl compounds. Monatshefte für Chemie, 2018, 149, 1389-1400.	0.9	4
4089	Copper(II) and Sodium(I) Complexes based on 3,7-Diacetyl-1,3,7-triazaphosphabicyclo[3.3.1]nonane-5-oxide: Synthesis, Characterization, and Catalytic Activity. Chemistry - an Asian Journal, 2018, 13, 2868-2880.	1.7	22
4090	Reaction of CO <sub>2</sub> with Atomic Transition Metal M <sup>+n</sup> Ions: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 5848-5860.	1.1	10
4091	A computational mechanistic study of substrate-controlled competitive O-H and C-H insertion reactions catalyzed by dirhodium(II) carbenoids: insight into the origin of chemoselectivity. Organic Chemistry Frontiers, 2018, 5, 2353-2363.	2.3	9
4092	Designing Metal-Free Frustrated Lewis Pairs Catalyst for the Efficient Dehydrogenation of Ammonia Borane. Chemistry - A European Journal, 2018, 24, 13238-13245.	1.7	14
4093	Thermochemical and Kinetics of the CH <sub>3</sub> OH + (S)N Reactional System. Journal of Physical Chemistry A, 2018, 122, 5905-5910.	1.1	2
4094	Origin of stereoselectivity in the amination of alcohols using cooperative asymmetric dual catalysis involving chiral counter-ions. Chemical Science, 2018, 9, 6126-6133.	3.7	23
4095	Formation of Nitrogen-Bearing Organic Molecules in the Reaction NH <sub>3</sub> +C <sub>2</sub> H <sub>5</sub> : A Theoretical Investigation and Main Implications for Prebiotic Chemistry in Space. Lecture Notes in Computer Science, 2018, , 773-782.	1.0	3
4096	Water catalyzed pyrolysis of oxygen functional groups of coal: A density functional theory investigation. Fuel, 2018, 233, 328-335.	3.4	13
4097	OH initiated oxidation mechanism of monoterpene (linalool) - A first comprehensive theoretical study. Atmospheric Environment, 2018, 189, 235-243.	1.9	6
4098	Structural and Computational Bases for Dramatic Skeletal Rearrangement in Anditomin Biosynthesis. Journal of the American Chemical Society, 2018, 140, 9743-9750.	6.6	43
4100	Computational investigation of M1/W6S8 (M=Fe, Ru, and Os) single-atom catalysts for CO <sub>2</sub> hydrogenation. Catalysis Surveys From Asia, 2018, 22, 195-207.	1.0	6
4101	Understanding the Diels-Alder reactivity of 1,2-azaborine analogues. Tetrahedron, 2018, 74, 4289-4294.	1.0	7
4102	Mechanistic and kinetic study on the reaction of Furan with O( <sup>3</sup> P). Journal of Physical Organic Chemistry, 2018, 31, e3864.	0.9	2
4103	Electrophilicity of aliphatic nitrilium closo-decaborate clusters: Hyperconjugation provides an unexpected inverse reactivity order. Journal of Organometallic Chemistry, 2018, 870, 97-103.	0.8	12
4104	Access to 3-aminobenzothiophenes and 3-aminothiophenes fused to 5-membered heteroaromatic rings through 6-electrocyclization reaction of keteniminium salts. Tetrahedron Letters, 2018, 59, 3242-3248.	0.7	17
4105	<i>o</i> -Substituted group-controlled selectivity in Rh(III)-catalyzed coupling of benzamides with 1,1-difluoromethylene alkynes: a computational mechanistic study. Catalysis Science and Technology, 2018, 8, 3590-3598.	2.1	14
4106	Theoretical exploration of H <sub>2</sub> X (X=O, S, Se) and HY (Y=F, Cl, Br) assisted H <sub>2</sub> -release from ammonia-borane and related compounds: mechanistic insights from theoretical viewpoint. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	5

#	ARTICLE	IF	CITATIONS
4107	When Applying the Mercury Poisoning Test to Palladacycle-Catalyzed Reactions, One Should Not Consider the Common Misconception of Mercury(0) Selectivity. <i>Organometallics</i> , 2018, 37, 2842-2858.	1.1	44
4108	Mechanistic investigation in the [1,4] and [1,2] Wittig rearrangement reactions: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21457-21473.	1.3	3
4109	BNPd single-atom catalysts for selective hydrogenation of acetylene to ethylene: a density functional theory study. <i>Royal Society Open Science</i> , 2018, 5, 171598.	1.1	3
4110	Theoretical study of the single noble metal stabilized on metal oxide clusters catalyze the water-gas shift reaction. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25767.	1.0	6
4111	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2018, 83, 10959-10973.	1.7	41
4112	Quantum chemical study on the role of water in the reaction of singlet methoxysulfonyl nitrene CH <sub>3</sub> OS(O)N. <i>Chemical Physics Letters</i> , 2018, 706, 548-552.	1.2	3
4113	Regioselective Arene and Heteroarene Functionalization: <i>N</i> -Alkenoxypyridinium Salts as Electrophilic Alkylating Agents for the Synthesis of <i>1</i> -Aryl/ <i>1</i> -Heteroaryl Ketones. <i>Journal of Organic Chemistry</i> , 2018, 83, 10051-10059.	1.7	31
4114	Insights on the Origin of Regiodivergence in the Parallel Kinetic Resolution of <i>rac</i> -Aziridines Using a Chiral Lanthanum-Yttrium Bimetallic Catalyst. <i>ACS Catalysis</i> , 2018, 8, 7633-7644.	5.5	9
4115	Oxidopyrylium-Alkene [5 + 2] Cycloaddition Conjugate Addition Cascade (C <sup>3</sup> ) Sequences: Scope, Limitation, and Computational Investigations. <i>Journal of Organic Chemistry</i> , 2018, 83, 9818-9838.	1.7	19
4116	An investigation of molecular mechanism and the role of Te-bridged-atom in the formation of polysubstituted pyridines via Hetero-Diels-Alder reaction of isotellurazole with acetylenic dienophile: a molecular electron density study. <i>Journal of Chemical Sciences</i> , 2018, 130, 1.	0.7	7
4117	Syntheses of Substituted 1,4-Disila-2,5-cyclohexadienes from Cyclic Hexasilane Si <sub>6</sub> Me <sub>12</sub> and Alkynes via Successive Si-Si Bond Activation by Pd/Isocyanide Catalysts. <i>Organometallics</i> , 2018, 37, 2531-2543.	1.1	11
4118	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aryl coumarins: mechanism and enantioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5474-5482.	1.5	6
4119	Regular patterns of the effects of hydrogen-containing additives on the formation of CdSe monomer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 20863-20873.	1.3	1
4120	A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in Ingenol Esters. <i>Australian Journal of Chemistry</i> , 2018, 71, 212.	0.5	4
4121	Base Mechanism to the Hydrolysis of Phosphate Triester Promoted by the Cd <sup>2+</sup> /Cd <sup>2+</sup> Active site of Phosphotriesterase: A Computational Study. <i>Inorganic Chemistry</i> , 2018, 57, 5888-5902.	1.9	6
4122	Study on the reaction mechanism between Pb <sub>3</sub> O <sub>4</sub> and Si in stored silicon delay composition. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 132, 327-336.	2.0	7
4123	Theoretical investigation on cyclohexane dehydrogenation catalyzed by V <sup>2+</sup> in gas-phase. <i>Structural Chemistry</i> , 2018, 29, 1129-1137.	1.0	2
4124	Exploration of unprecedented catalytic dehydrogenation mechanism of methylamine-water mixture in presence of Ru-pincer complex: A systematic DFT study. <i>Journal of Catalysis</i> , 2018, 363, 164-182.	3.1	10

#	ARTICLE	IF	CITATIONS
4125	Variation of the Intersection Point of the Potential Surface Crossing Induced by the Laser Phase Along the Reaction Path in Ion-Molecule Reactions: Application To $\text{Li}^+ + \text{CH}_4$ . <i>Journal of Structural Chemistry</i> , 2018, 59, 20-27.	0.3	0
4126	Photoelectrocatalytic application of palladium decorated zinc oxide-expanded graphite electrode for the removal of 4-nitrophenol: experimental and computational studies. <i>RSC Advances</i> , 2018, 8, 10255-10266.	1.7	25
4127	Computational Approach to Unravel the Role of Hydrogen Bonding in the Interaction of NAMI-A with DNA Nucleobases and Nucleotides. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8397-8411.	1.1	4
4128	Mechanistic and Kinetic Study on the Reaction of Thiophene ( $\text{C}_4\text{H}_4\text{S}$ ) with $\text{O}(\text{ }^3\text{P})$ . <i>ChemistrySelect</i> , 2018, 3, 8644-8650.	0.7	2
4129	A molecular mechanism for the enzymatic methylation of nitrogen atoms within peptide bonds. <i>Science Advances</i> , 2018, 4, eaat2720.	4.7	48
4130	Intramolecular $[3 + 2]$ Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET). <i>Journal of Physical Chemistry A</i> , 2018, 122, 7472-7481.	1.1	17
4131	The DFT Study of Single-Atom Pd1/g-C <sub>3</sub> N <sub>4</sub> Catalyst for Selective Acetylene Hydrogenation Reaction. <i>Catalysis Letters</i> , 2018, 148, 2992-3002.	1.4	21
4132	Theoretical investigations of the Ir-catalyzed direct borylation of B(3,6)- <i>carborane</i> : the actual catalyst, mechanism, and origin of regioselectivity. <i>Catalysis Science and Technology</i> , 2018, 8, 5165-5177.	2.1	22
4133	Mechanistic details of ethylene polymerization reaction using methyl nickel catalysts. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22915-22925.	1.3	5
4134	Catalytic Enantioselective $[10+4]$ Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13182-13186.	7.2	42
4135	Benzylic Thio and Seleno Newman-Kwart Rearrangements. <i>Journal of Organic Chemistry</i> , 2018, 83, 10786-10797.	1.7	9
4136	Gas-Phase Reactions of Carbon Dioxide with Copper Hydride Anions $\text{Cu}_2\text{H}_2^+$ : Temperature-Dependent Transformation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19379-19384.	1.5	26
4137	Reactions of sulfur and oxygen containing anions with nitrogen and oxygen atoms: A comparative study. <i>International Journal of Mass Spectrometry</i> , 2018, 433, 1-6.	0.7	5
4138	DFT study on the Au-catalyzed cyclization of indole-allenoate: counterion and solvent effects. <i>New Journal of Chemistry</i> , 2018, 42, 15618-15628.	1.4	14
4139	Catalytic Enantioselective $[10+4]$ Cycloadditions. <i>Angewandte Chemie</i> , 2018, 130, 13366-13370.	1.6	10
4140	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions. <i>Molecules</i> , 2018, 23, 1913.	1.7	13
4141	On-the-fly kinetics of hydrogen abstraction from polycyclic aromatic hydrocarbons by methyl/ethyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23578-23592.	1.3	5
4142	Effect of oligomerization reactions of Criegee intermediate with organic acid/peroxy radical on secondary organic aerosol formation from isoprene ozonolysis. <i>Atmospheric Environment</i> , 2018, 187, 218-229.	1.9	17

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4143	A molecular electron density theory study on the [3+2] cycloaddition reaction of thiocarbonyl ylides with hetaryl thioketones. <i>New Journal of Chemistry</i> , 2018, 42, 11819-11830.	1.4	7
4144	Lactamization of $sp^2$ C-H bonds with $CO_2$ under transition-metal-free and redox-neutral conditions: a computational mechanistic study. <i>Organic Chemistry Frontiers</i> , 2018, 5, 2189-2201.	2.3	8
4145	Questions in natural products synthesis research that can (and cannot) be answered using computational chemistry. <i>Chemical Society Reviews</i> , 2018, 47, 7845-7850.	18.7	28
4146	Theoretical insights into the reaction mechanisms between 2,3,7,8-tetrachlorodibenzofuran and the methylidyne radical. <i>RSC Advances</i> , 2018, 8, 21150-21163.	1.7	6
4147	Computational Study on Gold-Catalyzed Cascade Reactions of 1,4-Diynes and Pyrroles: Mechanism, Regioselectivity, Role of Catalyst, and Effects of Substituent and Solvent. <i>Organometallics</i> , 2018, 37, 1927-1936.	1.1	15
4148	The ion pair mechanism in the thermal deamination of primary amines catalyzed by HBr in the gas phase: DFT and AIM analysis. <i>Chemical Physics Letters</i> , 2018, 703, 117-123.	1.2	4
4149	A theoretical investigation on the mechanism of cycloaddition reactions of fulvenes with tetrazine and diazacyclopentadienone derivatives. <i>Structural Chemistry</i> , 2018, 29, 1511-1523.	1.0	5
4150	Electrostatic, sequential bond energies and structures of $Li^+ \cdot (N_2)_n$ complexes: computational study. <i>Structural Chemistry</i> , 2019, 30, 53-60.	1.0	6
4151	Theoretical investigation of $N(2D) + HOX (Cl, Br)$ reaction. <i>Molecular Physics</i> , 2019, 117, 228-240.	0.8	0
4152	Photodissociation of $CH_2BrI$ using cavity ring-down spectroscopy: in search of a BrI elimination channel. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13943-13949.	1.3	4
4153	Mechanistic study of the reaction of methyl peroxy radical ( $CH_3O_2$ ) with formaldehyde ( $CH_2O$ ). <i>Molecular Physics</i> , 2019, 117, 298-302.	0.8	6
4154	Mechanism and Substituent Effects of Benzene Arylation via a Phenyl Cation Strategy: A Density Functional Theory Study. <i>ChemCatChem</i> , 2019, 11, 5068-5076.	1.8	5
4155	An investigation of the molecular mechanism, chemoselectivity and regioselectivity of cycloaddition reaction between acetonitrile N-Oxide and 2,5-dimethyl-2H-[1,2,3]diazaphosphole: a MEDT study. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	15
4156	Theoretical Investigation of Excited-State Intramolecular Proton Transfer and Photoisomerization of 2-(Iminomethyl)phenol. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7246-7254.	1.1	5
4157	Mechanistic insights and origin of chemoselectivity for S=O bond cleavage in dinitrobenzenesulfonic carbamates. <i>New Journal of Chemistry</i> , 2019, 43, 14594-14602.	1.4	1
4158	Inherent atomic mobility changes in carbocation intermediates during the sesterterpene cyclization cascade. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 1890-1897.	1.3	6
4159	A density functional theory study on mechanisms of [4+2] annulation of enal with $\alpha$ -methylene cycloalkanone catalyzed by N-heterocyclic carbene. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e26039.	1.0	3
4160	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8185-8193.	1.5	11



#	ARTICLE	IF	CITATIONS
4179	Ligands and Bases Mediate Switching between Aminocarbonylations and Alkoxy carbonylations in Coupling of Aminophenols with Iodoarenes. <i>Inorganic Chemistry</i> , 2019, 58, 10217-10226.	1.9	8
4180	Mechanism and theory of $\alpha$ -glucopyranose homogeneous acid catalysis in the aqueous solution phase. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17993-18011.	1.3	9
4181	Chromium carbonyl complexes with aryl mono- and oligogermanes: Ability for haptotropic rearrangement. <i>Journal of Organometallic Chemistry</i> , 2019, 897, 217-227.	0.8	11
4182	The reactivity of CO on bimetallic Ni <sub>3</sub> M clusters (M = Sc, Ti, V, Cr, Mn, Fe, Co, Cu, Rh, Ru, Ag, Pd and Pt) by density functional theory. <i>New Journal of Chemistry</i> , 2019, 43, 11363-11373.	1.4	3
4183	A Computational Study of the Reaction N(2D) $\rightarrow$ C <sub>6</sub> H <sub>6</sub> Leading to Pyridine and Phenylnitrene. <i>Lecture Notes in Computer Science</i> , 2019, , 316-324.	1.0	10
4184	Comparative DFT study on the platinum catalyzed [3+2] and [2+2] cycloaddition reactions between the derivatives of allene and alkene. <i>Computational and Theoretical Chemistry</i> , 2019, 1163, 112507.	1.1	2
4185	Exploring the reactivity of carbene supported diboraanthracene towards dihydrogen activation. <i>Polyhedron</i> , 2019, 170, 666-673.	1.0	0
4186	Elucidating the origin of selectivity of [3+2]-cycloaddition reactions between thioketone and carbohydrate-derived nitrones by the DFT. <i>Journal of Molecular Modeling</i> , 2019, 25, 209.	0.8	8
4187	Hydrogen activation by isomeric aromatic phosphabenzene: A theoretical study. <i>Polyhedron</i> , 2019, 170, 690-694.	1.0	1
4188	Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3227.	1.8	6
4189	Electronic Structure and Kinetics Calculations for the Si+SH Reaction, a Possible Route of SiS Formation in Star-Forming Regions. <i>Lecture Notes in Computer Science</i> , 2019, , 306-315.	1.0	4
4190	Mechanistic Insights into the Chemo- and Regio-Selective B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> Catalyzed C-H Functionalization of Phenols with Diazoesters. <i>Journal of Organic Chemistry</i> , 2019, 84, 14508-14519.	1.7	27
4191	Transferring Colorization with Smaller Samples. <i>Journal of Physics: Conference Series</i> , 2019, 1302, 032047.	0.3	0
4192	DFT Studies on the Al-Speciation and Its Structure in Aqueous Aluminum Sol Formed by Aluminum Formoacetate. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9167-9179.	1.2	3
4193	The solvation effect on the rattling behaviour of the hydrated excess proton in water. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22385-22389.	1.3	1
4194	Insight into the mechanism of ethanol steam reforming on TM/Mo <sub>6</sub> S <sub>8</sub> clusters catalysts: A theoretical investigation. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 23947-23958.	3.8	3
4195	Dissection of the Mechanism of the Wittig Reaction. <i>Journal of Organic Chemistry</i> , 2019, 84, 14644-14658.	1.7	28
4196	Effectiveness of the bimetallic catalytic center over the monometallic one for catalyzing the rearrangement of cyclopropanated bicyclic derivatives. <i>Journal of Organometallic Chemistry</i> , 2019, 899, 120907.	0.8	1

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4197	On the Mechanism of the Asymmetric Aldol Addition of Chiral N- $\alpha$ -Amino Cyclic Carbamate Hydrazones: Evidence of Non-Curtin-Hammett Behavior. <i>Chemistry - A European Journal</i> , 2019, 25, 16037-16047.	1.7	3
4198	Base-Assisted Conversion of Protonated $D$ -Fructose to 5-HMF: Searching for Gas-Phase Green Models. <i>ChemistryOpen</i> , 2019, 8, 1190-1198.	0.9	10
4199	Computational Study on the Mechanisms and Pathways of the Atmospheric $NH_2 + BrO$ Reaction. <i>ChemistrySelect</i> , 2019, 4, 11002-11008.	0.7	0
4200	Advances in Spectroscopy: Molecules to Materials. <i>Springer Proceedings in Physics</i> , 2019, , .	0.1	4
4201	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. <i>Scientific Reports</i> , 2019, 9, 15361.	1.6	17
4202	Understanding the Reactivity of Neutral Geminal Group 14 Element/Phosphorus Frustrated Lewis Pairs. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10095-10101.	1.1	20
4203	Computationally Assisted Mechanistic Investigation into Hypervalent Iodine Catalysis: Cyclization of <i>N</i> -Allylbenzamide. <i>Journal of Organic Chemistry</i> , 2019, 84, 15605-15613.	1.7	13
4204	Computational Insight into the Mechanism of Ruthenium(II)-Catalyzed $\alpha$ -Alkylation of Arylmethyl Nitriles Using Alcohols. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10263-10272.	1.1	2
4205	Substituent Effect on the Hiltner Intramolecular Arene/Allene Diels-Alder Reaction: NBO Analysis and State Specific Dual Descriptors. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10730-10738.	1.1	7
4206	Formation of active species from ruthenium alkylidene catalysts—an insight from computational perspective. <i>Journal of Molecular Modeling</i> , 2019, 25, 331.	0.8	7
4207	Comprehensive Understanding of Bifunctional Behavior of PNP-Pincer Complexes Towards the Conversion of CO into Methanol and $CO_2$ : A DFT Approach. <i>ChemistrySelect</i> , 2019, 4, 10777-10786.	0.7	2
4208	Dehydrocyclization of diamine borane and amine-borane alcohol catalyzed by 1-lithio-2-alkyl-1,2-dihydropyridine and its Na & K analogues: A DFT analysis of the reaction mechanism. <i>International Journal of Hydrogen Energy</i> , 2019, 44, 28731-28745.	3.8	3
4209	Oxidation of Isoprene by Neutral Iron Oxide Nanoclusters in the Gas Phase. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25949-25956.	1.5	8
4210	A DFT Study of Acetylene Hydrogenation Catalyzed by S-Doped Pd <sub>1</sub> /g-C <sub>3</sub> N <sub>4</sub> . <i>Catalysts</i> , 2019, 9, 887.	1.6	7
4211	Density Functional Theory Studies on the Real and Apparent Water-Exchange Reaction Kinetics of $Al^{3+}$ in Aqueous Solution. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2315-2322.	1.2	2
4212	Stereoselective cyclopropanation of olefins through ammonium ylides: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e4008.	0.9	3
4213	Theoretical Investigation on Mechanism, Thermochemistry, and Kinetics of the Gas-phase Reaction of 2-Propargyl Radical with Formaldehyde. <i>Chemical Research in Chinese Universities</i> , 2019, 35, 884-891.	1.3	14
4214	N-Heterocyclic Carbene Ligand-Controlled Chemodivergent Suzuki-Miyaura Cross Coupling. <i>Journal of Organic Chemistry</i> , 2019, 84, 11799-11812.	1.7	26

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4215	Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical: Hydrogen and Chlorine Atom Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8954-8967.	1.1	13
4216	Further understanding of the Ru-centered [2+2] cycloreversion/cycloaddition involved into the interconversion of ruthenacyclobutane using the Grubbs catalysts from a reaction force analysis. <i>Journal of Molecular Modeling</i> , 2019, 25, 305.	0.8	4
4217	A molecular electron density theory study of the mechanism, chemo- and stereoselectivity of the epoxidation reaction of <i>R</i> -carvone with peracetic acid. <i>RSC Advances</i> , 2019, 9, 28500-28509.	1.7	15
4218	Theoretical study on desulfurization mechanisms of a coal-based model compound 2-methylthiophene during pyrolysis under inert and oxidative atmospheres. <i>Fuel</i> , 2019, 257, 116028.	3.4	15
4219	Exploration of tetra-branched multiple-site SO <sub>2</sub> capture materials. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18250-18258.	1.3	2
4220	Mechanistic insight into photocrosslinking reaction between triplet state 4-thiopyrimidine and thymine. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21305-21316.	1.3	3
4221	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 609.	1.8	3
4222	Mechanistic Insight into the Ring-Opening Polymerization of $\epsilon$ -Caprolactone and L-Lactide Using Ketiminate-Ligated Aluminum Catalysts. <i>Polymers</i> , 2019, 11, 1530.	2.0	7
4223	Molecular and dissociated adsorption of hydrogen on TiC <sub>6</sub> H <sub>6</sub> . <i>International Journal of Hydrogen Energy</i> , 2019, 44, 25800-25808.	3.8	8
4224	Single-Atom X/g-C <sub>3</sub> N <sub>4</sub> (X = Au <sub>1</sub> , Pd <sub>1</sub> , and Ru <sub>1</sub> ) Catalysts for Acetylene Hydrochlorination: A Density Functional Theory Study. <i>Catalysts</i> , 2019, 9, 808.	1.6	14
4225	Site Selectivity in Pd-Catalyzed Reactions of $\alpha$ -Dialkyl-(methoxycarbonyl)acetamides: Effects of Catalysts and Substrate Substitution in the Synthesis of Oxindoles and $\beta$ -Lactams. <i>Molecules</i> , 2019, 24, 3551.	1.7	5
4226	Chameleon-like Behavior of the Directing Group in the Rh(III)-Catalyzed Regioselective C-H Amidation of Indole: An Experimental and Computational Study. <i>ACS Catalysis</i> , 2019, 9, 10233-10244.	5.5	40
4227	Theoretical investigation of the reactivity of bispentamethylcyclopentadienyl uranium(IV) bithiolate complexes with the heteroallene molecules CS <sub>2</sub> and CO <sub>2</sub> . <i>Journal of Organometallic Chemistry</i> , 2019, 901, 120947.	0.8	5
4228	Deciphering the exceptional selectivity of semipinacol rearrangements in <i>cis</i> -fused $\beta$ -lactam diols using high-level quantum chemical methods. <i>Organic Chemistry Frontiers</i> , 2019, 6, 725-731.	2.3	5
4229	Understanding the <i>Z</i> -selectivity of the metal-free intermolecular aminoarylation of alkynes: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 125-133.	2.3	9
4230	Designing metal-free frustrated Lewis pairs for dihydrogen activation based on a carbene-borane system. <i>Polyhedron</i> , 2019, 162, 1-7.	1.0	3
4231	Molecular mechanism comparison of decarbonylation with deoxygenation and hydrogenation of 5-hydroxymethylfurfural catalyzed by palladium acetate. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 3795-3804.	1.3	8
4232	Hydrogen- and oxygen-atom transfers in the thermal activation of benzene mediated by Cu <sub>2</sub> O <sub>2</sub> <sup>+</sup> cations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1117-1122.	1.3	2



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4233	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 498-508.	1.5	11
4234	Pushing the limits of concertedness. A waltz of wandering carbocations. <i>Chemical Science</i> , 2019, 10, 2159-2170.	3.7	21
4235	Energy Landscapes in Photochemical Dissociation of Small Peroxides. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1353-1362.	1.1	5
4236	Insights into highly selective ring expansion of oxaziridines under Lewis base catalysis: a DFT study. <i>Organic Chemistry Frontiers</i> , 2019, 6, 679-687.	2.3	38
4237	Mechanism and chemoselectivity origins of bioconjugation of cysteine with Au(III)-aryl reagents. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1245-1253.	1.5	15
4238	Computational design of biofuels from terpenes and terpenoids. <i>Sustainable Energy and Fuels</i> , 2019, 3, 457-466.	2.5	23
4239	Carbones and Heavier Ylidones (EL <sub>2</sub> ) in Frustrated Lewis Pair Chemistry: Influence of the Nature of EL <sub>2</sub> on Dihydrogen Activation. <i>Inorganic Chemistry</i> , 2019, 58, 7828-7836.	1.9	26
4240	Organocatalytic Asymmetric Addition of Aldehyde to Nitroolefin by H-Pro-Glu-NH <sub>2</sub> : A Mechanistic Study. <i>ACS Omega</i> , 2019, 4, 8862-8873.	1.6	4
4241	An effective method to make polymers degrade readily: spatial isomerization. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16905-16909.	1.3	4
4242	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. <i>Dalton Transactions</i> , 2019, 48, 9214-9224.	1.6	4
4243	Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. <i>ChemPhysChem</i> , 2019, 20, 1812-1821.	1.0	5
4244	Experimental and Theoretical Approaches in the Study of Phenanthroline-tetrahydroquinolines for Alzheimer's Disease. <i>ChemistryOpen</i> , 2019, 8, 627-636.	0.9	4
4245	Hypercoordinate iodine for catalytic asymmetric diamination of styrene: insights into the mechanism, role of solvent, and stereoselection. <i>Chemical Science</i> , 2019, 10, 7082-7090.	3.7	14
4246	Synthesis and Catalytic Reactivity of Bis(molybdenum-trihalide) Complexes Bridged by Ferrocene Skeleton toward Catalytic Nitrogen Fixation. <i>Organometallics</i> , 2019, 38, 2863-2872.	1.1	13
4247	Unexpected intramolecular N-arylcyano- $\beta$ -diketiminato cyclization in new aminoquinoline derivative complexes of aluminium for CO <sub>2</sub> fixation into cyclic carbonates. <i>New Journal of Chemistry</i> , 2019, 43, 12059-12068.	1.4	3
4248	<sup>27</sup> Al NMR Chemical Shifts and Relative Stabilities of Aqueous Monomeric Al <sup>3+</sup> Hydrolytic Species with Different Coordination Structures. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1353-1361.	1.2	14
4249	A density functional theory study on the [3+2] cycloaddition of N-(p-methylphenacyl)benzothiazolium ylide and 1-nitro-2-(p-methoxyphenyl) ethene: the formation of two diastereomeric adducts via two different mechanisms. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	6
4250	Theoretical study on the mechanism and chemoselectivity in gold(I)-catalyzed cycloisomerization of $\beta,\beta$ -disubstituted ortho-(alkynyl)styrenes. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2701-2712.	2.3	13

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4251	Mechanistic investigation-inspired activation mode of DBU and the function of the $\hat{\pm}$ -diazo group in the reaction of the $\hat{\pm}$ -amino ketone compound and EDA: [DBU-H] <sup>+</sup> -DMF-H <sub>2</sub> O and $\hat{\pm}$ -diazo as strong N-terminal nucleophiles. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2678-2686.	2.3	2
4252	Radiation Damage Mechanisms of Chemotherapeutically Active Nitroimidazole Derived Compounds. <i>Frontiers in Chemistry</i> , 2019, 7, 329.	1.8	10
4253	[Cp <sub>2</sub> Mo(OH)(OH <sub>2</sub> )] <sup>+</sup> -Catalyzed Hydrolysis of Mono- and Difunctional Ethers: Theoretical Understanding of Their Divergent Reactivity. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2924-2932.	1.0	1
4254	Molecular Insights on the Role of (CTA <sup>+</sup> )(SiO <sup>+</sup> ) Ion Pair into the Catalytic Activity of [CTA <sup>+</sup> ] <sup>+</sup> Si <sup>+</sup> MCM-41. <i>Topics in Catalysis</i> , 2019, 62, 941-955.	1.3	4
4255	How effectively bonding evolution theory retrieves and visualizes curly arrows: The cycloaddition reaction of cyclic nitrones. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25985.	1.0	18
4256	H/D exchange in N-heterocycles catalysed by an NHC-supported ruthenium complex. <i>Catalysis Science and Technology</i> , 2019, 9, 3398-3407.	2.1	9
4257	Theory Research of Catalytic for Water-Gas Shift-Reaction by Copper Doping of TM Clusters (TM = Ag,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.3	0
4258	Impact of C=C/B <sup>N</sup> Replacement on the Diels-Alder Reactivity of Curved Polycyclic Aromatic Hydrocarbons. <i>Chemistry - A European Journal</i> , 2019, 25, 9771-9779.	1.7	7
4259	Computational Study of the Formation of C8, C5, and C4 Guanine:Lysine Adducts via Oxidation of Guanine by Sulfate Radical Anion. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5150-5163.	1.1	7
4260	Influence of H <sub>3</sub> O <sup>+</sup> on the structure formation of oligomers in aluminium sols prepared from basic aluminium acetate: Experiments and computations. <i>Journal of Molecular Liquids</i> , 2019, 289, 111052.	2.3	10
4261	Complexes of Zn(II)-Triazoles with CO <sub>2</sub> and H <sub>2</sub> O: Structures, Energetics, and Applications. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5555-5565.	1.1	5
4262	An Experimental and Theoretical Investigation of 1-Butanol Pyrolysis. <i>Frontiers in Chemistry</i> , 2019, 7, 326.	1.8	12
4263	Pressure-Dependent Rate Rules for the Intramolecular H-Shift Reactions of Hydroperoxy-Alkenyl-Peroxy Radicals in Low Temperature. <i>Energy &amp; Fuels</i> , 2019, 33, 5597-5609.	2.5	6
4264	Palladium- and Ruthenium-Catalyzed Intramolecular Carbene C Ar <sup>H</sup> Functionalization of $\hat{\pm}$ -Amino- $\hat{\pm}$ -diazoesters for the Synthesis of Tetrahydroquinolines. <i>Chemistry - A European Journal</i> , 2019, 25, 10239-10245.	1.7	11
4265	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. <i>Chemical Reviews</i> , 2019, 119, 8131-8191.	23.0	167
4266	Theoretical Study of the Mechanism of Catalytic Alkylation of Adamantane with 2,2,4-Trimethylpentane Cracking Products. <i>Petroleum Chemistry</i> , 2019, 59, 66-70.	0.4	3
4267	The Mechanism of the Propagation in the Anionic Polymerization of Polystyryllithium in Non-Polar Solvents Elucidated by Density Functional Theory Calculations. A Study of the Negligible Part Played by Dimeric Ion-Pairs under Usual Polymerization Conditions. <i>Polymers</i> , 2019, 11, 1022.	2.0	3
4268	Sulfate and hydroxyl radicals-initiated degradation reaction on phenolic contaminants in the aqueous phase: Mechanisms, kinetics and toxicity assessment. <i>Chemical Engineering Journal</i> , 2019, 373, 668-676.	6.6	124

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4269	Theoretical study of the reaction mechanism and kinetics of the OH <sup>-</sup> + <sup>-</sup> trimethyl orthoformate ((CH <sub>3</sub> O) <sub>3</sub> CH) <sup>-</sup> + <sup>-</sup> O <sub>2</sub> reaction. Computational and Theoretical Chemistry, 2019, 1159, 38-45.	1.1	5
4270	Doping Effects on the Reactivity of the MVO <sub>5</sub> <sup>-</sup> (M = V <sup>+</sup> Zn) Clusters in CO Oxidation Reaction. Journal of Physical Chemistry C, 2019, 123, 14180-14186.	1.5	8
4271	Insights into the mechanisms of Ag-catalyzed synthesis of CF <sub>3</sub> -substituted heterocycles via [3+2]-cycloaddition from $\hat{\pm}$ -trifluoromethylated methyl isocyanides: effects of DBU and exploration of diastereoselectivity. New Journal of Chemistry, 2019, 43, 9265-9273.	1.4	3
4272	Theoretical Study of the Possibility of Functionalization of C <sub>20</sub> Fullerene with the Simplest Ketene CH <sub>2</sub> CO. Journal of Structural Chemistry, 2019, 60, 524-535.	0.3	5
4273	Mechanisms investigation of the WGSR catalyzed by single noble metal atoms supported on vanadium oxide clusters. Applied Organometallic Chemistry, 2019, 33, e4960.	1.7	4
4274	Furthering the reaction mechanism of cationic vanadium clusters towards oxygen. Physical Chemistry Chemical Physics, 2019, 21, 11234-11241.	1.3	18
4275	Insight into the mechanism of secondary reactions in cellulose pyrolysis: interactions between levoglucosan and acetic acid. Cellulose, 2019, 26, 8279-8290.	2.4	25
4276	Formation of Protonated Glycine Isomers in the Interstellar Medium. ACS Earth and Space Chemistry, 2019, 3, 1170-1181.	1.2	7
4277	Gold(I)-catalyzed intermolecular dioxolane addition to alkynes: the role of water. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
4278	Mechanisms and Activity of 1-Phenylethanol Dehydrogenation Catalyzed by Bifunctional NHC <sup>III</sup> Complex. European Journal of Organic Chemistry, 2019, 2019, 3929-3936.	1.2	4
4279	An MEDT study of the mechanism and selectivities of the [3+2] cycloaddition reaction of tomentosin with benzonitrile oxide. International Journal of Quantum Chemistry, 2019, 119, e25980.	1.0	21
4280	The reaction mechanism study on the decarbonylation of 2-methyl-2-propenal assisted by hydrogen chloride, water, or sulfur acid. Structural Chemistry, 2019, 30, 2271-2277.	1.0	1
4281	Density functional calculations for Rh(I)-catalyzed C-C bond activation of siloxyvinylcyclopropanes and diazoesters. Applied Organometallic Chemistry, 2019, 33, e4869.	1.7	2
4282	Understanding the mechanism of the 1,3-dipolar cycloaddition reaction between a thioformaldehyde S-oxide and cyclobutadiene: Competition between the stepwise and concerted routes. Progress in Reaction Kinetics and Mechanism, 2019, 44, 213-221.	1.1	3
4283	Atmospheric reactions of glyoxal with NO <sub>2</sub> and NH <sub>2</sub> radicals: Hydrogen abstraction mechanism and natural bond orbital analysis. Progress in Reaction Kinetics and Mechanism, 2019, 44, 187-209.	1.1	7
4284	Kinetics of hydrogen abstraction from desflurane by OH and Cl radicals - A theoretical study. Chemical Physics Letters, 2019, 728, 142-147.	1.2	5
4285	A theoretical insight on the kinetics for the reaction of (E)/(Z)-CHF=CF(CF <sub>2</sub> ) <sub>x</sub> =1,2CF <sub>3</sub> with OH radicals under tropospheric conditions. Journal of Fluorine Chemistry, 2019, 222-223, 31-45.	0.9	6
4286	Amoxicillin on polyglutamic acid composite three-dimensional graphene modified electrode: Reaction mechanism of amoxicillin insights by computational simulations. Analytica Chimica Acta, 2019, 1073, 22-29.	2.6	30

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4287	Understanding the sequence of the electronic flow along the HCN/CNH isomerization within a bonding evolution theory quantum topological framework. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
4288	Unravelling the Origins of Hydroboration Chemoselectivity Inversion Using an N,O-Chelated Ir(I) Complex: A Computational Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 6709-6718.	1.7	10
4289	Mechanisms and Stereoselectivities of NHC-Catalyzed [3 + 4] Cycloaddition Reaction between Isatin-Derived Enal and N-(ortho-Chloromethyl)aryl Amide. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2989-2997.	1.2	22
4290	The structural aspects of the transformation of 3-nitroisoxazoline-2-oxide to 1-aza-2,8-dioxabicyclo[3.3.0]octane derivatives: Experimental and MEDT theoretical study. <i>Journal of Molecular Structure</i> , 2019, 1192, 27-34.	1.8	15
4291	A Computational Study of Model Parent Systems and Reported Aza-(Iso)Nazarov/Aza-(Iso)Piancatelli Electrocyclic Reactions. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2539-2551.	1.2	8
4292	High-level theoretical study of the hydrogen abstraction reaction $H_2S + O_2 = SH + HO_2$ and prediction of the rate constants. <i>Computational and Theoretical Chemistry</i> , 2019, 1155, 61-66.	1.1	3
4293	Direct Conversion of Acetylene and 1,2-Dichloroethane to Vinyl Chloride Monomer over a Supported Carbon Nitride Catalyst: Tunable Activity Controlled by the Synthesis Temperature. <i>Industrial &amp; Engineering Chemistry Research</i> , 2019, 58, 5404-5413.	1.8	4
4294	Thermochemistry and Kinetics of the Thermal Degradation of 2-Methoxyethanol as Possible Biofuel Additives. <i>Scientific Reports</i> , 2019, 9, 4535.	1.6	20
4295	Mechanisms and Kinetic Parameters for the Gas-Phase Reactions of 3-Methyl-3-buten-2-one and 3-Methyl-3-penten-2-one with Ozone. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2745-2755.	1.1	11
4296	Solvent effect on Hetero-Diels-Alder reaction of isoselenazole with symmetrical acetylenic dienophiles: A MEDT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1154, 17-25.	1.1	8
4297	Mechanistic study on iron(II)-mediated direct arylation of benzene with chlorobenzene. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25912.	1.0	1
4299	New Oxidovanadium(IV) Complexes with 2,2'-bipyridine and 1,10-phenanthroline Ligands: Synthesis, Structure and High Catalytic Activity in Oxidations of Alkanes and Alcohols with Peroxides. <i>Catalysts</i> , 2019, 9, 217.	1.6	24
4300	A DFT study on the mechanism of rhodium-catalyzed regioselective hydrothiolation of the allyl amine. <i>Molecular Catalysis</i> , 2019, 468, 62-74.	1.0	3
4301	DFT study on the regio- and stereoselectivity of the organocatalytic aza-Diels-Alder reaction of crotonaldehyde and cyclic 1-aza-1,3-butadiene. <i>Structural Chemistry</i> , 2019, 30, 1831-1842.	1.0	2
4302	Roles of Water Molecules and Counterion on HS <sup>-</sup> Sensing Reaction Utilizing a Pyrylium Derivative: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3334-3343.	1.1	2
4303	Role of (H <sub>2</sub> O) <sub>n</sub> (n = 1-2) in the Gas-Phase Reaction of Ethanol with Hydroxyl Radical: Mechanism, Kinetics, and Products. <i>ACS Omega</i> , 2019, 4, 5805-5817.	1.6	9
4304	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. <i>Journal of the American Chemical Society</i> , 2019, 141, 6234-6246.	6.6	42
4305	Palladium-catalysed alkyne alkoxy carbonylation with P,N-chelating ligands revisited: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8543-8552.	1.3	14

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4306	Influence of water on HFO-1234yf oxidation pyrolysis via ReaxFF molecular dynamics simulation. <i>Molecular Physics</i> , 2019, 117, 1768-1780.	0.8	18
4307	Novel aluminum complexes bearing 2-(aminomethylene)malonate ligands with high efficiency and controllability in ring-opening polymerization of $\mu$ -caprolactone. <i>European Polymer Journal</i> , 2019, 115, 399-408.	2.6	11
4308	A concerted addition mechanism in [Hmim]Br-triggered thiol-ene reactions: a typical ionic liquid effect revealed by DFT and experimental studies. <i>New Journal of Chemistry</i> , 2019, 43, 5752-5758.	1.4	8
4309	Quantum chemical study on isomerization and transformation of hexabromocyclododecanes. <i>Structural Chemistry</i> , 2019, 30, 899-910.	1.0	2
4310	Factors Controlling the Reactivity of Strained-Alkyne Embedded Cycloparaphenylenes. <i>Journal of Organic Chemistry</i> , 2019, 84, 4330-4337.	1.7	9
4311	Mechanism and stereoselectivity in NHC-catalyzed $\hat{I}^2$ -functionalization of saturated carboxylic ester. <i>RSC Advances</i> , 2019, 9, 7635-7644.	1.7	9
4312	Theoretical Study on the Transition-Metal-Catalyzed Cycloadditions of 2 <i>H</i> -Azirines with Alkynes: Implication of Carbenoid Intermediates. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 619-628.	2.0	3
4313	Molecular design of ionic liquids as novel non-metal catalysts for the acetylene hydrochlorination reaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7635-7644.	1.3	7
4314	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. <i>Tetrahedron</i> , 2019, 75, 2807-2816.	1.0	4
4315	Spectroscopic Characterization of Nicotinoyl and Isonicotinoyl Nitrenes and the Photointerconversion of 4-Pyridylnitrene with Diazacycloheptatetraene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3793-3801.	1.1	5
4316	Vanadium complexes of different nuclearities in the catalytic oxidation of cyclohexane and cyclohexanol an experimental and theoretical investigation. <i>New Journal of Chemistry</i> , 2019, 43, 17557-17570.	1.4	25
4317	The Driving Force for the Acylation of $\hat{I}^2$ Lactam Antibiotics by L, D-Transpeptidase 2: Quantum Mechanics/Molecular Mechanics (QM/MM) Study. <i>ChemPhysChem</i> , 2019, 20, 1126-1134.	1.0	13
4318	Dimerization and cyclotrimerization of terminal arylalkynes initiated by a phosphine-free ruthenium alkylidene complex. <i>Molecular Catalysis</i> , 2019, 469, 18-26.	1.0	9
4319	Synergistic Effects of Imidazolium-Functionalization on <i>fac</i> -Mn(CO) <sub>3</sub> Bipyridine Catalyst Platforms for Electrocatalytic Carbon Dioxide Reduction. <i>Journal of the American Chemical Society</i> , 2019, 141, 6569-6582.	6.6	104
4320	A DFT study on catalytic oxidative desulfurization with H <sub>2</sub> O <sub>2</sub> over Ti-MWW zeolite. <i>Journal of Molecular Modeling</i> , 2019, 25, 106.	0.8	4
4321	Reaction Mechanisms and Kinetics of the Hydrogen Abstraction Reactions of C <sub>4</sub> -C <sub>6</sub> Alkenes with Hydroxyl Radical: A Theoretical Exploration. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1275.	1.8	19
4322	Theoretical Investigation of Steric Effect Influence on Reactivity of Substituted Butadienes with Bromocyclobutenone. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2231-2241.	2.5	4
4323	Solid-State Catalytic Isotope Exchange of Hydrogen for Deuterium in Cyclopropylglycine. <i>Doklady Physical Chemistry</i> , 2019, 484, 15-19.	0.2	2

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4324	One catalyst, multiple processes: ligand effects on chemoselective control in Ru-catalyzed <i>anti</i> -Markovnikov reductive hydration of terminal alkynes. <i>Catalysis Science and Technology</i> , 2019, 9, 2315-2327.	2.1	4
4325	Theoretical study on the regioselective photoisomerization of asymmetric N,C-chelate organoboron compounds. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8376-8383.	1.3	10
4326	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. <i>Tetrahedron</i> , 2019, 75, 1961-1967.	1.0	36
4327	Mechanistic Insights into the Reaction of <i>N</i> -Propargylated Pyrrole and Indole Carbaldehyde with Ammonia, Alkyl Amines, and Branched Amines: A Synthetic and Theoretical Investigation. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 5261-5274.	1.2	15
4328	A molecular electron density theory study of Diels-Alder reaction between Danishefsky's diene and (2 <i>E</i> )-2-phenyl-2-(trifluoromethyl) acrylonitrile. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3937.	0.9	1
4329	Cooperative Catalytic Performance of Lewis and Brønsted Acids from AlCl <sub>3</sub> Salt in Aqueous Solution toward Glucose-to-Fructose Isomerization. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4879-4891.	1.5	28
4330	Understanding the Molecular Mechanism of the Rearrangement of Internal Nitronic Ester into Nitronorbornene in Light of the MEDT Study. <i>Molecules</i> , 2019, 24, 462.	1.7	16
4331	Exploration of assisting behavior of molecular-MO <sub>2</sub> (M = Ti, Zr) reagents towards the detoxication of tabun: A DFT study. <i>Chemical Physics Letters</i> , 2019, 717, 164-174.	1.2	2
4332	DFT study of response mechanism and selectivity of poly(3,4-ethylenedioxythiophene) towards CO <sub>2</sub> and SO <sub>2</sub> as gas sensor. <i>Structural Chemistry</i> , 2019, 30, 1427-1436.	1.0	8
4333	Quantitative descriptors of electronic structure in the framework of molecular orbital theory. <i>Advances in Inorganic Chemistry</i> , 2019, 73, 191-219.	0.4	1
4334	Theoretical study on the gas phase reaction of methyl chavicol with hydroxyl radical. <i>Computational and Theoretical Chemistry</i> , 2019, 1151, 78-90.	1.1	5
4335	Cooperative desorption of H <sub>2</sub> O and CO from photo-excited cobalt oxide clusters: The evidence of photo-catalytic coupling. <i>Chemical Physics Letters</i> , 2019, 719, 72-77.	1.2	1
4336	Hydrogen Evolution in [NiFe] Hydrogenases: A Case of Heterolytic Approach between Proton and Hydride. <i>Inorganic Chemistry</i> , 2019, 58, 2979-2986.	1.9	6
4337	Formaldehyde Generation in Photooxidation of Isoprene on Iron Oxide Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2019, 123, 5120-5127.	1.5	10
4338	Theoretical investigation on the mechanism of Cu(II)-catalyzed synthesis of 4-quinolones: effects of additives HOTf vs. HOTs. <i>New Journal of Chemistry</i> , 2019, 43, 4291-4305.	1.4	5
4339	Effects of solvents on the DACBO-catalyzed vinylogous Henry reaction of isatin with 3,5-dimethyl-4-nitroisoxazole in water and in solution from QM/MM MC simulations. <i>RSC Advances</i> , 2019, 9, 4932-4941.	1.7	5
4340	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from $\hat{\pm}$ -Santonin. <i>Molecules</i> , 2019, 24, 832.	1.7	39
4341	Theoretical studies of hydrogen abstraction from H <sub>2</sub> X and CH <sub>3</sub> XH (X = O, S) by trichloromethyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 6525-6534.	1.3	5

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4342	Mechanistic study of ethanol steam reforming on TM <sup>6</sup> S <sup>8</sup> clusters: a DFT study. <i>Catalysis Science and Technology</i> , 2019, 9, 1631-1643.	2.1	10
4343	Effect of the exchange correlation functional on the synchronicity/nonsynchronicity in bond formation in Diels-Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428.	1.3	31
4344	Synthesis, Structure, and Bonding Analysis of Tin(II) Dihalide and Cyclopentadienyltin(II) Halide (Alkyl)(amino)carbene Complexes. <i>Organometallics</i> , 2019, 38, 1052-1061.	1.1	23
4345	DFT Study on COS Oxidation Reaction Mechanism. <i>Minerals, Metals and Materials Series</i> , 2019, , 879-884.	0.3	0
4346	Understanding exo-selective Diels-Alder reactions involving Fischer-type carbene complexes. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 2985-2991.	1.5	4
4347	Exploring the mechanism of alkene hydrogenation catalyzed by defined iron complex from DFT computation. <i>Journal of Molecular Modeling</i> , 2019, 25, 61.	0.8	3
4348	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. <i>Chemistry of Materials</i> , 2019, 31, 1507-1519.	3.2	29
4349	A Quantum Mechanical Approach for Accurate Rate Parameters of Free-Radical Polymerization Reactions. , 2019, , 17-46.		1
4350	Simultaneous Formation of <i>cis</i> - and <i>trans</i> -CH <sub>3</sub> OCu(OH) Intermediates in Methane Activation by Cu in Solid Ar. <i>Inorganic Chemistry</i> , 2019, 58, 3237-3246.	1.9	1
4351	Chemical Insight on Decreased Sensitivity of CL-20/TNT Cocrystal Revealed by ReaxFF MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2079-2092.	2.5	30
4352	Theoretical Approaches to the Conformational Preference of 2,2-Di-tert-Butyl-1,3-Dioxane, 2,2-Di-tert-Butyl-1,3-Dithian, and 2,2-Di-tert-Butyl-1,3-Diselenan. <i>Russian Journal of Inorganic Chemistry</i> , 2019, 64, 1556-1564.	0.3	0
4353	A Molecular Electron Density Theory Study of the Synthesis of Spirobipyrazolines through the Domino Reaction of Nitrilimines with Allenates. <i>Molecules</i> , 2019, 24, 4159.	1.7	11
4354	The effect of interstitial boron on the mechanisms of acetylene hydrogenation catalyzed by Pd <sub>6</sub> : A DFT study. <i>Computational and Theoretical Chemistry</i> , 2019, 1170, 112636.	1.1	4
4355	CASPT2, CASSCF and non-adiabatic molecular dynamics (NAMD) studies on the low-lying electronic states of 1-H-1,2,3-triazole photolysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25809-25819.	1.3	3
4356	The control effects of different scaffolds in chiral phosphoric acids: a case study of enantioselective asymmetric arylation. <i>Catalysis Science and Technology</i> , 2019, 9, 6482-6491.	2.1	7
4357	Theoretical investigation of the mechanism, kinetics and subsequent degradation products of the NO <sub>3</sub> radical initiated oxidation of 4-hydroxy-3-hexanone. <i>Environmental Sciences: Processes and Impacts</i> , 2019, 21, 2080-2092.	1.7	0
4358	Organometallic chemistry of new carbon materials. Structure and dynamic behavior of group 6 metal tricarbonyl complexes of graphene and perforated graphene: a DFT study. <i>New Journal of Chemistry</i> , 2019, 43, 17991-18002.	1.4	2
4359	Aminonitrones as highly reactive bifunctional synthons. An expedient one-pot route to 5-amino-1,2,4-triazoles and 5-amino-1,2,4-oxadiazoles potential antimicrobials targeting multi-drug resistant bacteria. <i>New Journal of Chemistry</i> , 2019, 43, 17358-17366.	1.4	9

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4360	Expanstines Aâ€ˆD: four unusual isoprenoid epoxy cyclohexenones generated by <i>Penicillium expansum</i> YJ-15 fermentation and photopromotion. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3839-3846.	2.3	19
4361	Conversion of methane to benzene in CVI by density functional theory study. <i>Scientific Reports</i> , 2019, 9, 19496.	1.6	6
4362	Ab initio dynamics of hydrogen abstraction from N <sub>2</sub> H <sub>4</sub> by OH radicals: an RRKM-based master equation study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23733-23741.	1.3	12
4363	Proton-assisted air oxidation mechanisms of iron(ii) bis-thiosemicarbazone complexes at physiological pH: a kinetic-mechanistic study. <i>Dalton Transactions</i> , 2019, 48, 16578-16587.	1.6	4
4364	Insights into the mechanisms of Cu(i)-catalyzed heterocyclization of $\hat{\pm}$ -acyl- $\hat{\pm}$ -alkynyl ketene dithioacetals to form 3-cyanofurans: the roles of NH <sub>4</sub> OAc. <i>New Journal of Chemistry</i> , 2019, 43, 19149-19158.	1.4	4
4365	Origins of stereoselectivity in uncatalyzed and ZnBr <sub>2</sub> -catalyzed Dielsâ€ˆAlder reactions of a chiral sulfinylquinone. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 8756-8767.	1.5	0
4366	Cl Atoms and OH Radicals Initiated Kinetic and Mechanistic Study on the Degradation of Propyl Butanoate under Tropospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10976-10989.	1.1	5
4367	Mechanism and kinetics of the atmospheric reaction of 1,3,5-trimethylbenzene bicyclic peroxy radical with OH. <i>RSC Advances</i> , 2019, 9, 32594-32600.	1.7	3
4368	Computational study on the mechanism and kinetics for the reaction between HO <sub>2</sub> and <i>n</i> -propyl peroxy radical. <i>RSC Advances</i> , 2019, 9, 40437-40444.	1.7	5
4369	Computational study on the mechanisms and kinetics of the CH <sub>2</sub> =CHCH <sub>2</sub> F with O(3P) reaction. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 104-111.	2.0	1
4370	Theoretical studies on the mechanism and kinetic for CH <sub>3</sub> CH <sub>2</sub> O + HO <sub>2</sub> and CH <sub>3</sub> CHO + HO <sub>2</sub> reactions. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3895.	0.9	4
4371	Photodecomposition of 1 <i>H</i> -Pyrrole Carbonyl Azides: Direct Observation of Singlet 1 <i>H</i> -Pyrrole Carbonyl Nitrenes and Triplet 1 <i>H</i> -Pyrrolylnitrene. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 401-411.	1.2	5
4372	Steric Demand and Rate-determining Step for Photoenolization of Diortho-substituted Acetophenone Derivatives. <i>Photochemistry and Photobiology</i> , 2019, 95, 154-162.	1.3	4
4373	Understanding the Nature of Transition States in the Confined Nanospace of Different Acidic Zeolites on the Desulfurization Mechanism of Thiophene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1260-1278.	1.5	5
4374	Density Functional Theory Study on the Oxidative Addition of Chloroarenes to POP Rhodium Complexes. <i>Bulletin of the Korean Chemical Society</i> , 2019, 40, 189-191.	1.0	1
4375	Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by $\hat{\pm}$ Au(I) Complexes: Coordination Mode Determines Regioselectivity. <i>ACS Catalysis</i> , 2019, 9, 848-858.	5.5	45
4376	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 1605-1613.	1.2	4
4377	UV photolysis of tetrachloro- <i>p</i> -benzoquinone (TCBQ) in aqueous solution: Mechanistic insight from quantum chemical calculations. <i>Chemical Engineering Journal</i> , 2019, 361, 812-819.	6.6	14



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4378	DFT Research on Benzothiophene Pyrolysis Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2019, 123, 796-810.	1.1	20
4379	[3 + 2] cycloaddition reaction of N,N-cyclic azomethine imines toward highly electron-deficient nitroalkenes: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3925.	0.9	4
4380	A density functional theory study on mechanism and substituent effects of a base-free and catalyst-free synthesis of functionalized dihydrobenzoxazoles. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25836.	1.0	7
4381	The gas-phase pyrolysis of methyl azidoformate in the absence and presence of water: a theoretical study. <i>Molecular Physics</i> , 2019, 117, 34-41.	0.8	2
4382	Mechanisms and regioselectivities of DABCO/DMAP-catalyzed [2+4] annulation reactions of allenolate with $\beta,\gamma$ -unsaturated cyclic ketimine: A DFT study. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3914.	0.9	5
4383	H <sub>2</sub> -release from alcohols, diols, and compounds with amino functionality promoted by titanium(II) sandwich complex, [Cp <sub>2</sub> Ti]: a theoretical approach. <i>Structural Chemistry</i> , 2019, 30, 681-690.	1.0	3
4384	Quantum chemical and theoretical kinetics studies on the reaction of hydroperoxyl radical with chlorine atom. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	1
4385	Exploration of M(100)-2Å-1 (M=Si, Ge) surface termination through hydrogen passivation using ethane and ammonia-borane derivatives: A theoretical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 87, 11-21.	1.3	1
4386	Theoretical investigation on atmospheric reaction of O(3P) with CH <sub>2</sub> CN. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3913.	0.9	1
4387	Thermodynamic and kinetic studies of the retro-Diels-Alder reaction of 1,4-cyclohexadiene, 4H-pyran, 4H-thiopyran, 1,4-dioxine, and 1,4-dithiine: a theoretical investigation. <i>Structural Chemistry</i> , 2019, 30, 877-885.	1.0	6
4388	A theoretical study on the elimination reaction of acrylonitrile from 2'-O-cyanoethylated nucleosides by Bu <sub>4</sub> NF. <i>Tetrahedron</i> , 2019, 75, 1-9.	1.0	5
4389	Effective redox reactions by chromium oxide anions: Sulfur dioxide oxidation in the gas phase. <i>International Journal of Mass Spectrometry</i> , 2019, 436, 18-22.	0.7	10
4390	Metabolic Activation and Carcinogenesis of Tobacco-Specific Nitrosamine N <sup>o</sup> -Nitrosonoronicotine (NNN): A Density Function Theory and Molecular Docking Study. <i>International Journal of Environmental Research and Public Health</i> , 2019, 16, 178.	1.2	9
4391	Adsorption of multiple H <sub>2</sub> molecules on the complex TiC <sub>6</sub> H <sub>6</sub> : An unusual combination of chemisorption and physisorption. <i>Energy</i> , 2019, 171, 315-325.	4.5	22
4392	Insight into the Effects of Electrostatic Potentials on the Conversion Mechanism of the Hydrogen-Bonded Complexes and Carbon-Bonded Complexes: An Ab Initio and Quantum Theory of $\alpha$ -Atoms in Molecules Investigation. <i>ACS Omega</i> , 2019, 4, 231-241.	1.6	3
4393	CO hydrogenation on M <sub>1</sub> /W <sub>6</sub> S <sub>8</sub> (M=Co and Ni) single-atom catalysts: Competition between C <sub>2</sub> hydrocarbons and methanol synthesis pathways. <i>Molecular Catalysis</i> , 2019, 464, 10-21.	1.0	4
4394	Theoretical study on the [4+2] cycloaddition of 1,3-dimethylindole with 2,6-dimethylquinone. <i>Structural Chemistry</i> , 2019, 30, 1173-1184.	1.0	5
4395	Insight into the reaction mechanism of ethanol steam reforming catalysed by Co-Mo <sub>6</sub> S <sub>8</sub> . <i>Molecular Physics</i> , 2019, 117, 416-430.	0.8	5

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4396	Transformation Routes of P V and P III Substituted Acyclic Diaminocarbenes. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1621-1632.	1.0	2
4397	A three-component, one-pot synthesis of 1,8-naphthyridine and isoxazole derivatives and computational elucidation of the mechanism. <i>Research on Chemical Intermediates</i> , 2019, 45, 2119-2134.	1.3	4
4398	Theoretical study of the substituent effect of hydroxy group on tandem Cope rearrangement and [2+2] cycloaddition in cis-1,2-diethynylcyclopropane and its mono-hetero analogues. <i>Structural Chemistry</i> , 2019, 30, 1203-1210.	1.0	1
4399	Theoretical Insights into the Reaction Mechanism between 2,3,7,8-Tetrachlorodibenzofuran and Hydrogen Peroxide: A DFT Study. <i>ACS Omega</i> , 2019, 4, 358-367.	1.6	6
4400	Electronic Effect-Guided, Palladium-Catalyzed Regioselective B-H Activation and Multistep Diarylation of <i>o</i> -Carboranes with Aryl Iodides. <i>ACS Omega</i> , 2019, 4, 465-474.	1.6	9
4401	Theoretical Study on the Reaction of Nitric Oxide with Propargyl Radical. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1015-1021.	1.1	13
4402	A computational foray into the mechanism and catalysis of the adduct formation reaction of guanine with crotonaldehyde. <i>Journal of Computational Chemistry</i> , 2019, 40, 630-637.	1.5	2
4403	Imine hydrosilylation using an iron complex catalyst: A computational study. <i>Journal of Computational Chemistry</i> , 2019, 40, 62-71.	1.5	1
4404	Diterpene Synthase-Catalyzed Biosynthesis of Distinct Clerodane Stereoisomers. <i>ChemBioChem</i> , 2019, 20, 111-117.	1.3	13
4405	Reaction mechanism of NO with hydrolysates of NAMI: an MD simulation by combining the QM/MM (ABEEM) with the MD-FEP method. <i>Journal of Computational Chemistry</i> , 2019, 40, 1141-1150.	1.5	7
4406	Insight into the structures and reactivities of aqueous Al(III)-carboxylate complexes from cluster-based ab initio computational studies: Implications for the ligand-promoted mineral dissolution mechanism. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 244, 451-466.	1.6	2
4407	Participation of furoxancarboxitrile oxide in [3+2] cycloaddition reaction toward C≡N triple bond: a Molecular Electron Density Theory study of regioselectivity and mechanistic aspect. <i>Structural Chemistry</i> , 2019, 30, 317-326.	1.0	7
4408	Novel nonmetal catalyst of supported tetraphenylphosphonium bromide for acetylene hydrochlorination. <i>Catalysis Science and Technology</i> , 2019, 9, 188-198.	2.1	14
4409	Mechanism study on rhodium(III)-catalyzed C-H functionalization of <i>o</i> -vinylphenols with alkynes: Regioselectivity and chemoselectivity. <i>Computational and Theoretical Chemistry</i> , 2019, 1147, 40-50.	1.1	1
4410	An Extended Computational Study of Criegee Intermediate-Alcohol Reactions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 218-229.	1.1	45
4411	Unraveling the concerted catalytic mechanism of the human immunodeficiency virus type 1 (HIV-1) protease: a hybrid QM/MM study. <i>Structural Chemistry</i> , 2019, 30, 409-417.	1.0	15
4412	Designing Reactions with Post-Transition-State Bifurcations: Asynchronous Nitrene Insertions into C-C $\sigma$ Bonds. <i>CheM</i> , 2019, 5, 227-236.	5.8	28
4413	Interstellar dimethyl ether gas-phase formation: a quantum chemistry and kinetics study. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 482, 3567-3575.	1.6	48

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4414	Insights into the Oxidative Palladium-Catalyzed Regioselective Synthesis of 3-Arylindoles from N-Ts-Anilines and Styrenes: A Computational Study. <i>ChemCatChem</i> , 2019, 11, 780-789.	1.8	35
4415	Theoretical investigation of the gas-phase reaction of NiO <sup>+</sup> with ethane. <i>Structural Chemistry</i> , 2019, 30, 937-944.	1.0	0
4416	Theoretical study on the atmospheric reaction of CH <sub>3</sub> SH with O <sub>2</sub> . <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25822.	1.0	6
4417	Steric effects on normal and abnormal acyclic, cyclic-saturated, and cyclic-unsaturated diaminocarbenes using <i>scp</i> -DFT method. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3898.	0.9	8
4418	Computational studies on the formation of aza-oxypentadienyl intermediates from alkylidene oxaziridines and keteneimine oxides and their conversion to 1,5-dihydropyrrolones. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25796.	1.0	1
4419	Theoretical elucidation on the mechanism of 1H-1,2,4-diazaphospholes synthesis from 1,3-bis(amino)-phosphaallyl chlorides with hydrazine. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3899.	0.9	2
4420	N,N-dimethylformamide (DMF), and N,N-dimethylacetamide (DMA) reactions with NO <sub>3</sub> , OH and Cl: A theoretical study of the kinetics and mechanisms. <i>Arabian Journal of Chemistry</i> , 2019, 12, 4957-4970.	2.3	7
4421	DFT evidence for hydride transfer from aromatic C-H bond to superelectrophile in reactions of 1,3,5-Ad <sub>3</sub> C <sub>6</sub> H <sub>3</sub> with CBr <sub>3</sub> <sup>+</sup> Al <sub>2</sub> Br <sub>7</sub> <sup>-</sup> and 1,3,5-Ad <sub>3</sub> C <sub>6</sub> H <sub>3</sub> with CBr <sub>3</sub> <sup>+</sup> Al <sub>2</sub> Br <sub>7</sub> <sup>-</sup> and CO. <i>Molecular Catalysis</i> , 2020, 482, 100300.	1.0	0
4422	A theoretical study on the kinetics of multichannel Multiwell reaction of H <sub>2</sub> S(1A <sub>1</sub> ) with HO <sub>2</sub> (2A <sup>+</sup> ). <i>Molecular Physics</i> , 2020, 118, e1583387.	0.8	0
4423	Mechanistic studies and rate coefficients calculations of hydrogen abstraction from ethanol by methyl peroxy radical and hydroperoxyl radical. <i>Molecular Physics</i> , 2020, 118, .	0.8	5
4424	Atmospheric oxidation chemistry of 1-methoxy-propyl acetate initiated by OH radicals: kinetics and mechanisms. <i>Molecular Physics</i> , 2020, 118, e1601786.	0.8	4
4425	Computational study on mechanisms and pathways of the atmospheric NH <sub>2</sub> +O reaction. <i>Molecular Physics</i> , 2020, 118, e1658908.	0.8	2
4426	Basic-carbon nanocatalysts in the efficient synthesis of chromene derivatives. Valorization of both PET residues and mineral sources. <i>Chemical Engineering Journal</i> , 2020, 382, 122795.	6.6	10
4427	A Novel Spherical Boron Phosphide as a High-Efficiency Overall Water Splitting Catalyst: A Density Functional Theory Study. <i>Catalysis Letters</i> , 2020, 150, 544-554.	1.4	7
4428	First-principles approach to the first step of metal-phosphine bond formation to synthesize alloyed quantum dots using dissimilar metal precursors. <i>Chemical Physics</i> , 2020, 528, 110512.	0.9	0
4429	Theoretical understanding mechanisms and stereoselectivities of [2+2] cycloaddition of ketenes with ketimines catalyzed by bifunctional N-heterocyclic carbene. <i>Structural Chemistry</i> , 2020, 31, 181-190.	1.0	2
4430	Understanding the origin of the enantioselectivity and the mechanism of the asymmetric reduction of ketimine generated from acetophenone with oxazaborolidine catalyst. <i>Structural Chemistry</i> , 2020, 31, 253-261.	1.0	7
4431	Hydrolysis mechanism of double six-membered ring pentaborate anion. <i>Chemical Physics Letters</i> , 2020, 739, 136930.	1.2	4

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4432	Mechanism and Stereoselectivity of the Elementometalation Process of Activated Alkyne $R_2C=C(R)CO_2$ Tj $ETQ_0 0 0_7gBT /Over$	1.5	0
4433	Theoretical studies on chiral formamide-mediated asymmetric allylation of aldimines. Journal of the Iranian Chemical Society, 2020, 17, 623-630.	1.2	0
4434	Health care utilization and steroidâ€refractory toxicities from immune checkpoint inhibitors. Cancer, 2020, 126, 322-328.	2.0	13
4435	ZnO and TiO <sub>2</sub> clusters as catalyst in the addition and abstraction reaction of acrylic acid with the OH radical. International Journal of Chemical Kinetics, 2020, 52, 3-15.	1.0	2
4436	The effect of three-lobed bearing shapes in floating-ring bearings on the nonlinear oscillations of high-speed rotors. Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology, 2020, 234, 751-769.	1.0	6
4437	First principle studies on the atmospheric oxidation of HFC-C1436 initiated by the OH radical. New Journal of Chemistry, 2020, 44, 2070-2082.	1.4	8
4438	Tipping the balance: theoretical interrogation of divergent extended heterolytic fragmentations. Chemical Science, 2020, 11, 2231-2242.	3.7	13
4439	A Combined Experimental and Theoretical Study on the Gas Phase Reaction of OH Radicals with Ethyl Propyl Ether. Journal of Physical Chemistry A, 2020, 124, 721-730.	1.1	7
4440	Gas-Phase Reaction Kinetics of Pyruvic Acid with OH Radicals: The Role of Tunneling, Complex Formation, and Conformational Structure. Journal of Physical Chemistry A, 2020, 124, 790-800.	1.1	15
4441	Sulfurous and sulfonic acids: Predicting the infrared spectrum and setting the surface straight. Journal of Chemical Physics, 2020, 152, 024302.	1.2	8
4442	Insight into the reaction mechanism and chemoselectivity in the cycloaddition of ynamides and isoxazoles with H <sub>2</sub> O. Catalysis Science and Technology, 2020, 10, 240-251.	2.1	9
4443	Heterogeneous (de)chlorination-enabled control of reactivity in the liquid-phase synthesis of furanic biofuel from cellulosic feedstock. Green Chemistry, 2020, 22, 637-645.	4.6	32
4444	A one-pot route to <i>N</i> -acyl ureas: a formal four-component hydrolytic reaction involving aminonitrones and isocyanide dibromides. New Journal of Chemistry, 2020, 44, 1253-1262.	1.4	7
4445	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Dielsâ€Alder reactions. Organic and Biomolecular Chemistry, 2020, 18, 292-304.	1.5	24
4446	Theoretical insight into the degradation of p-nitrophenol by OH radicals synergized with other active oxidants in aqueous solution. Journal of Hazardous Materials, 2020, 389, 121901.	6.5	62
4447	S <sub>2</sub> Reactions of N <sub>2</sub> O <sub>5</sub> with Ions in Water: Microscopic Mechanisms, Intermediates, and Products. Journal of Physical Chemistry A, 2020, 124, 711-720.	1.1	8
4448	Synergistic Effect of Nitrogen Dopants on Carbon Nanotubes on the Catalytic Selective Epoxidation of Styrene. ACS Catalysis, 2020, 10, 129-137.	5.5	55
4449	Mechanistic Study on Catalytic Disproportionation of Hydrazine by a Protic Pincerâ€Type Iron Complex through Protonâ€Coupled Electron Transfer. European Journal of Inorganic Chemistry, 2020, 2020, 1472-1482.	1.0	8

#	ARTICLE	IF	CITATIONS
4450	Insight into the reaction mechanism of CH <sub>2</sub> SH with HO <sub>2</sub> : A density functional theory study. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26146.	1.0	2
4451	Scope, Kinetics, and Mechanism of On Water-Cu Catalysis in the N Cross-Coupling Reactions of Indole Derivatives. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 561-569.	1.2	11
4452	Atmospheric chemistry of the reaction between propylene carbonate and OH radical: An ab initio RRKM-based master equation study. <i>Chemical Physics Letters</i> , 2020, 739, 137020.	1.2	8
4453	The optimal adsorption pathway of H <sub>2</sub> molecules on Ti-Acetylene/ ethylene compounds: A DFT study. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 2105-2118.	3.8	3
4454	Keteniminium Salts: Reactivity and Propensity toward Electrocyclization Reactions. <i>Journal of Organic Chemistry</i> , 2020, 85, 449-463.	1.7	7
4455	A Comparative Study on C <sub>2</sub> Hydrocarbons and Methanol Synthesis from CO Hydrogenation Catalyzed by M <sub>1</sub> /W <sub>6</sub> S <sub>8</sub> (M = Ir and Ca) Single-Atom Catalysts. <i>Catalysis Letters</i> , 2020, 150, 1515-1526.	1.4	2
4456	Unraveling the sequence of electron flows along the reaction mechanism by quantum topological tools: The 32CA reaction of acetonitrile oxide with 7-bromo-oxanorborn-5-en-2-one. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 96, 107513.	1.3	4
4457	A computational study on the [3+2] cycloaddition of para-quinone methides with nitrile imines: a two-stage one-step mechanism. <i>Monatshefte für Chemie</i> , 2020, 151, 51-61.	0.9	8
4458	Shedding light on the energetics, regioselectivity, stereoselectivity, and mechanistic aspects of [3 + 2] cycloaddition reaction between azomethine imines and 2-sulfolene through molecular electron density theory. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4042.	0.9	3
4459	Ab-initio studies of thermal unimolecular decomposition of furan: A complementary deterministic and stochastic master equation model. <i>Fuel</i> , 2020, 264, 116492.	3.4	14
4460	Oxidation reaction mechanism and kinetics between OH radicals and alkyl-substituted aliphatic thiols: H-abstraction pathways. <i>Progress in Reaction Kinetics and Mechanism</i> , 2020, 45, 146867831988612.	1.1	3
4461	Exploring effects of the trifluoromethyl substituent on the chemoselectivity and regioselectivity of [3+2] cycloadditions of thiocarbonyl S-methanides with $\alpha,\beta$ -unsaturated ketones. <i>Journal of the Chinese Chemical Society</i> , 2020, 67, 703-710.	0.8	2
4462	Mechanism for hydrolysis of double six-membered ring tetraborate anion. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26118.	1.0	3
4463	A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of 3-chloro-2-methyl-1-propene with OH radical. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	0
4464	First-principles study of the reaction mechanism governing the S <sub>N</sub> Ar of the dimethylamine on 2-methoxy-5-nitrothiophenes. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	5
4465	Addition of Re-Bonded Nucleophilic Ligands to Activated Alkynes: A Theoretical Rationalization. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 269-280.	1.0	1
4466	VUV Photofragmentation of Chloriodomethane: The Iso-CH <sub>2</sub> I <sup>+</sup> Cl and Iso-CH <sub>2</sub> Cl <sup>+</sup> I Radical Cation Formation. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7491-7499.	1.1	5
4467	Theoretical Study of the Mechanism of Palladium(0)-Catalyzed Intramolecular [2+2+2] Cycloaddition of Ester-Substituted Alkynes. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 7455-7465.	1.2	3

#	ARTICLE	IF	CITATIONS
4468	Theoretical survey of the photochemical deracemization mechanism of chiral allene 3-(3,3-dimethyl-1-buten-1-ylidene)-2-piperidinone. <i>Organic Chemistry Frontiers</i> , 2020, 7, 3656-3663.	2.3	3
4469	Spiro[1,2]oxaphosphetanes of Nonstabilized and Semistabilized Phosphorus Ylide Derivatives: Synthesis and Kinetic and Computational Study of Their Thermolysis. <i>Journal of Organic Chemistry</i> , 2020, 85, 14570-14591.	1.7	4
4470	Mechanistic Insights into the N-Heterocyclic Carbene Catalyzed Synthesis of $\alpha,\beta$ -Diketones: A DFT Approach. <i>ChemistrySelect</i> , 2020, 5, 11996-12008.	0.7	4
4471	Palladium-catalysed methoxycarbonylation of ethene with bidentate diphosphine ligands: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24330-24336.	1.3	11
4472	Catalytic CO Oxidation by O <sub>2</sub> Mediated with Single Gold Atom Doped Titanium Oxide Cluster Anions AuTi <sub>2</sub> O <sub>4</sub> . <i>ChemPhysChem</i> , 2020, 21, 2550-2556.	1.0	6
4473	Theoretical investigations on mechanisms and pathways of CH <sub>2</sub> FO <sub>2</sub> /CHF <sub>2</sub> O <sub>2</sub> with ClO reactions in the atmosphere. <i>Journal of Fluorine Chemistry</i> , 2020, 236, 109595.	0.9	0
4474	Manganese-Catalyzed Multicomponent Synthesis of Tetrasubstituted Propargylamines: System Development and Theoretical Study. <i>Advanced Synthesis and Catalysis</i> , 2020, 362, 3872-3885.	2.1	18
4475	Effect of formal CH/P exchange on tandem Cope rearrangement and [2+2] cycloaddition of <i>cis</i> -1,2-diethylnylcyclopropane and its mono-hetero analogues. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2020, 195, 677-686.	0.8	0
4476	DFT Case Study of the Mechanism of a Metal-Free Oxygen Atom Insertion into a <i>p</i> -Quinone Methide C(sp <sup>3</sup> )-C(sp <sup>2</sup> ) Bond. <i>Journal of Organic Chemistry</i> , 2020, 85, 10110-10117.	1.7	0
4477	Unveiling the high reactivity of strained dibenzocyclooctyne in [3 + 2] cycloaddition reactions with diazoalkanes through the molecular electron density theory. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4100.	0.9	21
4478	Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1959-1972.	1.1	12
4479	Theoretical study on the desulfurization mechanisms of thiophene and benzothiophene under inert and oxidative atmospheres. <i>Fuel</i> , 2020, 280, 118683.	3.4	11
4480	Computational insights into the coupling mechanism of benzoic acid, phenoxy acetylene and dihydroisoquinoline catalyzed by silver ion as polarizer and stabilizer. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5903.	1.7	4
4481	Amine-functionalized ionic liquids for CO <sub>2</sub> capture. <i>Journal of Molecular Modeling</i> , 2020, 26, 345.	0.8	13
4482	Oxidation of isoprene by titanium oxide cluster cations in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27357-27363.	1.3	4
4483	Comparison of the Reactivity and Structures for the Neutral and Cationic Bis(imino)pyridyl Iron and Cobalt Species by DFT Calculations. <i>Catalysts</i> , 2020, 10, 1396.	1.6	6
4484	Mechanism exploring of acetylene hydrochlorination using hexamethylenetetramine as a single active site metal-free catalyst. <i>Catalysis Communications</i> , 2020, 147, 106147.	1.6	6
4485	Understanding the Origin of the Regioselectivity in Non-Polar [3+2] Cycloaddition Reactions through the Molecular Electron Density Theory. <i>Organics</i> , 2020, 1, 19-35.	0.6	12

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4486	Crystal Structure and Mechanistic Molecular Modeling Studies of Mycobacterium tuberculosis Diterpene Cyclase Rv3377c. <i>Biochemistry</i> , 2020, 59, 4507-4515.	1.2	6
4487	Selective hydrogenation of acetylene catalyzed by nickel and nitrogen-doped C34: A density functional theory study. <i>Chemical Physics Letters</i> , 2020, 757, 137871.	1.2	4
4488	An n $\pi^*$ gated decay mediates excited-state lifetimes of isolated azaindoles. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18639-18645.	1.3	3
4489	Methanol and glycolaldehyde production from formaldehyde in massive star-forming regions. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 497, 4486-4494.	1.6	2
4490	Kinetics of hydrogen abstraction from CH <sub>3</sub> SH by OH radicals: An ab initio RRKM-based master equation study. <i>Atmospheric Environment</i> , 2020, 242, 117833.	1.9	12
4491	Microscopic mechanism for effect of sodium on NO heterogeneous reduction by char. <i>Journal of Fuel Chemistry and Technology</i> , 2020, 48, 663-673.	0.9	16
4492	One-pot synthesis of oxazolidinones and five-membered cyclic carbonates from epoxides and chlorosulfonyl isocyanate: theoretical evidence for an asynchronous concerted pathway. <i>Beilstein Journal of Organic Chemistry</i> , 2020, 16, 1805-1819.	1.3	9
4493	A theoretical study of the hydrolysis mechanism of A-234; the suspected novichok agent in the Skripal attack. <i>RSC Advances</i> , 2020, 10, 27884-27893.	1.7	31
4494	Theoretical Insight into the Reaction Mechanism and Kinetics for the Criegee Intermediate of anti-PhCHO with SO <sub>2</sub> . <i>Molecules</i> , 2020, 25, 3041.	1.7	2
4495	A theoretical study on the metal-free triazole formation through tandem [3+2] cycloaddition/retro-Diels-Alder reaction of benzyl azide and oxanorbornadienedicarboxylate. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 97, 107552.	1.3	3
4496	Theoretical Study on Photoisomerization Mechanisms of Diphenyl $\pi$ -Conjugated N $\pi$ -Chelate Organoboron Compounds. <i>Chemistry - A European Journal</i> , 2020, 26, 12891-12897.	1.7	6
4497	Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory. <i>Tetrahedron</i> , 2020, 76, 131458.	1.0	11
4498	Computational study on the mechanisms and kinetics of the CH <sub>2</sub> BrO + ClO reaction in the atmosphere. <i>RSC Advances</i> , 2020, 10, 24308-24318.	1.7	2
4499	Theoretical investigation of the reaction mechanisms and kinetics of CFCI <sub>2</sub> CH <sub>2</sub> O and ClO in the atmosphere. <i>RSC Advances</i> , 2020, 10, 26433-26442.	1.7	1
4500	Computational study on the mechanisms and kinetics of the CH <sub>2</sub> CCl + O <sub>2</sub> reaction. <i>Canadian Journal of Chemistry</i> , 2020, 98, 395-402.	0.6	0
4501	Comparison of the Photochemistry of Acyclic and Cyclic 4-(4-Methoxy-phenyl)-4-oxo-but-2-enoate Ester Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7346-7354.	1.1	7
4502	A computational study on the kinetics of pyrolysis of isopropyl propionate as a biodiesel model: DFT and ab initio investigation. <i>Fuel</i> , 2020, 281, 118798.	3.4	18
4503	Unravelling the strain-promoted [3+2] cycloaddition reactions of phenyl azide with cycloalkynes from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2020, 44, 13633-13643.	1.4	30

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4504	Nb( <i>i</i> PrNPMe <sub>2</sub> ) <sub>3</sub> Fe <sup>+</sup> PMe <sub>3</sub> : A potential high reactivity heterobimetallic catalyst for acetylene cycloadditions. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5966.	1.7	4
4505	Substituent-regulated mechanism on reaction Cp <sub>2</sub> NbH <sub>3</sub> (Cp = $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ) with RCi <sup>+</sup> CR (R = COOMe and Me). <i>Dalton Transactions</i> , 2020, 49, 15376-15384.	1.6	0
4506	Production and Characterization of Molecular Dications: Experimental and Theoretical Efforts. <i>Molecules</i> , 2020, 25, 4157.	1.7	9
4507	Hydrolysis versus aminolysis of a potential nerve agent tabun: a computational reaction mechanism study. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	7
4508	Mechanistic Insights into the Hydrolysis of <i>o</i> -GlcNAcylation Catalyzed by Human <i>o</i> -GlcNAcase. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9310-9322.	1.2	4
4509	Understanding the Influence of the Trifluoromethyl Group on the Selectivities of the [3+2] Cycloadditions of Thiocarbonyl <i>s</i> -methanides with $\alpha,\beta$ -Unsaturated Ketones. A MEDT study. <i>ChemistrySelect</i> , 2020, 5, 12791-12806.	0.7	4
4510	Theoretical study on COS oxidation mechanism. <i>Combustion and Flame</i> , 2020, 221, 311-325.	2.8	9
4511	A mechanistic study on Cu(i) catalyzed carboxylation of the C-F bond with CO <sub>2</sub> : a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 9065-9071.	1.5	7
4512	Lithium Cation-Catalyzed Benzene Diels-Alder Reaction: Insights on the Molecular Mechanism Within the Molecular Electron Density Theory. <i>Journal of Organic Chemistry</i> , 2020, 85, 13121-13132.	1.7	13
4513	Construction of Benzo-1,2,3-thiazaphosphole Heterocycles by Annulations of <i>ortho</i> -Phosphinoarenesulfonyl Fluorides with Trimethylsilyl Azide. <i>Journal of Organic Chemistry</i> , 2020, 85, 14785-14794.	1.7	11
4514	Bouncing off walls - widths of exit channels from shallow minima can dominate selectivity control. <i>Chemical Science</i> , 2020, 11, 9937-9944.	3.7	17
4515	Computational insight into the mechanism and origin of high regioselectivity in the ring-opening cyclization of spirocyclopropanes with stabilized sulfonium ylides by the DFT. <i>Journal of Molecular Modeling</i> , 2020, 26, 255.	0.8	0
4516	Exploiting the Potential of Meroterpenoid Cyclases to Expand the Chemical Space of Fungal Meroterpenoids. <i>Angewandte Chemie</i> , 2020, 132, 23980-23989.	1.6	9
4517	Unveiling the mechanism and selectivity of [3+2] cycloaddition reactions of benzonitrile oxide to ethyl trans-cinnamate, ethyl crotonate and trans-2-penten-1-ol through DFT analysis. <i>Journal of Molecular Modeling</i> , 2020, 26, 279.	0.8	10
4518	Acenaphthoquinoxaline as a selective fluorescent sensor for Hg (II) detection: experimental and theoretical studies. <i>Heliyon</i> , 2020, 6, e04986.	1.4	12
4519	Reactivity of Iron Hydride Anions Fe <sub>2</sub> H <sub>n</sub> <sup>+</sup> ( <i>n</i> = 0-3) with Carbon Dioxide. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8414-8420.	1.1	7
4520	Deciphering the Curly Arrow Representation and Electron Flow for the 1,3-Dipolar Rearrangement between Acetonitrile Oxide and (1 <i>S</i> ,2 <i>R</i> ,4 <i>S</i> )-2-Cyano-7-oxabicyclo[2.2.1]hept-5-en-2-yl Acetate Derivatives. <i>ACS Omega</i> , 2020, 5, 22215-22225.	1.6	10
4521	Catalytic effect of water, ammonia, formic acid, or sulfuric acid on the HCN + H <sub>2</sub> O reaction in the aqueous solution. <i>Structural Chemistry</i> , 2020, 31, 2533-2542.	1.0	2



#	ARTICLE	IF	CITATIONS
4522	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
4523	DFT study of VOC pollutants catalyzed by optimal MoxOy: exploration of reaction mechanism of CH3R (R=CHO, CH2OH) by MoO2. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	0
4524	Reactivity of Neutral Tantalum Sulfide Clusters Ta3Sn (n = 0-4) with N2. Journal of Physical Chemistry A, 2020, 124, 7749-7755.	1.1	20
4525	Exploiting the Potential of Meroterpenoid Cyclases to Expand the Chemical Space of Fungal Meroterpenoids. Angewandte Chemie - International Edition, 2020, 59, 23772-23781.	7.2	28
4526	Nb2BN2 cluster anions reduce four carbon dioxide molecules: reactivity enhancement by ligands. Dalton Transactions, 2020, 49, 14081-14087.	1.6	7
4527	Experimental and theoretical studies on the thermal decomposition of trans-1-chloro-3,3,3-trifluoropropene and 2-chloro-3,3,3-trifluoropropene and their fire-extinguishing performance. New Journal of Chemistry, 2020, 44, 12932-12941.	1.4	7
4528	Experimental and Density Functional Theory Studies on 1,1,1,4,4,4-Hexafluoro-2-Butene Pyrolysis. Molecules, 2020, 25, 3799.	1.7	6
4529	Adsorption and dissociation of molecular hydrogen on Na3Al5 and Na5Al5 clusters. Chemical Physics Letters, 2020, 758, 137922.	1.2	3
4530	Kinetic Studies on the Photo-oxidation Reactions of Methyl-2-methyl Butanoate and Methyl-3-methyl Butanoate with OH Radicals. Journal of Physical Chemistry A, 2020, 124, 10923-10936.	1.1	1
4531	Theoretical Study of Ozonation of Methylparaben and Ethylparaben in Aqueous Solution. Journal of Physical Chemistry A, 2020, 124, 10967-10976.	1.1	3
4532	Electrospray ionization collision induced dissociation of thieno[3,2-d]pyrimidine derivatives. International Journal of Mass Spectrometry, 2020, 457, 116411.	0.7	1
4533	A computational study on NHC-Catalyzed [3+4] annulation between isatin-derived enal and aurone-derived azadiene: Insights into mechanism and stereoselectivity. Molecular Catalysis, 2020, 496, 111183.	1.0	8
4534	Understanding the Reactivity of Trimethylsilyldiazoalkanes Participating in [3+2] Cycloaddition Reactions towards Diethylfumarate with a Molecular Electron Density Theory Perspective. Organics, 2020, 1, 3-18.	0.6	13
4535	Reagent addition sequence and equivalent in N-heterocyclic carbene-catalyzed nonpolar inversion enable conversion from aldimine to benzoxazole. International Journal of Quantum Chemistry, 2020, 120, e26249.	1.0	2
4536	A computational investigation on the HO2 and isopropyl peroxy radical reaction: Mechanism and kinetics. Chemical Physics Letters, 2020, 749, 137442.	1.2	4
4537	Mechanism of accelerating soot oxidation by NO2 from diesel engine exhaust. Environmental Pollution, 2020, 264, 114708.	3.7	17
4538	Mechanism of thermal decomposition of HFO-1234ze(E) under supercritical fluid conditions. Journal of Supercritical Fluids, 2020, 160, 104792.	1.6	12
4539	Quantum chemical study of the reaction of trichloroethylene with O(3P). International Journal of Chemical Kinetics, 2020, 52, 589-598.	1.0	2

#	ARTICLE	IF	CITATIONS
4540	Theoretical investigation on the Cu( $\eta^5$ -Cp) $\eta^5$ -Cp)-catalyzed <i>N</i> -carboxamidation of indoles with isocyanates to form indole-1-carboxamides: effects of solvents. <i>New Journal of Chemistry</i> , 2020, 44, 9878-9887.	1.4	2
4541	Atmospheric chemistry of CHBr <sub>2</sub> O <sub>2</sub> : a theoretical study on mechanisms and kinetics of the CHBr <sub>2</sub> O <sub>2</sub> + ClO reaction. <i>Structural Chemistry</i> , 2020, 31, 1897-1908.	1.0	0
4542	Insights on Absolute and Relative Stereocontrol in Stereodivergent Cooperative Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 9612-9624.	6.6	29
4543	Stereoselectivity and nonmigratory insertion mechanism of dimethylacetylene dicarboxylate into metallocene-hydride of Cp <sub>2</sub> M(L)H [Cp = $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ; M = Nb, V; L = CO, P(OMe) <sub>3</sub> ]: A DFT study. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5601.	1.7	2
4544	Theoretical analysis of the regio- and stereoselective synthesis of spiroisoxazolines. <i>Journal of Molecular Modeling</i> , 2020, 26, 117.	0.8	2
4545	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. <i>Scientific Data</i> , 2020, 7, 137.	2.4	71
4546	Catalytic hydration of cyanamides with phosphinous acid-based ruthenium( $\eta^2$ ) and osmium( $\eta^2$ ) complexes: scope and mechanistic insights. <i>Catalysis Science and Technology</i> , 2020, 10, 4084-4098.	2.1	9
4547	The Mechanism of the Intramolecular Hydrocarbyl Metathesis within a Planar Triruthenium Cluster: Combining Core Flexibility with Hydride Mobility. <i>Chemistry - A European Journal</i> , 2020, 26, 13880-13889.	1.7	1
4548	$\beta$ -Functionalized ketene N,S-acetals as two-carbon synthons in the reaction with 1,2-naphthoquinone 1-methide. Synthesis of 3-amino-1H-benzo[f]chromenes. <i>Chemistry of Heterocyclic Compounds</i> , 2020, 56, 521-528.	0.6	4
4549	Using Polypeptide Bearing Furan Side Chains as a General Platform to Achieve Highly Effective Preparation of Smart Glycopolypeptide Analogue-Based Nano-Prodrugs for Cancer Treatment. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020, 194, 111165.	2.5	5
4550	Density Functional Theory Study of the Metal-Catalyzed Cycloaddition of Indolyl-Allenenes: Possible Reaction Pathways, Stereoselectivity, and Regioselectivity. <i>Organometallics</i> , 2020, 39, 1782-1789.	1.1	7
4551	Thermal unimolecular decomposition of ethyl 2-oxoacetate and its reactivity toward OH radicals: A theoretical study. <i>International Journal of Chemical Kinetics</i> , 2020, 52, 580-588.	1.0	1
4552	Advanced concepts in electronic structure (ACES) software programs. <i>Journal of Chemical Physics</i> , 2020, 152, 184105.	1.2	24
4553	Why [2+2]-cycloaddition reactions between isocyanates and imines do not occur in Pd-activation conditions?. <i>Inorganica Chimica Acta</i> , 2020, 510, 119758.	1.2	3
4554	A quantum chemical study on $\text{Cl}^{\cdot}$ -initiated atmospheric degradation of CH <sub>2</sub> BrO <sub>2</sub> . <i>Molecular Physics</i> , 2020, 118, e1734244.	0.8	0
4555	3-Benzylbenzothiazolidene Carbene Catalyzed Isomerization of Dimethyl Maleate to Dimethyl Fumarate: Experimental and Theoretical Results. <i>Current Organocatalysis</i> , 2020, 7, 108-117.	0.3	1
4556	Substituent Effect on the Thermodynamics and Kinetics of Carbyne Complex [( $\eta^5$ -C <sub>5</sub> H <sub>5</sub> )(CO)(COMe)Re( $\eta^6$ -C <sub>6</sub> H <sub>4</sub> X)] Isomerization to Carbene Complex		

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4558	Theoretical investigations on mechanisms and kinetics of CH <sub>2</sub> XO <sub>2</sub> (X=F, Cl) with Cl reaction in the atmosphere. <i>Journal of Molecular Modeling</i> , 2020, 26, 139.	0.8	1
4559	Ozonation of diclofenac in the aqueous solution: Mechanism, kinetics and ecotoxicity assessment. <i>Environmental Research</i> , 2020, 188, 109713.	3.7	19
4560	A DFT mechanistic study of the synthesis of trans-Z,Z-[PtII(Cl)(NH <sub>3</sub> ){HN=C(NH <sub>2</sub> )Me} <sub>2</sub> ]Cl from addition of NH <sub>3</sub> to trans-[PtII(Cl) <sub>2</sub> (N CMe) <sub>2</sub> ]. <i>Inorganica Chimica Acta</i> , 2020, 511, 119847.	1.2	2
4561	Mechanistic Insight for Targeting Biomolecules by Ruthenium(II) NSAID Complexes. <i>ACS Applied Bio Materials</i> , 2020, 3, 4600-4612.	2.3	11
4562	Theoretical understanding the effects of external electric field on the hydrolysis of anticancer drug titanocene dichloride. <i>Molecular Physics</i> , 2020, 118, .	0.8	4
4563	Mechanisms and origins of stereoselectivity of NHC-catalyzed reaction of aldehyde and butadienoate. <i>Molecular Catalysis</i> , 2020, 492, 111030.	1.0	6
4564	Unveiling the Lewis Acid Catalyzed Diels-Alder Reactions Through the Molecular Electron Density Theory. <i>Molecules</i> , 2020, 25, 2535.	1.7	34
4565	Atmospheric chemistry of CFCI <sub>2</sub> O <sub>2</sub> : a theoretical study on mechanisms and kinetics of the CFCI <sub>2</sub> O <sub>2</sub> + ClO reaction. <i>Journal of Molecular Modeling</i> , 2020, 26, 177.	0.8	0
4566	Energetics of Dynamic Kinetic Asymmetric Transformation in Suzuki-Miyaura Coupling. <i>ACS Catalysis</i> , 2020, 10, 4349-4360.	5.5	6
4567	Shimalactone Biosynthesis Involves Spontaneous Double Bicyclic Ring Formation with 8π Electrocyclization. <i>Angewandte Chemie</i> , 2020, 132, 8542-8548.	1.6	5
4568	The oxo exchange reaction mechanism of americium(VI): a density functional theory study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2020, 324, 857-868.	0.7	1
4569	Monoalkylation of aniline with trichloroacetimidate catalyzed by (±)-camphorsulfonic acid through an S <sub>N</sub> 1 reaction based on dual hydrogen-bonding activation modes. <i>New Journal of Chemistry</i> , 2020, 44, 5526-5534.	1.4	1
4570	Dynamics of imidogen reaction with hydroxyl radical: a theoretical approach. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 1987-2000.	1.2	2
4571	Theoretical study on thermal curing mechanism of arylethynyl-containing resins. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6468-6477.	1.3	10
4572	1,3-Dipolar cycloaddition of N-allyl substituted polycyclic derivatives of isoindole-1,3-dione with nitrones and nitrile oxides: An experimental and theoretical investigation. <i>Tetrahedron</i> , 2020, 76, 131104.	1.0	11
4573	Stability and anion diffusion kinetics of Yttria-stabilized zirconia resolved from machine learning global potential energy surface exploration. <i>Journal of Chemical Physics</i> , 2020, 152, 094703.	1.2	15
4574	Ag <sup>+</sup> -Catalyzed Hydroazidation of Terminal Alkynes and Mechanistic Studies. <i>Journal of the American Chemical Society</i> , 2020, 142, 7083-7091.	6.6	19
4575	Criegee intermediate decomposition pathways for the formation of o-toluic acid and 2-methylphenylformate. <i>Chemical Physics Letters</i> , 2020, 748, 137399.	1.2	0

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4576	Describing Polytopyal Rearrangements of Fluxional Molecules with Curvilinear Coordinates Derived from Normal Vibrational Modes: A Conceptual Extension of Cremer–Pople Puckering Coordinates. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3162-3193.	2.3	8
4577	Reactions of Transition-Metal Carbyne Cations with Ethylene in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2628-2633.	1.1	12
4578	A [1+2] cycloaddition instead of usual [2+3] cycloaddition between the B <sub>12</sub> N <sub>12</sub> cluster and methyl azide: Potential energy surface calculations and Born–Oppenheimer molecular dynamics simulations. <i>Progress in Reaction Kinetics and Mechanism</i> , 2020, 45, 146867831990058.	1.1	1
4579	Unveiling the Different Chemical Reactivity of Diphenyl Nitrilimine and Phenyl Nitrile Oxide in [3+2] Cycloaddition Reactions with (R)-Carvone through the Molecular Electron Density Theory. <i>Molecules</i> , 2020, 25, 1085.	1.7	27
4580	Spectral Decomposition of the Reaction Force Constant. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2372-2379.	1.1	6
4581	Shimalactone Biosynthesis Involves Spontaneous Double Bicyclic Ring Formation with 8π Electrocyclization. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 8464-8470.	7.2	20
4582	Natural acridones and coumarins as free radical scavengers: Mechanistic and kinetic studies. <i>Chemical Physics Letters</i> , 2020, 746, 137312.	1.2	12
4583	Elusive Cyanoforn: Computational Probing Its Stability and Reactivity with Accurate Ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2634-2648.	1.1	0
4584	Mechanisms and energetics for catalytic combustion from methane to methanol and methanol to formaldehyde on single site palladium oxide species supported on AL-MCM-41 silica. <i>Chemical Physics Letters</i> , 2020, 751, 137523.	1.2	3
4585	Computational study on NHC catalyzed [4+2] annulation between $\beta$ -chloroenals and pyrazolinones: mechanism and stereoselectivity. <i>New Journal of Chemistry</i> , 2020, 44, 11643-11651.	1.4	8
4586	Crystal Structure and Theoretical Investigation of Thiobarbituric Acid Derivatives as Nonlinear Optical (NLO) Materials. <i>Crystals</i> , 2020, 10, 442.	1.0	2
4587	Rate rules for hydrogen abstraction reaction kinetics of polycyclic aromatic hydrocarbons and vinyl radical. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	6
4588	Benchmarking of DFT methods using experimental free energies and volumes of activation for the cycloaddition of alkynes to cuboidal Mo <sub>3</sub> S <sub>4</sub> clusters. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26353.	1.0	3
4589	Generation and trapping of non-aromatic cycloimines via diazotization/dediazotization of N-amino cyclic amines: theoretical and experimental results. <i>Structural Chemistry</i> , 2020, 31, 2179-2187.	1.0	2
4590	Theoretical investigations on mechanisms and kinetics of the CH <sub>3</sub> CFClO <sub>2</sub> · with ClO· reaction in the atmosphere. <i>Scientific Reports</i> , 2020, 10, 11078.	1.6	0
4591	A Kinetic Approach to Double Proton Transfer in Watson–Crick DNA Base Pairs. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1715-1722.	1.2	10
4592	Unravelling the regio- and stereoselective synthesis of bicyclic N,O-nucleoside analogues within the molecular electron density theory perspective. <i>Structural Chemistry</i> , 2020, 31, 2147-2160.	1.0	13
4593	Density functional theory study of non-metal catalysts with different CN ratios for acetylene hydrochlorination. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2020, 603, 125230.	2.3	2

#	ARTICLE	IF	CITATIONS
4594	Theoretical kinetics of the C <sub>2</sub> H <sub>4</sub> +NH <sub>2</sub> reaction. <i>Combustion and Flame</i> , 2020, 215, 193-202.	2.8	5
4595	Atmospheric chemistry of CF <sub>2</sub> ClO <sub>2</sub> : a theoretical study on mechanisms and kinetics of the CF <sub>2</sub> ClO <sub>2</sub> + HO <sub>2</sub> reaction. <i>Environmental Science and Pollution Research</i> , 2020, 27, 33965-33974.	2.7	0
4596	Unveiling the Role of Hydrogen Bonding and g-Tensor in the Interaction of Ru-Bis-DMSO with Amino Acid Residue and Human Serum Albumin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6459-6474.	1.2	2
4597	A molecular electron density theory study of the Grignard reagent-mediated regioselective direct synthesis of 1,5-disubstituted 1,2,3-triazoles. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4062.	0.9	20
4598	Theoretical investigations on $\text{Cl}^-$ -initiated atmospheric degradation of CH <sub>2</sub> O <sub>2</sub> (X = F, Cl). <i>Journal of Fluorine Chemistry</i> , 2020, 234, 109501.	0.9	0
4599	Dual reactivity of B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> enables the silylative cascade conversion of <i>N</i> -aryl piperidines to sila- <i>N</i> -heterocycles: DFT calculations. <i>Organic Chemistry Frontiers</i> , 2020, 7, 944-952.	2.3	20
4600	Evidence and evolution of Criegee intermediates, hydroperoxides and secondary organic aerosols formed via ozonolysis of 1-pinene. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6528-6537.	1.3	14
4601	A quantum chemical study on $\text{Cl}^-$ -initiated atmospheric degradation of CH <sub>3</sub> CFClO <sub>2</sub> . <i>Journal of Molecular Structure</i> , 2020, 1209, 127830.	1.8	2
4602	Cl Atom-Initiated Photo-Oxidation Reactions of Vinyl Trifluoroacetate and Allyl Trifluoroacetate in Tropospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2123-2139.	1.1	0
4603	Hydrolysis of HNSO <sub>2</sub> : A potential route for atmospheric production of H <sub>2</sub> SO <sub>4</sub> and NH <sub>3</sub> . <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26182.	1.0	5
4604	Quantum chemical calculation to elucidate the biodegradation pathway of methylphenanthrene by green microalgae. <i>Water Research</i> , 2020, 173, 115598.	5.3	6
4605	Insights into the Photoinduced Isomerization Mechanisms of a <i>N</i> -Chelate Organoboron Compound: A Theoretical Study. <i>ChemPhysChem</i> , 2020, 21, 510-517.	1.0	12
4606	Synthesis of <i>N</i> -Substituted 1,2-Diamino Acids via Stereoselective <i>N</i> -Michael Additions to a Chiral Bicyclic Dehydroalanine. <i>Journal of Organic Chemistry</i> , 2020, 85, 3134-3145.	1.7	13
4607	Degradation of prosulfocarb by hydroxyl radicals in gas and aqueous phase: Mechanisms, kinetics and toxicity. <i>Ecotoxicology and Environmental Safety</i> , 2020, 191, 110175.	2.9	15
4608	Theoretical Study of the Kinetics of the Gas-Phase Reaction between Phenyl and Amino Radicals. <i>ACS Omega</i> , 2020, 5, 1277-1286.	1.6	8
4609	Isotopic Studies for Tracking Biogenic Carbon during Co-processing of Biomass and Vacuum Gas Oil. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 2652-2664.	3.2	14
4610	Dinuclear Zn(II) and tetranuclear Co(II) complexes of a tetradentate N <sub>2</sub> O <sub>2</sub> Schiff base ligand: Synthesis, crystal structure, characterization, DFT studies, cytotoxicity evaluation, and catalytic activity toward benzyl alcohol oxidation. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5493.	1.7	17
4611	Theoretical Insight towards Mechanism, Role of NHC and DBU in the Synthesis of Substituted Quinolines. <i>ChemistrySelect</i> , 2020, 5, 1300-1307.	0.7	4

#	ARTICLE	IF	CITATIONS
4612	A DFT study on the reaction mechanism of enantioselective reduction of ketones with borane catalyzed by a B-methoxy-oxazaborolidine catalyst derived from (â€“)Î²-pinene. Journal of Molecular Modeling, 2020, 26, 27.	0.8	3
4613	Hydrogen bonding and non-covalent interaction assisted nickel(0) catalysed reversible alkenyl functional group swapping: a computational study. Catalysis Science and Technology, 2020, 10, 1747-1760.	2.1	3
4614	DFT Study on the Gold(I)â€Catalyzed Dehydrogenative Heterocyclization of Alkynyl Alkenones to form Furan Fused Carbocycles: Effects of Additives C <sub>5</sub> H <sub>5</sub> NO vs. PhNO. Applied Organometallic Chemistry, 2020, 34, e5443.	1.7	3
4615	Sulfurâ€doped Graphene as an Efficient Metalâ€free Carbocatalyst for the Synthesis of 1,5â€Benzodiazepines Derivatives. ChemistrySelect, 2020, 5, 968-978.	0.7	7
4616	Mechanism and kinetics of diuron oxidation by hydroxyl radical addition reaction. Environmental Science and Pollution Research, 2020, 27, 12080-12095.	2.7	14
4617	The DFT Quest for Possible Reaction Pathways, Catalytic Species, and Regioselectivity in the InCl <sub>3</sub> -Catalyzed Cycloaddition of N-Tosyl Formaldimine with Olefins or Allenes. Journal of Organic Chemistry, 2020, 85, 3676-3688.	1.7	7
4618	Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen. Green Chemistry, 2020, 22, 2403-2418.	4.6	26
4619	Selective Hydrogenation of Acetylene Catalysed by a B12N12 Cluster Doped with a Single Nickel Atom: A DFT Study. Catalysts, 2020, 10, 115.	1.6	7
4620	Insights into the reaction mechanism of criegee intermediate with NO radical. Computational and Theoretical Chemistry, 2020, 1175, 112731.	1.1	3
4621	A molecular electron density theory investigation of the molecular mechanism, regioselectivity, stereoselectivity and chemoselectivity of cycloaddition reaction between acetonitrile N-oxide and 2,5-dimethyl-2H-[1,2,3]diazarsole. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	21
4622	Hexamethylphosphanetriamineâ€mediated aziridination of imines with alphaâ€ketoesters: A molecular electron density theory study. Journal of Physical Organic Chemistry, 2020, 33, e4058.	0.9	6
4623	How does cross-conjugation influence thiol additions to enones? A computational study of thiol trapping by the naturally occurring divinyl ketones zerumbone and Î±-santonin. Organic and Biomolecular Chemistry, 2020, 18, 1426-1435.	1.5	7
4624	Photolysis of 5-Azido-3-Phenylisoxazole at Cryogenic Temperature: Formation and Direct Detection of a Nitrosoalkene. Molecules, 2020, 25, 543.	1.7	5
4625	Computational study on mechanisms and kinetics of the atmospheric CFC12CH2O2 with Cl reaction. Journal of Molecular Graphics and Modelling, 2020, 99, 107618.	1.3	1
4626	A mechanistic study of the activation of small molecules (H2 and C2H2) by group 14 analogues of selenophene. New Journal of Chemistry, 2020, 44, 8922-8936.	1.4	0
4627	On the Catalytic Activity of [RuH <sub>2</sub> (PPh <sub>3</sub> ) <sub>3</sub> (CO)] (PPh <sub>3</sub> =triphenylphosphine) in Rutheniumâ€Catalysed Generation of Hydrogen from Alcohols: a Combined Experimental and DFT study. ChemCatChem, 2020, 12, 2995-3009.	1.8	4
4628	A theoretical elucidation for the formation of unusual zwitterionic sandwich and terminal ruthenium complexes. Journal of Physical Organic Chemistry, 2020, 33, e4070.	0.9	0
4629	Understanding the mechanism of [3+2] cycloaddition reaction of benzoisothiazole-2,2-dioxide-3-ylidene with nitrones. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1

#	ARTICLE	IF	CITATIONS
4630	Theoretical study on the activation of C-H bond in ethane by PdX <sup>+</sup> (X = F, Cl, Br, H, and CH <sub>3</sub> ) in the gas phase. <i>Journal of Molecular Modeling</i> , 2020, 26, 91.	0.8	0
4631	Rate rules for hydrogen abstraction reaction kinetics of alkenes from allylic sites by HO <sub>2</sub> radical. <i>Computational and Theoretical Chemistry</i> , 2020, 1179, 112795.	1.1	4
4632	The use of control experiments as the sole route to correct the mechanistic interpretation of mercury poisoning test results: The case of P,C-palladacycle-catalysed reactions. <i>Journal of Organometallic Chemistry</i> , 2020, 916, 121245.	0.8	3
4633	Enantioselective hydrosilylation of unsaturated carbon-heteroatom bonds (C=N, C=O) catalyzed by [Ru-S] complexes: a theoretical study. <i>RSC Advances</i> , 2020, 10, 9431-9437.	1.7	5
4634	Theoretical study of the mechanism behind the site- and enantio-selectivity of C-H functionalization catalysed by chiral dirhodium catalyst. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9561-9572.	1.3	5
4635	Rationalizing the Al I -Promoted Oxidative Addition of C <sup>~</sup> C Versus C <sup>~</sup> H Bonds in Arenes. <i>Chemistry - A European Journal</i> , 2020, 26, 11806-11813.	1.7	18
4636	A molecular electron density theory study to understand the interplay of theory and experiment in nitrone-enone cycloaddition. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	0.7	13
4637	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions. <i>RSC Advances</i> , 2020, 10, 15394-15405.	1.7	94
4638	[Mo <sub>2</sub> O <sub>2</sub> S <sub>8</sub> ] <sup>2-</sup> small molecule dimer as a basis for hydrogen evolution reaction (HER) catalyst materials. <i>SN Applied Sciences</i> , 2020, 2, 1.	1.5	8
4639	Multi-molar CO <sub>2</sub> capture beyond the direct Lewis acid-base interaction mechanism. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11354-11361.	1.3	10
4640	Theoretical investigations on mechanisms and pathways of CH <sub>2</sub> ClO <sub>2</sub> /CHCl <sub>2</sub> O <sub>2</sub> with ClO reactions in the atmosphere. <i>Environmental Science and Pollution Research</i> , 2020, 27, 20457-20468.	2.7	0
4641	Quantum-chemical study of organic reaction mechanisms. IX. The interaction of benzoylacetylene with dithio- and diselenomalonamides. <i>Journal of Organometallic Chemistry</i> , 2020, 915, 121242.	0.8	6
4642	Synthesis of bodinieric acids A and B, both C-18 and C-19-functionalized abietane diterpenoids: DFT study of the key aldol reaction. <i>RSC Advances</i> , 2020, 10, 15015-15022.	1.7	1
4643	3-Nitrene-2-formylthiophene and 3-Nitrene-2-formylfuran: Matrix Isolation, Conformation, and Rearrangement Reactions. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3786-3794.	1.1	4
4644	High-efficiency dynamic sensing of biothiols in cancer cells with a fluorescent $\beta$ -cyclodextrin supramolecular assembly. <i>Chemical Science</i> , 2020, 11, 4791-4800.	3.7	35
4645	Mechanistic details of metal-free cyclization reaction of organophosphorus oxide with alkynes mediated by 2,6-lutidine and Tf <sub>2</sub> O. <i>Journal of Computational Chemistry</i> , 2020, 41, 1709-1717.	1.5	5
4646	A density functional theory exploration on the Zn catalyst for acetylene hydration. <i>Journal of Molecular Modeling</i> , 2020, 26, 105.	0.8	9
4647	A theoretical investigation on the mechanism and kinetics of the thermal isomerization of Trimethylsilylcyclopropane using CBS-QB3. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 130, 55-74.	0.8	3

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4648	Three-component coupling reaction of the C60 fullerene, indole and propargyl bromide: a theoretical study. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2020, 130, 75-90.	0.8	4
4649	Complete degradation of glyoxal by NO radicals through two steps: The first at high-temperatures and the second at low-temperatures. <i>Computational and Theoretical Chemistry</i> , 2020, 1180, 112822.	1.1	2
4650	Environmentally benign benzyl alcohol oxidation and C-C coupling catalysed by amide functionalized 3D Co(II) and Zn(II) metal organic frameworks. <i>Journal of Catalysis</i> , 2020, 385, 324-337.	3.1	59
4651	A Close Look to the Oxaphosphetane Formation along the Wittig Reaction: A [2+2] Cycloaddition?. <i>Journal of Organic Chemistry</i> , 2020, 85, 6675-6686.	1.7	31
4652	Density Functional Theory Investigation of the Binding of ThioTEPA to Purine Bases: Thermodynamics and Bond Evolution Theory Analysis. <i>Journal of Physical Chemistry A</i> , 2020, 124, 4068-4080.	1.1	12
4653	CO Oxidation Catalyzed by the Neutral Cluster IrAl <sub>2</sub> O <sub>8</sub> with Iridium in a High Oxidation State of VI. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8869-8875.	1.5	10
4654	Synthetic Studies on Pactamycin: A Synthesis of Johnson's Intermediate. <i>Organic Letters</i> , 2020, 22, 3515-3518.	2.4	8
4655	The Activation Strain Model in the Light of Real Space Energy Partitions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2020, 646, 1062-1072.	0.6	7
4656	Elimination of Thiophenic Compounds by Cycloaddition with Ethylene for an Efficient Purification of Fuels: A DFT Study. <i>Topics in Catalysis</i> , 2021, 64, 288-296.	1.3	3
4657	A theoretical kinetic study on the reaction of atomic bromine with toluene. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 390-402.	1.0	3
4658	Theoretical insights into the synthesis reaction mechanism of 1,2,3-triazole based on sakai reaction. <i>Tetrahedron</i> , 2021, 77, 131737.	1.0	7
4659	Structural and thermochemical studies of pyrrolidine borane and piperidine borane by gas electron diffraction and quantum chemical calculations. <i>Structural Chemistry</i> , 2021, 32, 205-213.	1.0	1
4660	Reaction kinetics of a series of alkenes with ClO and BrO radicals: A theoretical study. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 250-264.	1.0	2
4661	Mechanistic insights into the reaction Cp <sub>2</sub> Nb(CO)H (Cp <sup>-</sup> = $\eta^5$ -C <sub>5</sub> H <sub>5</sub> ) with acetylenedicarboxylic acid (ADCA): DFT studies. <i>Inorganica Chimica Acta</i> , 2021, 514, 119990.	1.2	0
4662	A molecular electron density theory study of polar Diels-Alder reaction between 2,4-dimethyl-5-ethoxyoxazole and ethyl 4,4-trifluorocrotonate. <i>Structural Chemistry</i> , 2021, 32, 805-817.	1.0	2
4663	Regio- and stereochemistry in the intramolecular [4+2] and intermolecular [3+2] cycloaddition reactions in the synthesis of epoxy pyrrolo[3,4-g]indazoles: a density functional theory study. <i>Chemical Papers</i> , 2021, 75, 951-965.	1.0	3
4664	DFT study on the [4+4] domino cycloaddition of ynones with benzylidenepyrazolones to access eight-membered cyclic ethers: effects of DBU vs. Et <sub>3</sub> N. <i>New Journal of Chemistry</i> , 2021, 45, 131-140.	1.4	4
4665	A DFT study on NHC catalyzed [4+2] annulation of 2-hazirines with ketones: Mechanism and selectivity. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26557.	1.0	6



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4666	Understanding the C~F Bond Activation Mediated by Frustrated Lewis Pairs: Crucial Role of Non~covalent Interactions. <i>Chemistry - A European Journal</i> , 2021, 27, 3823-3831.	1.7	26
4667	Quantum chemical study on the ozonolysis mechanism of guaiacol and the structure-reactivity relationship of phenols with hydroxyl, methoxy, and methyl substituents. <i>Chemical Engineering Journal</i> , 2021, 420, 127629.	6.6	7
4668	Theoretical study of the hydrogen abstraction reactions from substituted phenolic species. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113120.	1.1	6
4669	Mechanistic Investigation on Chemiluminescent Formaldehyde Probes. <i>Chemistry - A European Journal</i> , 2021, 27, 5712-5720.	1.7	7
4670	Computational prediction on the catalytic activity of heterobimetallic complex featuring M~M triple bond in acetylene cyclotrimerization: Mechanistic study. <i>Journal of Computational Chemistry</i> , 2021, 42, 484-491.	1.5	3
4671	The density functional theory study of 2D nonmetallic catalyst defective graphene for acetylene hydration. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26561.	1.0	1
4672	Cooperative Noncovalent Interactions Lead to a Highly Diastereoselective Sulfonyl-Directed Fluorination of Steroidal 1,2-Unsaturated Hydrazones. <i>Journal of Organic Chemistry</i> , 2021, 86, 1300-1307.	1.7	0
4673	Theoretical study on the atmospheric degradation mechanism and subsequent products of E,4-hexadienal with hydroxyl radical. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26563.	1.0	7
4674	DFT Investigation of the 6-Inter-ring Haptotropic Rearrangement of the Group 8 Metals Complexes [(graphene)MCp] <sup>+</sup> (M = Fe, Ru, Os). <i>Journal of Physical Chemistry A</i> , 2021, 125, 366-375.	1.1	1
4675	~ Catalysis in Carbon Flatland~Flipping [8]Annulene on Graphene. <i>Chemistry - A European Journal</i> , 2021, 27, 3420-3426.	1.7	12
4676	Sulfur-assisted large-scale synthesis of graphene microspheres for superior potassium-ion batteries. <i>Energy and Environmental Science</i> , 2021, 14, 965-974.	15.6	164
4677	The kinetic mechanism of acetylene hydrogenation to prepare ethane over Fe <sub>x</sub> O <sub>y</sub> clusters: A DFT study. <i>Chemical Engineering Science</i> , 2021, 230, 116170.	1.9	6
4678	CBS-QB3 study on the pyrolysis mechanism of 3-ethynylbenzo[b]thiophene. <i>Chemical Physics Letters</i> , 2021, 762, 138120.	1.2	5
4679	Reaction kinetics of a series of alkanes with ClO and BrO radicals: A theoretical study. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 189-206.	1.0	3
4680	Rapid computational evaluation of small-molecule hydrolase mimics for preorganized H~bond networks. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26423.	1.0	1
4681	Theoretical study on the reaction of nitric oxide with 2-hydroxyethyl radical. <i>Molecular Physics</i> , 2021, 119, e1811906.	0.8	1
4682	Mechanistic and kinetic study on the reaction of the Cl~initiated atmospheric degradation of CFCl <sub>2</sub> O. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4130.	0.9	0
4683	Competition and conversion between pnictogen bonds and hydrogen bonds involving prototype organophosphorus compounds. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18794-18805.	1.3	2

#	ARTICLE	IF	CITATIONS
4684	Understanding the regioselectivity of the copper(I)- and ruthenium(II)- catalyzed [3 + 2] cycloadditions of azido derivative of ribose with terminal alkyne: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	3
4685	Unveiling the high regioselectivity and stereoselectivity within the synthesis of spirooxindolenitropyrrolidine: A molecular electron density theory perspective. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4189.	0.9	21
4686	Mechanistic Studies of Reduction and Initiation over the Vanadium-Oxide Polyethylene Catalyst. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2393-2402.	1.5	2
4687	Iron-promoted dealkylative carbene aminocyclization of $\hat{I}$ -arylamino- $\hat{I}$ -diazoesters. <i>Dalton Transactions</i> , 2021, 50, 2167-2176.	1.6	1
4689	A Computational Study on the Attack of Nitrogen and Oxygen Atoms to Toluene. <i>Lecture Notes in Computer Science</i> , 2021, , 620-631.	1.0	6
4690	Theoretical insight into the origins of chemo- and diastereo-selectivity in the palladium-catalysed (3 +) Tj ETQq1 1 0,784314 rgBT /Over	2.3	3
4691	Exploring water adsorption and reactivity in a series of doped aluminum cluster anions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23896-23908.	1.3	3
4692	Conversion of carbon dioxide to a novel molecule $\text{NCNBO}^{\sim}$ mediated by $\text{NbBN}^{\sim}$ anions at room temperature. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22613-22619.	1.3	2
4693	Dynamic Effects on Migratory Aptitudes in Carbocation Reactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 1088-1097.	6.6	18
4694	Mandrel degradation model of combined fast and slow processes. <i>High Power Laser Science and Engineering</i> , 2021, 9, .	2.0	5
4695	Non-peripherally substituted metallocphthalocyanines catalyzed diastereoselective carbonyl-ylide reactions: Synthesis and DFT calculations. <i>Tetrahedron</i> , 2021, 80, 131892.	1.0	0
4696	Efficient $\text{N}^{\sim}$ -sulfopropylation of chitosan with 1,3-propane sultone in aqueous solutions: neutral pH as the key condition. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 2146-2158.	1.9	7
4697	Mechanism and regio- and stereoselectivity in an NHC-catalyzed Mannich/lactamization domino reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6204-6212.	1.3	7
4698	Three-component reaction involving isoquinoline and dimethyl acethylenedicarboxylate in the presence of indole: Theoretical and experimental investigations of the reaction mechanism. <i>Progress in Reaction Kinetics and Mechanism</i> , 2021, 46, 146867832095686.	1.1	1
4699	Perylene bisimide cyclophanes as receptors for planar transition structures $\hat{\epsilon}$ catalysis of stereoinversions by shape-complementarity and noncovalent $\hat{\epsilon}$ interactions. <i>Organic Chemistry Frontiers</i> , 2021, 8, 4408-4418.	2.3	8
4700	DFT insights into the Ni-catalyzed regioselective hydrocarboxylation of unsaturated alkenes with $\text{CO}^{\sim}$ . <i>Dalton Transactions</i> , 2021, 50, 15084-15093.	1.6	4
4701	Computational Investigation of Substituent Effect on the Thermodynamics and Kinetics of $\hat{2}$ -Hydrocarbyl Elimination from a Rhodium(I) Iminyl Complex. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 163-171.	0.1	0
4702	Study on the Reaction of Nanosized Yttrium Oxide Cluster Anions with $\text{N}^{\sim}$ -Butane in the Gas Phase. <i>Acta Chimica Sinica</i> , 2021, 79, 490.	0.5	1

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4703	Acceptorless dehydrogenative condensation: synthesis of indoles and quinolines from diols and anilines. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 677-683.	1.5	13
4704	Silica-supported Nb(iii)â€“CH <sub>3</sub> species can act as an efficient catalyst for the non-oxidative coupling of methane. <i>New Journal of Chemistry</i> , 2021, 45, 12260-12270.	1.4	1
4705	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021, 3, 74-93.	0.9	9
4706	Nucleophilic catalysis of <i>p</i> -substituted aniline derivatives in acylhydrazone formation and exchange. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7202-7210.	1.5	2
4707	A W1 computational study on the kinetics of initial pyrolysis of a biodiesel model: methyl propanoate. <i>New Journal of Chemistry</i> , 2021, 45, 19531-19541.	1.4	7
4708	Photodissociation of CH <sub>2</sub> BrCHBrC(O)Cl at 248 nm: probing Br <sub>2</sub> as the primary fragment using cavity ring-down spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22492-22500.	1.3	0
4709	A computational approach to understand the role of metals and axial ligands in artificial heme enzyme catalyzed Câ€“H insertion. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9500-9511.	1.3	15
4710	Probing the anomeric effect and mechanism of isomerization of oxazinane rings by DFT methods. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 1066-1082.	1.5	8
4711	Michael addition of ethyl anthranilate and phenyl monothioanthranilate to acetylenic esters: experimental and theoretical results. <i>Structural Chemistry</i> , 2021, 32, 1611-1618.	1.0	0
4712	Mechanistic study on the NHC-catalyzed [3+4] annulation of enals and thiazolones. <i>New Journal of Chemistry</i> , 2021, 45, 12129-12137.	1.4	7
4713	Theoretical study of the reaction mechanism between triphenylphosphine with dialkyl acetylenedicarboxylates in the presence of benzotriazole. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	1
4714	Pyridine-pyrazole based Al( <sup>iii</sup> )â€“turn onâ€™ sensor for MCF7 cancer cell imaging and detection of picric acid. <i>RSC Advances</i> , 2021, 11, 10094-10109.	1.7	22
4715	Topological unraveling of the [3+2] cycloaddition (32CA) reaction between <i>N</i> -methylphenylnitrene and styrene catalyzed by the chromium tricarbonyl complex using electron localization function and catastrophe theory. <i>New Journal of Chemistry</i> , 2021, 45, 20342-20351.	1.4	6
4716	The platination mechanism of RNase A by arsenoplatin: insight from the theoretical study. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1795-1803.	3.0	5
4717	Metal Bound or Free Ylides as Reaction Intermediates in Metal-Catalyzed [2,3]-Sigmatropic Rearrangements? It Depends. <i>ACS Catalysis</i> , 2021, 11, 829-839.	5.5	30
4718	Brønsted Acid Organocatalyzed Three-Component Hydroamidation Reactions of Vinyl Ethers. <i>Journal of Organic Chemistry</i> , 2021, 86, 4171-4181.	1.7	2
4719	Deciphering the Differential Influence of Organic Additives on Coal Fluidity Development: A First-Principles Investigation. <i>Energy &amp; Fuels</i> , 2021, 35, 4053-4066.	2.5	1
4720	Kinetics of the Reactions of Methyl Radical with Hydrogen, Methyl and Ethyl Peroxides. <i>ChemistrySelect</i> , 2021, 6, 1548-1554.	0.7	0

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4721	An experimental and mechanism study on the regioselective click reaction toward the synthesis of thiazolidinone-triazole. <i>Heliyon</i> , 2021, 7, e06113.	1.4	9
4722	CO <sub>2</sub> Activation and Hydrogenation by Palladium Hydride Cluster Anions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1747-1753.	1.1	10
4723	Ammonia and borane activation by Tantalum Carbide cluster anion Ta <sub>2</sub> C <sub>4</sub> <sup>3-</sup> : A theoretical approach. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 8401-8410.	3.8	5
4724	Solid-State Catalytic Hydrogen/Deuterium Exchange in Mexidol. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 273-278.	0.1	1
4725	Modeling (Prediction) of the Structure of Possible Transition States of Aromatic Hydrocarbons. <i>Russian Journal of Organic Chemistry</i> , 2021, 57, 135-142.	0.3	1
4726	Regioselectivity Patterns in Radical Cyclization of Diosphenol Derivatives with Different Ring Size: A Combined Experimental and DFT Study. <i>ChemistrySelect</i> , 2021, 6, 1748-1755.	0.7	0
4727	Mechanistic Insight into Chemical Reactions of Acyclic Diboryloxy Carbenes: the Activation Strain Model Study. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 929-938.	1.0	0
4728	Degradation mechanisms, kinetics and eco-toxicity assessment of 2,4-Dinitrophenol by oxygen-containing free radicals in aqueous solution. <i>Molecular Physics</i> , 2021, 119, e1886365.	0.8	6
4729	The sequential activation of H <sub>2</sub> and N <sub>2</sub> mediated by the gas-phase Sc <sub>3</sub> N <sup>+</sup> clusters: Formation of amido unit. <i>Journal of Chemical Physics</i> , 2021, 154, 054307.	1.2	11
4730	Dynamics of the isotope exchange reaction of D with H <sub>3</sub> <sup>+</sup> , H <sub>2</sub> D <sup>+</sup> , and D <sub>2</sub> H <sup>+</sup> . <i>Journal of Chemical Physics</i> , 2021, 154, 084307.	1.2	3
4731	Photooxidation of Isoprene by Titanium Oxide Cluster Anions with Dimensions up to a Nanosize. <i>Journal of the American Chemical Society</i> , 2021, 143, 3951-3958.	6.6	15
4732	Combined NMR and Computational Study of Cysteine Oxidation during Nucleation of Metallic Clusters in Biological Systems. <i>Inorganic Chemistry</i> , 2021, 60, 4144-4161.	1.9	3
4733	Control of the Regioselectivity of Alkyne Hydrostannylation by Tuning the Metal Pair of Heterobimetallic Catalysts: A Theoretical Study. <i>Organometallics</i> , 2021, 40, 654-662.	1.1	6
4734	Catalysis by Bidentate Iodine(III)-Based Halogen Donors: Surpassing the Activity of Strong Lewis Acids. <i>Journal of Organic Chemistry</i> , 2021, 86, 5317-5326.	1.7	41
4735	Dynamic Effects in Intramolecular Schmidt Reactions: Entropy, Electrostatic Drag, and Selectivity Prediction. <i>ChemPhysChem</i> , 2021, 22, 649-656.	1.0	2
4736	The conductor-like polarizable continuum model study of indenyl effect on the ligand substitution reaction in the (Ī <sup>5+</sup> )-C <sub>9</sub> H <sub>7</sub> Co(CO) <sub>2</sub> complex. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 901-912.	1.0	6
4737	Theoretical investigation of Prolyl-Histidine-catalyzed intermolecular aldol reaction. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4203.	0.9	0
4738	Atmospheric oxidation chemistry of hexafluoroisobutylene initiated by OH radical: Kinetics and mechanism. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113137.	1.1	2

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4739	Kinetic Study of Gas-Phase Reactions of Pyruvic Acid with HO <sub>2</sub> . Journal of Physical Chemistry A, 2021, 125, 2232-2242.	1.1	4
4740	Investigation of the reaction mechanism between cyclohexyl isocyanide and dimethyl acetylenedicarboxylate in the presence of 2-mercaptobenzoxazole: a theoretical study. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 656-663.	0.8	0
4741	Atomic insights into the thermal runaway process of hydrogen peroxide and 1,3,5-trimethylbenzene mixture: Combining ReaxFF MD and DFT methods. Chemical Engineering Research and Design, 2021, 147, 578-588.	2.7	17
4742	The key role of adsorbate-catalyst interactions into catalytic activity of [CTA <sup>+</sup> ]-Si-MCM-41 from electron density analysis. Molecular Catalysis, 2021, 504, 111472.	1.0	1
4743	Atmospheric oxidation of 4-(2-methoxyethyl) phenol initiated by OH radical in the presence of O <sub>2</sub> and NO <sub>x</sub> : A mechanistic and kinetic study. International Journal of Quantum Chemistry, 2021, 121, e26650.	1.0	4
4744	The reaction of dimethyl sulfide with the Criegee intermediates CH <sub>2</sub> OO and (CH <sub>3</sub> ) <sub>2</sub> COO: Theoretical investigations. Computational and Theoretical Chemistry, 2021, 1197, 113145.	1.1	1
4745	An investigation of the regio-, chemo-, and stereoselectivity of cycloaddition reactions of 2-phenylsulfonyl-1,3-butadiene and its 3-phenylsulfanyl derivative: a DFT study. Structural Chemistry, 2021, 32, 1819-1831.	1.0	1
4746	Tuning catalytic activity of dimolybdenum paddlewheel complexes by ligands: mechanism study on the radical addition reaction of CCl <sub>4</sub> to 1-hexene. Structural Chemistry, 2021, 32, 2139-2145.	1.0	0
4747	Theoretical study of the reactions of hydrogen atom with methyl and ethyl hydroperoxides. Molecular Physics, 0, , e1919324.	0.8	1
4748	Unimolecular Pyrolysis Mechanism of Thiophene and Furan: An Ab Initio Comparative Study. Energy & Fuels, 2021, 35, 7819-7832.	2.5	5
4749	Theoretical insights into the degradation of tyrosol stimulated by hydroxyl and sulfate radicals in wastewater and ecotoxicity evaluation. Journal of Cleaner Production, 2021, 293, 126161.	4.6	16
4750	Kinetics and mechanisms of OH-induced 2-ethoxyethanol oxidation in the atmosphere. Structural Chemistry, 2021, 32, 2147-2157.	1.0	3
4751	Theoretical insights into phosphine-catalyzed [4+2] annulation of allenolates with thiazolone-derived alkenes. Journal of Physical Organic Chemistry, 2021, 34, e4215.	0.9	0
4752	Revisited the reaction mechanism of cobalt catalyzed [3+2] cycloaddition reactions between the derivatives of cyclopropanols and allenes: A DFT study. Journal of Organometallic Chemistry, 2021, 937, 121744.	0.8	4
4753	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. Fuel, 2021, 290, 119970.	3.4	22
4754	Comparative DFT Study on Dehydrogenative C(sp) <sup>3</sup> -H Elementation (E = Si, Ge, and Sn) of Terminal Alkynes Catalyzed by a Cationic Ruthenium(II) Thiolate Complex. Inorganic Chemistry, 2021, 60, 6228-6238.	1.9	4
4755	Mechanistic insights into the autocatalyzed rearrangement of 2-bromooxazolines to 2-bromoisocyanates by means of high-level quantum chemical methods. Journal of Physical Organic Chemistry, 2021, 34, e4214.	0.9	0
4756	Homotropic Cooperativity of Midazolam Metabolism by Cytochrome P450 3A4: Insight from Computational Studies. Journal of Chemical Information and Modeling, 2021, 61, 2418-2426.	2.5	17

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4757	Lewis Structures from Open Quantum Systems Natural Orbitals: Real Space Adaptive Natural Density Partitioning. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4013-4025.	1.1	6
4758	Activation of Carbon Dioxide by CoCDn <sup>4-</sup> (n = 0-4) Anions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3710-3717.	1.1	4
4759	Atmospheric Oxidation of Propanesulfinic Acid Initiated by OH Radicals: Reaction Mechanism, Energetics, Rate Coefficients, and Atmospheric Implications. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 1498-1510.	1.2	10
4760	Modeling Hydrogen Spillover on Oxide Catalytic Centers. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 944-948.	0.1	2
4761	Structures of a non-ribosomal peptide synthetase condensation domain suggest the basis of substrate selectivity. <i>Nature Communications</i> , 2021, 12, 2511.	5.8	53
4762	A DFT study on the mechanism and selectivity of [3+2] cycloaddition reactions leading to pyrrole[2,1-a] phthalazine compounds. <i>Theoretical Chemistry Accounts</i> , 2021, 140, .	0.5	1
4763	New Mechanistic Insights into Atmospheric Oxidation of Aniline Initiated by OH Radicals. <i>Environmental Science &amp; Technology</i> , 2021, 55, 7858-7868.	4.6	20
4764	Theoretical study of the reactions of nitrogen dioxide with hydrogen and methyl peroxides. <i>Chemical Physics Letters</i> , 2021, 771, 138498.	1.2	4
4765	Kinetics of three reactions involving the azide radical: H <sub>2</sub> N <sub>3</sub> , thermal decomposition of N <sub>3</sub> , and N <sub>3</sub> <sup>+</sup> N <sub>3</sub> . <i>Chemical Physics Letters</i> , 2021, 771, 138515.	1.2	0
4766	Theoretical insights into the dimerization mechanism of aluminum species at two different pH conditions. <i>Inorganica Chimica Acta</i> , 2021, 520, 120311.	1.2	5
4767	Insights into evolution mechanism of PAHs in coal thermal conversion: A combined experimental and DFT study. <i>Energy</i> , 2021, 222, 119970.	4.5	17
4768	A density functional theory investigation on bis(diethylamino)cyclopropenylidene catalyzed synthesis of 1,4-bifunctional compounds. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4219.	0.9	2
4769	Density Functional Theory Investigation of the Conversion of 5-(Hydroxymethyl)furfural into 2,5-Dimethylfuran over the Pd(111), Cu(111), and Cu <sub>3</sub> Pd(111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10295-10317.	1.5	18
4770	Fritsch <sup>1</sup> –Buttenberg <sup>2</sup> –Wiechell rearrangement of magnesium alkylidene carbenoids leading to the formation of alkynes. <i>Beilstein Journal of Organic Chemistry</i> , 2021, 17, 1352-1359.	1.3	1
4771	Solvent and temperature effects on the tautomerization of a carbonitrile molecule: A conductor-like polarizable continuum model (CPCM) study. <i>Main Group Chemistry</i> , 2021, 20, 59-68.	0.4	3
4772	A theoretical study on screening ionic liquids for SO <sub>2</sub> capture under low SO <sub>2</sub> partial pressure and high temperature. <i>Journal of Industrial and Engineering Chemistry</i> , 2021, 98, 161-167.	2.9	8
4773	Asymmetric Nucleophilic Allylation of $\alpha$ -Chloro Glycinate via Squaramide Anion-Abstraction Catalysis: S <sub>N</sub> 1 or S <sub>N</sub> 2 Mechanism, or Both?. <i>Journal of Organic Chemistry</i> , 2021, 86, 8414-8424.	1.7	5
4774	Non-noble metal single atom catalysts with S, N co-doped defective graphene support: A theoretical study of highly efficient acetylene hydration. <i>Materials Today Communications</i> , 2021, 27, 102216.	0.9	2

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4775	A molecular electron density theory study of the [3+2] cycloaddition reaction of nitronic ester with methyl acrylate. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
4776	Reinvestigation of tandem dimerization and 1,3-alkyl shift in 3-benzylbenzothiazolydene carbene: Experimental and theoretical results. <i>Journal of Molecular Structure</i> , 2021, 1233, 130103.	1.8	0
4777	Theoretical study on CO <sub>2</sub> hydrogenation mediated by Ru-PNP pincer complexes: An implication towards rational catalyst design. <i>Journal of Organometallic Chemistry</i> , 2021, 943, 121842.	0.8	0
4778	Theoretical study of the reactions of propargyl radical with methanol and ethanol. <i>Molecular Physics</i> , 2021, 119, .	0.8	0
4779	A DFT study of graphene-FeN <sub>x</sub> (x = 4, 3, 2, 1) catalysts for acetylene hydrochlorination. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 618, 126495.	2.3	10
4780	Structural Transitions in Glassy Atactic Polystyrene Using Transition-State Theory. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7273-7289.	1.2	5
4781	Unveiling the Ionic Diels-Alder Reactions within the Molecular Electron Density Theory. <i>Molecules</i> , 2021, 26, 3638.	1.7	3
4782	Investigation of the thermal stability of the antihypertensive drug nebivolol under different conditions: Experimental and computational analysis. <i>Journal of Thermal Analysis and Calorimetry</i> , 2022, 147, 5779-5786.	2.0	8
4783	Comparison of (5 + 2) Cycloadditions Involving Oxidopyrylium and Oxidopyridinium Ions: Relative Reactivities. <i>Journal of Organic Chemistry</i> , 2021, 86, 8652-8659.	1.7	6
4784	A Density Functional Theory Study on Et-BAC-Catalyzed 1,6-Conjugate Addition of <i>p</i> -Chlorobenzaldehyde to <i>p</i> -Quinone Methide for the Synthesis of $\beta,\beta$ -Diarylated Ketones. <i>Journal of Organic Chemistry</i> , 2021, 86, 9040-9054.	1.7	6
4785	Degradation mechanism of tris(2-chloroethyl) phosphate (TCEP) as an emerging contaminant in advanced oxidation processes: A DFT modelling approach. <i>Chemosphere</i> , 2021, 273, 129674.	4.2	12
4786	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
4787	Theoretical investigations on mechanisms and kinetics of methylketene with O(3P) reaction in the atmosphere. <i>Journal of Molecular Modeling</i> , 2021, 27, 228.	0.8	0
4788	Combined crossed molecular beams and computational study on the N( <sup>2</sup> D) + HCCN(X <sup>1</sup> ) reaction and implications for extra-terrestrial environments. <i>Molecular Physics</i> , 2022, 120, .	0.8	9
4789	Mechanism and regioselectivity of [Cu-Fe] heterobimetallic-catalyzed hydroboration of pyridines: DFT investigation. <i>Molecular Catalysis</i> , 2021, 511, 111722.	1.0	4
4790	Unveiling [3+2] cycloaddition reactions of benzonitrile oxide and diphenyl diazomethane to cyclopentene and norbornene: a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	8
4791	Mechanism and kinetic study for the reaction of allyl cyanide with Cl atom in the presence of O <sub>2</sub> . <i>Computational and Theoretical Chemistry</i> , 2021, 1201, 113286.	1.1	1
4792	An IrVO <sub>4</sub> Cluster Catalytically Oxidizes Four CO Molecules: Importance of Ir-V Multiple Bonding. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6519-6525.	2.1	9

#	ARTICLE	IF	CITATIONS
4793	Theoretical study of the Diels-Alder reaction of 3-bromo-1-phenylprop-2-ynone with furan and 2-methylfuran. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	5
4794	DFT Study on the Biosynthesis of Verrucosane Diterpenoids and Mangicol Sesterterpenoids: Involvement of Secondary-Carbocation-Free Reaction Cascades. <i>Jacs Au</i> , 2021, 1, 1231-1239.	3.6	15
4795	Experimental and Computational Evaluation of Tantalocene Hydrides for C-H Activation of Arenes. <i>Organometallics</i> , 2021, 40, 2666-2677.	1.1	3
4796	Theoretical Study on the Unimolecular Pyrolysis of Thiophene and Modeling. <i>ACS Omega</i> , 2021, 6, 20471-20482.	1.6	6
4797	Understanding the Catalytic Sites in Porous Hexagonal Boron Nitride for the Epoxidation of Styrene. <i>ACS Catalysis</i> , 2021, 11, 8872-8880.	5.5	20
4798	Theoretical Investigation of HER Mechanism Using Density Functional and Ab Initio Calculations. <i>Bulletin of the Korean Chemical Society</i> , 2021, 42, 1289.	1.0	1
4799	A DFT Study on the Mechanism of Catalytic Oxidation Desulfurization Over Ti-MWW Zeolite. <i>Journal of Cluster Science</i> , 2022, 33, 2103-2112.	1.7	3
4800	Fate of Cobaltacycles in Cp*Co-Mediated C-H Bond Functionalization Catalysis: Cobaltacycles May Collapse upon Oxidation via Co(IV) Species. <i>Organometallics</i> , 2021, 40, 2624-2642.	1.1	4
4801	Quantum Chemical Study of Mechanisms of Organic Reactions: X. Reaction of Dipotassium Propane-1,3-bis(thiolate) with 1,3-Dichloropropene in the System Hydrazine Hydrate-KOH. <i>Russian Journal of Organic Chemistry</i> , 2021, 57, 1073-1083.	0.3	0
4802	Factors Controlling the Aluminum(I)-meta-Selective C-H Activation in Arenes. <i>Chemistry - A European Journal</i> , 2021, 27, 12422-12429.	1.7	8
4803	Viable route and DFT study for the synthesis of optically active limonaketone: A barely available natural feedstock in <i>Cedrus atlantica</i> . <i>Journal of Molecular Structure</i> , 2021, 1235, 130221.	1.8	4
4804	Metal-free and iron(II)-assisted oxidation of cyclohexane to adipic acid with ozone: A theoretical mechanistic study. <i>Journal of Catalysis</i> , 2021, 399, 52-66.	3.1	17
4805	Computational Investigation on the Formation and Decomposition Reactions of the C <sub>4</sub> H <sub>3</sub> O Compound. <i>ACS Omega</i> , 2021, 6, 17965-17976.	1.6	5
4806	Mechanistic Insights into the Dual Directing Group-Mediated C-H Functionalization/Annulation <i>via</i> a Hydroxyl Group-Assisted M <sup>III</sup> -M <sup>V</sup> -M <sup>III</sup> Pathway. <i>ACS Omega</i> , 2021, 6, 17642-17650.	1.6	5
4807	Exploring The Sequence of Electron Density Along The Chemical Reactions Between Carbonyl Oxides And Ammonia/Water Using Bond Evolution Theory. <i>ChemPhysChem</i> , 2021, 22, 1792-1801.	1.0	10
4808	Unveiling the Different Reactivity of Bent and Linear Three-Atom-Components Participating in [3 + 2] Cycloaddition Reactions. <i>Organics</i> , 2021, 2, 274-286.	0.6	6
4809	Amino-grafted Cu and Sc Metal-Organic Frameworks involved in the green synthesis of 2-amino-4H-chromenes. Mechanistic understanding. <i>Microporous and Mesoporous Materials</i> , 2021, 323, 111232.	2.2	6
4810	Ozonolysis of Permethrin in the Atmosphere: Mechanism, Kinetics, and Evaluation of Toxicity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7705-7715.	1.1	9



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4811	Scale for Cyclopropenium Ions with Applications in CO <sub>2</sub> Capture. <i>Journal of Organic Chemistry</i> , 2021, 86, 11835-11844.	1.7	2
4812	Counterion Effect on the Mechanism of Gold(I)-Catalyzed Cycloisomerization of 3-Allenylmethylindoles to 4,9-Dihydro-1-H-Carbazoles: A Computational Study. <i>ChemistrySelect</i> , 2021, 6, 7482-7488.	0.7	0
4813	Combined Experimental and Computational Mechanistic Investigation of the Palladium-Catalyzed Decarboxylative Cross-Coupling of Sodium Benzoates with Chloroarenes. <i>Journal of Organic Chemistry</i> , 2021, 86, 11419-11433.	1.7	5
4814	Enhanced catalytic performance of oxidized Ru supported on N-doped mesoporous carbon for acetylene hydrochlorination. <i>Applied Catalysis A: General</i> , 2021, 623, 118236.	2.2	11
4815	A theoretical study on gas-phase reaction of methylketene with OH: mechanism, kinetics, and insights. <i>Structural Chemistry</i> , 0, , 1.	1.0	1
4816	Quantum Mechanical Investigation of the Oxidative Cleavage of the C-C Backbone Bonds in Polyethylene Model Molecules. <i>Polymers</i> , 2021, 13, 2730.	2.0	8
4817	A theoretical study on mechanism and kinetics of the C <sub>2</sub> H <sub>3</sub> +C <sub>2</sub> H <sub>3</sub> recombination and the isomerization and dissociation of butadiene. <i>Chemical Physics</i> , 2021, 548, 111217.	0.9	7
4818	Theoretical Studies on the Reaction Mechanism and Kinetics of Ethylbenzene-OH Adduct with O <sub>2</sub> and NO <sub>2</sub> . <i>Atmosphere</i> , 2021, 12, 1118.	1.0	4
4819	Multi-Ion Bridged Pathway of N-Oxides to 1,3-Dipole Dilithium Oxide Complexes. <i>Journal of Organic Chemistry</i> , 2021, 86, 11502-11518.	1.7	1
4820	Computational Study of the Effect of Doping with Ti on NaAlH <sub>4</sub> Nanocluster Dehydrogenation. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, 1646-1654.	0.1	0
4821	Theoretical investigations on mechanisms and kinetics of methylketene with H reaction in the atmosphere. <i>Journal of Physical Organic Chemistry</i> , 0, , e4274.	0.9	0
4822	Catalytic performance of Pt <sub>3</sub> Ni cluster toward ethane activation. <i>Chemical Physics</i> , 2021, 548, 111204.	0.9	2
4823	Network structure and properties of crosslinked bio-based epoxy resin composite: An in-silico multiscale strategy with dynamic curing reaction process. <i>Giant</i> , 2021, 7, 100063.	2.5	7
4824	Understanding the Participation of Fluorinated Azomethine Ylides in Carbenoid-Type [3 + 2] Cycloaddition Reactions with Ynal Systems: A Molecular Electron Density Theory Study. <i>Journal of Organic Chemistry</i> , 2021, 86, 12644-12653.	1.7	17
4825	Mechanistic study of vanadium-modified and sulfation-modified Phillips catalyst. <i>Molecular Catalysis</i> , 2021, 513, 111777.	1.0	1
4826	Unveiling the Intramolecular Ionic Diels-Alder Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021, 3, 834-853.	0.9	0
4827	Catalytic decomposition of N <sub>2</sub> O on iron-embedded C <sub>2</sub> N monolayer: A DFT study. <i>Materials Today Communications</i> , 2021, 28, 102585.	0.9	4
4828	Kinetics study on the reactions of dimethyl ether with triplet oxygen and hydrogen atoms. <i>Chemical Physics Letters</i> , 2021, 779, 138855.	1.2	4

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4829	Theoretical insight into the mechanisms of the gas-phase decomposition of azidoacetone. <i>Chemical Physics Letters</i> , 2021, 778, 138833.	1.2	0
4830	Computational Mechanistic Study of Fused Phenol Formations from 1,6-Heptadiyne Involving Carbyne Complexes. <i>ChemCatChem</i> , 0, , .	1.8	2
4831	Quadruple C-H Bond Activations of Methane by Dinuclear Rhodium Carbide Cation $[Rh_2C_3]^+$ . <i>Jacs Au</i> , 2021, 1, 1631-1638.	3.6	6
4832	BF <sub>3</sub> -catalyzed oxa-Diels-Alder reaction of ethyl vinyl sulfide and 2-methyl-phenylacrolein: a molecular electron density theory study. <i>Monatshefte für Chemie</i> , 2021, 152, 1209-1221.	0.9	6
4833	Application of density functional theory on the NO-char heterogeneous reduction mechanism in the presence of CO <sub>2</sub> . <i>Journal of Fuel Chemistry and Technology</i> , 2021, 49, 1231-1238.	0.9	1
4834	Theoretical insights into the enhancement of 1-Methyl-2,4,5-trinitroimidazole yield by exchanging of group introduction order. <i>Chemical Physics Letters</i> , 2021, 779, 138834.	1.2	2
4835	Theoretical study of the reactions of triplet Oxygen atom with methyl and ethyl hydroperoxides. <i>Molecular Physics</i> , 0, , .	0.8	0
4836	Synthesis of Pentacoordinated Spiro[4,4]phosphoranes by Reaction of Cyclic Phosphazanyl Anions with Epoxides. Study of their P-Remote Functionalization and Hydrolysis. <i>Synthesis</i> , 0, 0, .	1.2	2
4837	The role of electric field on decomposition of $CL \cdot 20 \cdot HMX$ cocrystal: A reactive molecular dynamics study. <i>Journal of Computational Chemistry</i> , 2021, 42, 2202-2212.	1.5	8
4838	Experimental and DFT research on role of sodium in NO reduction on char surface under H <sub>2</sub> O/Ar atmosphere. <i>Fuel</i> , 2021, 302, 121105.	3.4	13
4839	Facile and green preparation of colorimetric and fluorescent sensors for mercury, silver, and carbonate ions visual detecting: Spectroscopy and theoretical studies. <i>Journal of Molecular Structure</i> , 2021, 1241, 130626.	1.8	21
4840	Transformation of 1,1-biphosphirane-M(CO) <sub>5</sub> (M=Mo, Cr, W) complexes: Possible mechanisms and reactivity of active intermediates. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113420.	1.1	1
4841	Shapeshifting radicals. <i>Chemical Physics</i> , 2022, 552, 111373.	0.9	1
4842	Theoretical study of the reactions of triplet oxygen atom with 1-propanol and 2-propanol. <i>Chemical Physics Letters</i> , 2021, 781, 138990.	1.2	2
4843	Atmospheric ozonolysis of crotonaldehyde in the absence and presence of hydroxylated silica oligomer cluster adsorption. <i>Chemosphere</i> , 2021, 281, 130996.	4.2	4
4844	Theoretical investigations on the OH radical mediated kinetics of cis- and trans-CH <sub>3</sub> CF=CHF and CH <sub>3</sub> CH=CF <sub>2</sub> over temperature range of 200-400K. <i>Journal of Fluorine Chemistry</i> , 2021, 250, 109884.	0.9	1
4845	Mechanistic and kinetics study on the reaction of methylallyl alcohol with Cl: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2021, 1204, 113388.	1.1	0
4846	N-Acetylcysteine versus arsenic poisoning: A mechanistic study of complexation by molecular spectroscopy and density functional theory. <i>Journal of Molecular Liquids</i> , 2021, 340, 117168.	2.3	6

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4847	Theoretical Study on the Mechanism of Spirocyclization in Spiroviolene Biosynthesis. <i>Chemical and Pharmaceutical Bulletin</i> , 2021, 69, 1034-1038.	0.6	10
4848	Photochromism of dye containing Schiff base-metal complex: A revisit through spectro-kinetic, thermodynamic and theoretical analyses for the design of a molecular logic gate. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 420, 113505.	2.0	18
4849	Chemical reactivities and molecular docking studies of parthenolide with the main protease of HEP-G2 and SARS-CoV-2. <i>Journal of Molecular Structure</i> , 2021, 1243, 130705.	1.8	17
4850	Divulging the regioselectivity of epoxides in the ring-opening reaction, and potential himachalene derivatives predicted to target the antibacterial activities and SARS-CoV-2 spike protein with docking study. <i>Journal of Molecular Structure</i> , 2021, 1244, 130864.	1.8	10
4851	A Sensitization-Free Dimethyl Fumarate Prodrug, Isosorbide Di-(Methyl Fumarate), Provides a Topical Treatment Candidate for Psoriasis. <i>JID Innovations</i> , 2021, 1, 100040.	1.2	8
4852	Theoretical study of gas-phase detoxication of DMMP and DMPT using ammonia-borane and its analogous compound. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 109, 108037.	1.3	0
4853	Theoretical insight into the initial reaction of ozone with peroxide: Single electron transfer or adduct formation. <i>Chemical Engineering Journal</i> , 2022, 429, 132308.	6.6	4
4854	Synthesis of an industrial by-product-based polymeric additive for use with non-coking coal in metallurgical coke making and a combined density functional theory assessment of its molecular mechanism in fluidity development. <i>Soft Matter</i> , 2021, 17, 4122-4132.	1.2	2
4855	Understanding the different reactivity of ( <i>Z</i> )- and ( <i>E</i> )- <i>l</i> <sup>2</sup> -nitrostyrenes in [3+2] cycloaddition reactions. An MEDT study. <i>RSC Advances</i> , 2021, 11, 9698-9708.	1.7	7
4856	Insights into the mechanism and regioselectivity of the [3+2] cycloaddition reactions of cyclic nitron to nitrile functions with a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	0.5	13
4857	The keto $\rightleftharpoons$ enol tautomerization of ethyl acetoacetate in choline ionic liquids: the role of cation and anion in switching the tautomeric equilibrium. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 7386-7397.	1.3	4
4858	Computational study on the reactivity of imidazolium-functionalized manganese bipyridyl tricarbonyl electrocatalysts [Mn[bpyMe(Im-R)](CO) <sub>3</sub> Br] <sup>+</sup> (R = Me, Me <sub>2</sub> and Tj ETQq1 1.0.784314 rgBT /Ov 1.3	1.3	0
4859	Mechanism of iron complexes catalyzed in the <i>N</i> -formylation of amines with CO <sub>2</sub> and H <sub>2</sub> : the superior performance of $\sigma$ -H ligand methylated complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16675-16689.	1.3	3
4860	The CH <sub>2</sub> + OH Gas Phase Reaction: Formaldehyde and Acetaldehyde Formation Routes. <i>Lecture Notes in Computer Science</i> , 2021, , 581-593.	1.0	0
4861	Long-Range Complex in the HC <sub>3</sub> N + CN Potential Energy Surface: Ab Initio Calculations and Intermolecular Potential. <i>Lecture Notes in Computer Science</i> , 2021, , 413-425.	1.0	2
4862	Mechanistic insight into B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> catalyzed imine reduction with PhSiH <sub>3</sub> under stoichiometric water conditions. <i>RSC Advances</i> , 2021, 11, 20961-20969.	1.7	4
4863	Mechanistic insights of the degradation of an O-anisidine carcinogenic pollutant initiated by OH radical attack: theoretical investigations. <i>New Journal of Chemistry</i> , 2021, 45, 5907-5924.	1.4	10
4864	A theoretical investigation of iron-catalyzed selective hydrogenation of nitriles to secondary imines. <i>Chemical Physics Letters</i> , 2021, 762, 138130.	1.2	1

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4865	Mechanistic insights into rhodium-catalyzed enantioselective allylic alkylation for quaternary stereogenic centers. <i>Chemical Science</i> , 2021, 12, 2527-2539.	3.7	9
4866	Probing BrCl from photodissociation of CH <sub>2</sub> BrCl and CHBr <sub>2</sub> Cl at 248 nm using cavity ring-down spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6098-6106.	1.3	2
4867	DFT Quest of the Active Species of the Gallium-Mediated Coupling of Methylidenemalonates and Acetylenes. <i>Inorganic Chemistry</i> , 2021, 60, 995-1006.	1.9	3
4868	Stability of neutral molecular polynitrogens: energy content and decomposition mechanisms. <i>RSC Advances</i> , 2021, 11, 21567-21578.	1.7	4
4869	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. <i>New Journal of Chemistry</i> , 2021, 45, 13626-13638.	1.4	10
4870	N-Heterocyclic Carbenes-CuI Complexes as Catalysts: A Theoretical Insight. <i>Australian Journal of Chemistry</i> , 2021, 74, 503.	0.5	3
4871	Toward Better Halon Substitutes: Theoretical and Experimental Studies on the Pyrolysis Mechanism and Fire-Suppressing Performance of C <sub>5</sub> F <sub>10</sub> O (Perfluoro-3-methyl-2-butanone). <i>ACS Sustainable Chemistry and Engineering</i> , 2021, 9, 1272-1285.	3.2	9
4872	Theoretical Investigation of the Mechanisms and Kinetics of the Bimolecular and Unimolecular Reactions Involving in the C <sub>4</sub> H <sub>6</sub> Species. <i>Journal of Physical Chemistry A</i> , 2021, 125, 585-596.	1.1	10
4873	Rationalization of the mechanism and chemoselectivity of versatile Au-catalyzed reactions of diazoesters with allyl-functionalized sulfides, selenides, amines, or ethers by DFT. <i>Organic Chemistry Frontiers</i> , 2021, 8, 6053-6062.	2.3	3
4874	Topological investigation of the reaction mechanism of glycerol carbonate decomposition by bond evolution theory. <i>RSC Advances</i> , 2021, 11, 10083-10093.	1.7	12
4875	On the Catalytic Effects of the Thiazolium Salt in the Oxa-Diel-Alder Reaction between Benzaldehyde and Danishefsky's Diene: A Molecular Electron Density Theory Study. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9306-9317.	1.5	0
4876	Organocatalytic Enantioselective Higher-Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. <i>Angewandte Chemie</i> , 2018, 130, 1260-1264.	1.6	16
4877	Nitrite Reduction in Aqueous Solution Mediated by Amavadin Homologues: N <sub>2</sub> O Formation and Water Oxidation. <i>Chemistry - A European Journal</i> , 2018, 24, 2474-2482.	1.7	9
4878	Mechanistic Insights into the Regio- and Stereoselectivities of Testosterone and Dihydrotestosterone Hydroxylation Catalyzed by CYP3A4 and CYP19A1. <i>Chemistry - A European Journal</i> , 2020, 26, 6214-6223.	1.7	7
4879	Computational Insights into the CH <sub>3</sub> Cl+OH Chemical Reaction Dynamics at the Air-Water Interface. <i>ChemPhysChem</i> , 2017, 18, 2747-2755.	1.0	4
4880	Mechanism, Chemoselectivity, and Stereoselectivity of NHC-Catalyzed Asymmetric Desymmetrization of Enal-ethered Cyclohexadienones. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 3726-3733.	1.2	8
4881	Combined ab initio and density functional study of ring chain tautomerism in benzofurazan-1-oxide. <i>Journal of Computational Chemistry</i> , 1996, 17, 1848-1856.	1.5	25
4883	A Computational Study of the Reaction Cyanoacetylene and Cyano Radical Leading to 2-Butynedinitrile and Hydrogen Radical. <i>Lecture Notes in Computer Science</i> , 2020, , 707-716.	1.0	3

#	ARTICLE	IF	CITATIONS
4884	A Theoretical Investigation of the Reactions of N(2D) with Small Alkynes and Implications for the Prebiotic Chemistry of Titan. <i>Lecture Notes in Computer Science</i> , 2020, , 717-729.	1.0	3
4885	A Computational Study on the Insertion of N(2D) into a C-H or C-C Bond: The Reactions of N(2D) with Benzene and Toluene and Their Implications on the Chemistry of Titan. <i>Lecture Notes in Computer Science</i> , 2020, , 744-755.	1.0	7
4886	Design of Catalysts for Asymmetric Organic Reactions Through Density Functional Calculations. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 107-136.	0.6	2
4887	Theoretical Investigation of the NO <sub>3</sub> Initiated Reaction of VOCs. <i>NATO Science for Peace and Security Series C: Environmental Security</i> , 2013, , 163-171.	0.1	1
4888	Solvent Effects on the Diels-Alder Reaction of Methyl Vinyl Ketone and Cyclopentadiene from Computer Simulations. , 1993, , 377-387.		2
4889	Theory of Gas Phase Ion Chemistry: Energetics, Kinetics and Dynamics of Unimolecular and Bimolecular Reactions of Polyatomic Ions. , 1999, , 235-262.		1
4890	Direct Dynamics Method for the Calculation of Reaction Rates. , 1995, , 229-255.		106
4891	Loose Definitions of Reaction Paths. , 1995, , 39-75.		1
4892	Density Functional Theory, Calculations of Potential Energy Surfaces and Reaction Paths. , 1995, , 161-189.		4
4893	Using the Reaction Path Concept to Obtain Rate Constants From ab initio Calculations. , 1995, , 191-228.		2
4894	Density functional theory studies of the uncatalysed gas-phase oxidative dehydrogenation conversion of n-hexane to hexenes. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 153-164.	1.1	10
4895	Density functional theory investigation on the mechanism of dehydrogenation of cyclohexane catalyzed by heteronuclear NiTi+. <i>Computational and Theoretical Chemistry</i> , 2020, 1184, 112820.	1.1	3
4896	Regio-, diastereo- and enantioselectivity in the synthesis of CF <sub>3</sub> -containing spiro[pyrrolidin-3,2-oxindole] through the organocatalytic [3+2] cycloaddition reaction: A molecular electron density theory study. <i>Journal of Fluorine Chemistry</i> , 2020, 236, 109566.	0.9	8
4897	Thermochemical and Kinetics of Hydrazine Dehydrogenation by an Oxygen Atom in Hydrazine-Rich Systems: A Dimer Model. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12607-12614.	1.1	7
4898	Cracking under Internal Pressure: Photodynamic Behavior of Vinyl Azide Crystals through N <sub>2</sub> Release. <i>Journal of the American Chemical Society</i> , 2020, 142, 18565-18575.	6.6	23
4899	Understanding the role of frustrated Lewis pairs as ligands in transition metal-catalyzed reactions. <i>Dalton Transactions</i> , 2020, 49, 3129-3137.	1.6	10
4900	The ortho-to-para ratio of H <sub>2</sub> Cl <sup>+</sup> : Quasi-classical trajectory calculations and new simulations in light of new observations. <i>Astronomy and Astrophysics</i> , 2017, 608, A96.	2.1	6
4901	Hydrogen-assisted C-C coupling on reaction of Cu <sub>3</sub> H <sup>+</sup> Cluster anion with CO. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 628-634.	0.6	2

#	ARTICLE	IF	CITATIONS
4902	A Sesquiterpene Isonitrile with a New Tricyclic Skeleton from the Indo-Pacific Nudibranch <i>Phyllidiella pustulosa</i> : Spectroscopic and Computational Studies. <i>Australian Journal of Chemistry</i> , 2020, 73, 129.	0.5	9
4903	Effect of Substitution for Insertion of CO <sub>2</sub> into Epoxides and Aziridines: An Ab Initio Study. <i>Australian Journal of Chemistry</i> , 2020, 73, 30.	0.5	1
4904	Utilizing the Combined Power of Theory and Experiment to Understand Molecular Structure â€“ Solid-State and Gas-Phase Investigation of Morpholine Borane. <i>Australian Journal of Chemistry</i> , 2020, 73, 794.	0.5	4
4905	Azoxy rearrangement reactions. <i>Molecular Physics</i> , 1997, 91, 789-804.	0.8	5
4906	On the Concerted Ring Opening of Protonated Squalene Oxide and A-Ring Formation in the Biosynthesis of Lanosterol. <i>Collection of Czechoslovak Chemical Communications</i> , 2003, 68, 202-210.	1.0	12
4907	Formation of Ring A in the Biosynthesis of Hopanoids from Squalene. A Density Functional Study. <i>Collection of Czechoslovak Chemical Communications</i> , 2004, 69, 261-266.	1.0	8
4908	Sorption and Diffusion of Small Molecules Using Transition-State Theory. , 2004, , .		2
4909	Reaction Force. , 2009, , .		5
4910	Biapenem Inactivation by B <sub>2</sub> Metallo $\beta$ -Lactamases: Energy Landscape of the Post-Hydrolysis Reactions. <i>PLoS ONE</i> , 2012, 7, e30079.	1.1	14
4911	Biapenem Inactivation by B <sub>2</sub> Metallo $\beta$ -Lactamases: Energy Landscape of the Hydrolysis Reaction. <i>PLoS ONE</i> , 2013, 8, e55136.	1.1	11
4912	In Silico Studies in Probing the Role of Kinetic and Structural Effects of Different Drugs for the Reactivation of Tabun-Inhibited AChE. <i>PLoS ONE</i> , 2013, 8, e79591.	1.1	10
4914	Estimation of Solvent Effects for the Complexing Reaction of Propylene and Nickel Dithiolene. <i>Data Science Journal</i> , 2007, 6, S837-S846.	0.6	8
4915	Elucidation of Selectivity Difference in the Diels-Alder Reactions of 6,6-Disubstituted Cyclohexa-2,4-dienone. <i>Bulletin of the Korean Chemical Society</i> , 2002, 23, 829-837.	1.0	5
4916	The Rearrangement Reaction of CH <sub>3</sub> SNO <sub>2</sub> to CH <sub>3</sub> SONO Studied by a Density Functional Theory Method. <i>Bulletin of the Korean Chemical Society</i> , 2004, 25, 1657-1660.	1.0	5
4917	Theoretical Studies on the Addition Reactions of Ketene with NH <sub>3</sub> in the Gas Phase and in Non-Aqueous Solutions. <i>Bulletin of the Korean Chemical Society</i> , 2008, 29, 1335-1343.	1.0	4
4918	Ab Initio Study on the Thermal Decomposition of CH <sub>3</sub> CF <sub>2</sub> O Radical. <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 2973-2978.	1.0	4
4919	Adsorption Reactions of Trimethylgallium and Arsine on H/Si(100)-2x1 Surface. <i>Bulletin of the Korean Chemical Society</i> , 2009, 30, 1805-1810.	1.0	5
4920	Density Functional Theoretical Study on the C-H Coupling Reaction from Ir(III) Complexes. <i>Bulletin of the Korean Chemical Society</i> , 2010, 31, 500-502.	1.0	5

#	ARTICLE	IF	CITATIONS
4921	Intramolecular Ion-Molecule Reactions within $Ti^{+}(CH_3)_3COCH_3)_n$ Heteroclusters: Oxidation Pathway via C=O Bond Activation. Bulletin of the Korean Chemical Society, 2010, 31, 953-958.	1.0	4
4922	Density Functional Theoretical Study on the N-H Bond Activation by Ir Pincer Complexes. Bulletin of the Korean Chemical Society, 2010, 31, 1421-1423.	1.0	6
4923	Density Functional Theoretical Study on the Oxidative Additions of Silyl Halides to the Rh Pincer Complex. Bulletin of the Korean Chemical Society, 2011, 32, 2479-2481.	1.0	5
4924	Density Functional Theoretical Study on the Substituent Effect in Aryl Halide Oxidative Additions to a Rh Pincer Complex. Bulletin of the Korean Chemical Society, 2012, 33, 3838-3840.	1.0	2
4925	Density Functional Theoretical Study on the Carbon-Halide Oxidative Additions to a Rh Pincer Complex. Bulletin of the Korean Chemical Society, 2012, 33, 1052-1054.	1.0	3
4926	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
4927	Infrared Multiphoton Dissociation Spectroscopy of Protonated 1,2-Diaminoethane-water Clusters: Vibrational Assignment via the MP2 Method. Bulletin of the Korean Chemical Society, 2013, 34, 3327-3334.	1.0	3
4928	Theoretical Investigation of the Reaction of Ce <sup>+</sup> with Water in the Gas Phase: Density Functional Theory Calculations. Bulletin of the Korean Chemical Society, 2013, 34, 1551-1554.	1.0	1
4929	Stability and Interconversion of Acetylcholine Conformers. Bulletin of the Korean Chemical Society, 2014, 35, 2911-2916.	1.0	3
4930	Density Functional Theory Study of Competitive Reaction Pathways of $Ti^{+}$ with Fluorinated Acetone in the Gas Phase. Journal of the Korean Chemical Society, 2012, 56, 14-19.	0.2	1
4931	Regio- and stereoselective (3 + 2)-cycloaddition reactions of nitrones with cyclic allenes. Organic and Biomolecular Chemistry, 2021, 19, 9773-9784.	1.5	3
4932	Theoretical Insights into the Cooperative Catalytic Mechanism of a PW-Containing Keggin Heteropolyacid Anion and Ethanol toward Conversion of Fructose into 5-Ethoxymethylfurfural in Ethanol Solution. ACS Sustainable Chemistry and Engineering, 2021, 9, 14789-14799.	3.2	5
4933	Acceleration Mechanisms of C-H Bond Functionalization Catalyzed by Electron-Deficient CpRh(III) Complexes. ACS Catalysis, 2021, 11, 13591-13602.	5.5	21
4934	Theoretical studies of the reactions of 1,2-Ethanediol with triplet oxygen and hydrogen atoms. Molecular Physics, 2022, 120, .	0.8	0
4935	Nazarov Cyclizations Catalyzed by BINOL Phosphoric Acid Derivatives: Quantum Chemistry Struggles To Predict the Enantioselectivity. Journal of Organic Chemistry, 2022, 87, 1710-1722.	1.7	5
4936	Computational Study for CO <sub>2</sub> -to-CO Conversion over Proton Reduction Using $[Re[bpyMe(Im-R)](CO)_3Cl]^{+}$ (R = Me, Me <sub>2</sub> , and Me <sub>4</sub> ) Electro-catalysts and Comparison with Manganese Analogues. ACS Catalysis, 2021, 11, 12989-13000.	5.5	5
4937	Computational insights into the multi- $\pi$ -Diels-Alder reactions of neutral C <sub>60</sub> and its Li <sup>+</sup> encapsulated analogue: A density functional theory study. International Journal of Quantum Chemistry, 0, , .	1.0	4
4938	Computational Insights into Active Site Formation during Alkene Metathesis over a $MoO_x/SiO_2$ Catalyst: The Role of Surface Silanols. ACS Catalysis, 2021, 11, 13575-13590.	5.5	15

#	ARTICLE	IF	CITATIONS
4939	Theoretical insights of solvent effect on tautomerism, stability, and electronic properties of 6-alkyl-1-phenanthridine. <i>Journal of Physical Organic Chemistry</i> , 0, , e4294.	0.9	0
4940	Influence of the CH/B replacement on the Reactivity of Boranthrene and Related Compounds. <i>ACS Organic &amp; Inorganic Au</i> , 0, , .	1.9	6
4941	Insight into the Mechanism and Regioselectivity of Pd(OAc) <sub>2</sub> -Catalyzed C–O Bond Activation via a $\beta$ -O Elimination Approach: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9267-9278.	1.1	2
4942	The Reaction N( <sup>2</sup> D) + CH <sub>3</sub> CCH (Methylacetylene): A Combined Crossed Molecular Beams and Theoretical Investigation and Implications for the Atmosphere of Titan. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8846-8859.	1.1	12
4943	Detection of Ylide Formation between an Alkylidene carbene and Acetonitrile by Femtosecond Transient Absorption Spectroscopy. <i>Journal of the American Chemical Society</i> , 2021, 143, 17090-17096.	6.6	10
4944	Finding Transition States Using the LTP Algorithm. <i>Biocomputing</i> , 2002, , 107-128.	0.2	0
4948	Exploring the Catalytic Cycle of the Hydrosilylation of Alkenes Catalyzed by Hydrido-Bridged Diplatinum Complexes Using Electronic Structure Calculation Methods. , 2004, , 619-643.		0
4949	Theoretical study on thermal decomposition of azoisobutyronitrile in ground state. <i>Science in China Series B: Chemistry</i> , 2004, 47, 373.	0.8	0
4950	Sorption and Diffusion of Small Molecules Using Transition-State Theory. , 2004, , 409-466.		1
4951	Ab initio and DFT Study for the Internal Rotations of Cyclopropyldifluoroborane Molecule. <i>Journal of the Korean Chemical Society</i> , 2006, 50, 291-297.	0.2	0
4952	Modeling Chemical Reactions with First-Principle Molecular Dynamics. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 225-274.	0.6	0
4953	Ab Initio and DFT Investigations of the Mechanistic Pathway of Singlet Bromocarbenes Insertion into C-H Bonds of Methane and Ethane. <i>Lecture Notes in Computer Science</i> , 2007, , 288-295.	1.0	0
4955	Density Functional Study on the Reductive Elimination at an (NCN)Pt(IV) Center. <i>Bulletin of the Korean Chemical Society</i> , 2008, 29, 537-538.	1.0	1
4956	Theoretical Study of Cycloaddition Reactions of C <sub>60</sub> on the Si(100)-2 $\times$ 1 Surface. <i>Bulletin of the Korean Chemical Society</i> , 2010, 31, 1681-1688.	1.0	2
4957	Qualitative Approaches to Reactivity Phenomena. , 2011, , 649-674.		0
4958	Chemical Information from Information Discrimination and Relative Complexity. , 2011, , 251-291.		0
4959	Mechanism of ketone hydrosilylation using NHC–Cu(I) catalysts: a computational study. <i>Highlights in Theoretical Chemistry</i> , 2014, , 135-147.	0.0	0
4960	Thermochemistry of the reactions of F+(3P) and F+(1D) with hydrogen sulphide: a molecular orbital study. <i>Molecular Physics</i> , 1997, 91, 503-512.	0.8	3



#	ARTICLE	IF	CITATIONS
4961	Exploration of the Potential Energy Landscape of Aniline Using CASSCF and XMCQDPT2 Electronic Structure Calculations. Springer Theses, 2016, , 41-65.	0.0	0
4962	Basic Concepts and Methodology. Springer Theses, 2016, , 13-40.	0.0	0
4963	A Theoretical Study on the Relevance of Protonated and Ionized Species of Methanimine and Methanol in Astrochemistry. Lecture Notes in Computer Science, 2016, , 296-308.	1.0	1
4964	A Theoretical Investigation of the Decomposition and Reactivity of the CHF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> OCH <sub>2</sub> O Radical from HFE-356pcc3 between 200 and 400 K. Progress in Reaction Kinetics and Mechanism, 2017, 42, 154-162.	1.1	0
4965	Formation of Acetaldehyde in the Interstellar Medium from the Reaction of Methanol and Atomic Carbon in Interstellar Water Ice. Springer Proceedings in Physics, 2019, , 415-422.	0.1	2
4967	DFT study on the E-stereoselective reductive A <sup>3</sup> -coupling reaction of terminal alkynes with aldehydes and 3-pyrroline. Organic Chemistry Frontiers, 2020, 7, 2047-2054.	2.3	16
4968	DFT Study on the Biosynthesis of Preaspterpenoid A: Role of Secondary Carbocations in the Carbocation Cascade. Chemical and Pharmaceutical Bulletin, 2020, 68, 487-490.	0.6	5
4969	QUANTUM-CHEMICAL STUDY OF THE MECHANISM OF REACTION OF BENZOELACETHYLENE WITH DITIO- AND DISELENOMALONAMIDES. Scientific Papers Collection of the Angarsk State Technical University, 2020, 2020, 127-135.	0.1	0
4970	Decarbonylative Fluoroalkylation at Palladium(II): From Fundamental Organometallic Studies to Catalysis. Journal of the American Chemical Society, 2021, 143, 18617-18625.	6.6	25
4971	Theoretical hydrolysis mechanism of anticancer Pt(II) and Pd(II) dichloro complexes with N, N bidentate chelator in aqueous medium and their molecular docking. Chemical Physics, 2021, 553, 111390.	0.9	3
4972	Computational Exploration of the Efficacy of Fe(II)PNN Versus Fe(II)NNN Pincer Complexes in the Hydrogenation of Carbon Dioxide to Methanol. Journal of Physical Chemistry C, 2021, 125, 24350-24362.	1.5	5
4973	Ascendancy of Nitrogen Heterocycles in the Computationally Designed Mn(I)PNN Pincer Catalysts on the Hydrogenation of Carbon Dioxide to Methanol. Inorganic Chemistry, 2022, 61, 1851-1868.	1.9	8
4974	Microwave-assisted 1,3-Dioxo[3,3]-sigmatropic Rearrangement of Substituted Allylic Carbamates: Application to the Synthesis of Novel 1,3-Oxazine-2,4-Dione Derivatives. European Journal of Organic Chemistry, 0, , .	1.2	0
4975	DFT quest for mechanism and stereoselectivity in B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> -catalyzed cyclopropanation of alkenes with aryldiazoacetates. Molecular Catalysis, 2021, 516, 111980.	1.0	3
4976	Bridged-Selective Intramolecular Diels-Alder Reactions in the Synthesis of Bicyclo[2.2.2]octanes. Chemical and Pharmaceutical Bulletin, 2020, 68, 1201-1209.	0.6	0
4977	Stereoselective Cyclopropanation of Arylmethylidenemalononitriles by 2,6-Dimethylquinoline: A Molecular Electron Density Theory Study. Russian Journal of Organic Chemistry, 2020, 56, 2171-2178.	0.3	0
4978	Effects of External Electric Field on the Hydrolysis of Cisplatin: A Density Functional Theory Approach. Russian Journal of Inorganic Chemistry, 2020, 65, 2053-2061.	0.3	4
4979	Structure and Computational Basis for Backbone Rearrangement in Marine Oxasqualenoids. Journal of Organic Chemistry, 2021, 86, 2437-2446.	1.7	7

#	ARTICLE	IF	CITATIONS
4980	Prevailing charge transfer in the reaction of protonated and neutral nitric oxide: A theoretical and experimental study. <i>International Journal of Mass Spectrometry</i> , 2022, 471, 116724.	0.7	0
4981	Insights into the interaction between NO and char(N) containing different functional forms: Mechanistic, thermodynamic and kinetic studies. <i>Combustion and Flame</i> , 2022, 237, 111823.	2.8	13
4982	A Theoretical Investigation of the Reaction Between Glycolaldehyde and H <sup>+</sup> and Implications for the Organic Chemistry of Star Forming Regions. <i>Lecture Notes in Computer Science</i> , 2020, , 730-743.	1.0	0
4983	Ugi Adducts of Isatin as Promising Antiproliferative Agents with Druglike Properties. <i>Asian Journal of Organic Chemistry</i> , 2021, 10, 3434-3455.	1.3	6
4984	Computational Study on the Mechanism of Cycloaddition Reactions of Bissulfonyl-1,3-butadiene with Some Alkenes. <i>Letters in Organic Chemistry</i> , 2020, 17, 735-742.	0.2	0
4985	Rationalizing the influence of $\delta^+$ -cationic phospholes on $\delta^-$ -catalysis. <i>Dalton Transactions</i> , 2021, 50, 18036-18043.	1.6	3
4986	A mechanistic study on the regioselective Ni-catalyzed methylation $\rightarrow$ alkenylation of alkyne with AlMe <sub>3</sub> and allylic alcohol. <i>Organic Chemistry Frontiers</i> , 2021, 9, 163-172.	2.3	9
4987	Exploring the mechanism and kinetics of the reaction of carbon disulfide, CS <sub>2</sub> , with the Criegee intermediates CH <sub>2</sub> OO and (CH <sub>3</sub> ) <sub>2</sub> COO. <i>Computational and Theoretical Chemistry</i> , 2022, 1207, 113529.	1.1	0
4988	Three decades of unveiling the complex chemistry of <i>C</i> -nitroso species with computational chemistry. <i>Organic Chemistry Frontiers</i> , 2021, 9, 223-264.	2.3	11
4989	Mechanistic Study of Tungsten Bipyridyl Tetracarbonyl Electrocatalysts for CO <sub>2</sub> Fixation: Exploring the Roles of Explicit Proton Sources and Substituent Effects. <i>Topics in Catalysis</i> , 2022, 65, 325-340.	1.3	4
4990	Theoretical insights into the degradation of swep by hydroxyl radicals in atmosphere and water environment: Mechanisms, kinetics and toxicity. <i>Science of the Total Environment</i> , 2022, 816, 151651.	3.9	3
4991	A DFT and MP2 mechanistic and kinetic study on hypohalogenation reaction of cysteine and N-acetylcysteine in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022, 349, 118191.	2.3	1
4992	Isomers of Biologically Active 2-Aminopyrimidinium Picrate through Intrinsic Reaction Coordinate Analysis and Spectroscopic Measurements. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-12.	1.4	0
4993	The Participation of 3,3,3-Trichloro-1-nitroprop-1-ene in the [3 + 2] Cycloaddition Reaction with Selected Nitrile N-Oxides in the Light of the Experimental and MEDT Quantum Chemical Study. <i>Molecules</i> , 2021, 26, 6774.	1.7	18
4994	Ultraviolet photolysis of monochloro-p-benzoquinone (MCBQ) in aqueous solution: Theoretical investigation into the dechlorination. <i>Chemosphere</i> , 2022, 291, 132884.	4.2	3
4995	Mechanism, Kinetics, and Ecotoxicity Assessment of $\hat{A}$ -OH-Initiated Oxidation Reactions of Sulfoxaflo. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10052-10064.	1.1	3
4996	Spontaneous Isomerization of a Hydroxynaphthalene-Containing Spiropyran in Polar Solvents Enhanced by Hydrogen Bonding Interactions. <i>ACS Omega</i> , 2021, 6, 35619-35628.	1.6	4
4997	Assessing and rationalizing the performance of Hessian update schemes for reaction path Hamiltonian rate calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 204112.	1.2	1

#	ARTICLE	IF	CITATIONS
4998	Adsorption of hazardous gases on poly(3,4-ethylenedioxythiophene): Density functional theory study. <i>International Journal of Chemical Kinetics</i> , 2022, 54, 121-129.	1.0	5
4999	Phosphine-oxide organic ligand improved Cu-based catalyst for acetylene hydrochlorination. <i>Applied Catalysis A: General</i> , 2022, 630, 118461.	2.2	13
5000	Theoretical Studies of the Reactions of Methyl radical with Dimethyl Ether and 1,2-Ethandiol. <i>Computational and Theoretical Chemistry</i> , 2021, 1207, 113538.	1.1	1
5001	Theoretical study on molecular mechanism of aerobic oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran catalyzed by VO <sub>2</sub> <sup>+</sup> with counterpart anion in N,N-dimethylacetamide solution. <i>RSC Advances</i> , 2021, 11, 39888-39895.	1.7	1
5002	Mechanistic Study of Cu-Catalyzed Addition Reaction of Isocyanates. <i>Chinese Journal of Organic Chemistry</i> , 2021, 41, 4347.	0.6	4
5003	Computational studies on the sterol-like cyclization of a monodomain class II terpene cyclase. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 10647-10651.	1.5	0
5004	Platinum Assisted Tandem C Bond Cleavage and N Bond Formation in Amide Functionalized Bisphosphine Ph <sub>2</sub> PC <sub>6</sub> H <sub>4</sub> C(O)N(H)C <sub>6</sub> H <sub>4</sub> PPH <sub>2</sub> : Synthesis, Mechanistic, and Catalytic Studies. <i>Inorganic Chemistry</i> , 2022, 61, 857-868.	1.9	5
5005	Ag <sub>2</sub> O versus Cu <sub>2</sub> O in the Catalytic Isomerization of Coordinated Diaminocarbenes to Formamidines: A Theoretical Study. <i>Materials</i> , 2022, 15, 491.	1.3	1
5006	Construction of sulfur-containing compounds with anti-cancer stem cell activity using thioacrolein derived from garlic based on nature-inspired scaffolds. <i>Organic and Biomolecular Chemistry</i> , 2021, 20, 196-207.	1.5	4
5007	Theoretical Studies of the Reactions of Methyl Ethyl Ether with Hydrogen Atom, Triplet Oxygen Atom and Methyl Radical. <i>Chemical Physics Letters</i> , 2022, 790, 139346.	1.2	1
5008	Theoretical study of mechanisms and kinetics of reactions of the O(3P) atom with alkyl hydroperoxides (ROOH) where (R = CH <sub>3</sub> & C <sub>2</sub> H <sub>5</sub> ). <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113547.	1.1	2
5009	Temperature dependent kinetics for the reaction between OH radicals and (E)- and (Z)- CHF=CHCl: A dual-level computational study. <i>Computational and Theoretical Chemistry</i> , 2022, 1208, 113558.	1.1	1
5010	Direct observation of the particle-phase bicyclic products from OH-initiated oxidation of 1,3,5-trimethylbenzene under NO <sub>x</sub> -free conditions. <i>Atmospheric Environment</i> , 2022, 271, 118914.	1.9	4
5011	Theoretical investigation on atmospheric reaction mechanism, kinetics and SAR estimations of four-carbon ketones and alcohols. <i>Atmospheric Environment</i> , 2022, 271, 118915.	1.9	2
5012	Enhanced oxygen transfer over bifunctional Mo-based oxametallacycle catalyst for epoxidation of propylene. <i>Journal of Colloid and Interface Science</i> , 2022, 611, 564-577.	5.0	12
5013	Combined in situ XAS and DFT studies on the role of Pt in zeolite-supported metal catalysts for selective n-hexane isomerization. <i>Fuel</i> , 2022, 314, 123099.	3.4	7
5014	A detailed kinetic study on the tautomerization reactions of barbituric acid: A combined DFT-QTAIM analysis. <i>Main Group Chemistry</i> , 2022, , 1-16.	0.4	0
5015	Perylene Bisimide Cyclophanes as Biaryl Enantiomerization Catalysts – Explorations into C Catalysis and Host-Guest Chirality Transfer. <i>Journal of Organic Chemistry</i> , 2022, 87, 5485-5496.	1.7	7

#	ARTICLE	IF	CITATIONS
5016	Analytical Energy Gradient for State-Averaged Orbital-Optimized Variational Quantum Eigensolvers and Its Application to a Photochemical Reaction. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 741-748.	2.3	13
5017	Unveiling the synthesis of spirocyclic, tricyclic, and bicyclic triazolooxazines from intramolecular [3 + 2] azide-alkyne cycloadditions with a molecular electron density theory perspective. <i>Structural Chemistry</i> , 2022, 33, 555-570.	1.0	6
5018	A molecular electron density theory study of the higher-order cycloaddition reactions of tropone with electron-rich ethylenes. The role of the Lewis acid catalyst in the mechanism and pseudocyclic selectivity. <i>New Journal of Chemistry</i> , 2021, 46, 294-308.	1.4	4
5019	Role of Anion in Determining the Stereoselectivity of Mg-Ph-BOX-Catalyzed Diels-Alder Reactions: A Computational Study. <i>Organometallics</i> , 2022, 41, 105-114.	1.1	2
5020	Computational Study of the Rh/phanephos-Catalyzed Enantioselective [2+2+2] Cyclization of Enediyne, Affording Lactone-Fused Cyclohexadiene Bearing a Quaternary Bridgehead Carbon. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 221-229.	2.0	0
5021	Evaluation of the mechanism, regio-, and diastereoselectivity of aza-Diels-Alder reactions of 2H-azirine under a Lewis acid catalyst. <i>Structural Chemistry</i> , 2022, 33, 445.	1.0	0
5022	Mechanism of Fuel Gas Denitration on the KOH-Activated Biochar Surface. <i>Journal of Physical Chemistry A</i> , 2022, 126, 296-305.	1.1	6
5023	Remote N-H activation of indole aldehydes: an investigation of the mechanism, origin of selectivities, and role of the catalyst. <i>New Journal of Chemistry</i> , 2022, 46, 2761-2776.	1.4	1
5024	Insights into the gold-catalyzed intermolecular annulations of alkynes with <i>N</i> -allenamides: a mechanistic DFT study. <i>Dalton Transactions</i> , 2022, 51, 3734-3739.	1.6	3
5025	The mechanism and origin of selectivities for NHC-catalyzed synthesis of axially chiral benzothiophene/benzofuran-fused biaryls. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 1662-1670.	1.5	11
5026	CO self-promoted oxidation by gas-phase cluster anions IrVO <sub>4</sub> <sup>-</sup> . <i>Chemical Physics Letters</i> , 2022, 787, 139276.	1.2	2
5027	Quantum tunneling of hydrogen atom transfer affects mandrel degradation in inertial confinement fusion target fabrication. <i>IScience</i> , 2022, 25, 103674.	1.9	4
5028	Intensifying strategy of ionic liquids for Pd-based catalysts in anthraquinone hydrogenation. <i>Catalysis Science and Technology</i> , 2022, 12, 1766-1776.	2.1	3
5029	The Mechanism and Kinetics Model of Degradation of Dicarboxylic Acids by Hydroxyl Radicals under Atmospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 787-799.	1.1	1
5030	Dehydrogenation of ammonia-borane to functionalize neutral and Li <sup>+</sup> -encapsulated C <sub>60</sub> , C <sub>70</sub> and C <sub>36</sub> fullerene cages: a DFT approach. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4022-4041.	1.3	2
5031	New 1,2,3-Triazoles from (R)-Carvone: Synthesis, DFT Mechanistic Study and In Vitro Cytotoxic Evaluation. <i>Molecules</i> , 2022, 27, 769.	1.7	14
5032	Optimization and design for the curing process of solid azide propellant: Influence of typical components on the curing reactions of PBT binders with TDI. <i>Journal of the Chinese Chemical Society</i> , 2022, 69, 419-439.	0.8	1
5033	Molecular insights into chirality transfer from double axially chiral phosphoric acid in a synergistic enantioselective intramolecular amination. <i>Chemical Science</i> , 2022, 13, 1323-1334.	3.7	6

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5034	Automatic Approach to Explore the Multireaction Mechanism for Medium-Sized Bimolecular Reactions via Collision Dynamics Simulations and Transition State Searches. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 910-924.	2.3	6
5035	A Theoretical Evaluation of the Behavior of Nitrosoamidine upon Reacting with Methoxy Butadiene, as Potential Heterodiene or Heterodienophile. <i>Letters in Organic Chemistry</i> , 2022, 19, .	0.2	0
5036	A theoretical investigation on the hydrodesulphurisation mechanism of hydrogenated thiophene over Cuâ€“Mo-modified FAU zeolite. <i>Molecular Simulation</i> , 0, , 1-22.	0.9	0
5037	Mechanistic studies of the reactions of nitrogen dioxide with dimethyl ether and methyl ethyl ether. <i>Chemical Physics Letters</i> , 2022, 793, 139430.	1.2	2
5038	Ab initio and DFT benchmark study for the calculations of isotopic shifts of fundamental frequencies for 2,3-dihydropyran. <i>Structural Chemistry</i> , 0, , 1.	1.0	1
5039	Unraveling the sequence of electron flow along the cyclocondensation reaction between ciprofloxacin and thiosemicarbazide through the bonding evolution theory. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 113, 108141.	1.3	3
5040	Effect of K-decoration on the generation and reduction of N $\text{O}$ onto a biochar surface. <i>Fuel</i> , 2022, 316, 123148.	3.4	6
5041	Phenolic Compounds to Hinder Sulfur Crystallization in Sulfur-Extended Bitumen. <i>Resources, Conservation and Recycling</i> , 2022, 180, 106184.	5.3	4
5042	Computational discoveries of reaction mechanisms: recent highlights and emerging challenges. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 2028-2042.	1.5	4
5043	Tuning the metathesis performance of a molybdenum oxide-based catalyst by silica support acidity modulation and high temperature pretreatment. <i>Catalysis Science and Technology</i> , 2022, 12, 2134-2145.	2.1	2
5044	The cycloaddition reaction of ethylene and methane mediated by Ir <sup>+</sup> to generate a half-sandwich structure IrHCp <sup>+</sup> . <i>Chinese Chemical Letters</i> , 2023, 34, 107196.	4.8	1
5045	Experimental and Theoretical Studies of Trans-2-Pentenal Atmospheric Ozonolysis. <i>Atmosphere</i> , 2022, 13, 291.	1.0	1
5046	Ab initio kinetics of OH-initiated oxidation of cyclopentadiene. <i>Fuel</i> , 2022, 317, 123305.	3.4	5
5047	Unveiling the intramolecular [3 + 2] cycloaddition reactions of <i>C</i> -, <i>N</i> -disubstituted nitrones from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2022, 46, 7721-7733.	1.4	9
5048	Thiolate-assisted copper( <sup>i</sup> ) catalyzed Câ€“S cross coupling of thiols with aryl iodides: scope, kinetics and mechanism. <i>New Journal of Chemistry</i> , 2022, 46, 6283-6295.	1.4	5
5049	Competing Mechanisms of CO Hydrogenation to Ethanol Over TM/Mo &lt;sub>6</sub>S &lt;sub>8</sub> Catalysts. <i>S&amp;S&amp;R&amp;N Electronic Journal</i> , 0, , .	0.4	0
5050	Reaction kinetics of 1,4-cyclohexadienes with OH radicals: an experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7836-7847.	1.3	3
5051	Effect of O-substitution in imidazole based Zn( <sup>ii</sup> ) dual fluorescent probes in the light of arsenate detection in potable water: a combined experimental and theoretical approach. <i>Dalton Transactions</i> , 2022, 51, 7174-7187.	1.6	8

#	ARTICLE	IF	CITATIONS
5052	Mechanism and origin of the stereoselectivity of manganese-catalyzed hydrosilylation of alkynes: a DFT study. <i>Catalysis Science and Technology</i> , 2022, 12, 2649-2658.	2.1	6
5053	Lithium-Assisted Dinitrogen Reduction Mediated by Nb <sub>2</sub> LiNO <sub>4</sub> <sup>+</sup> Cluster Anions: Electron Donors or Structural Units. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1511-1517.	1.1	14
5054	Thermodynamic and Kinetic Studies on the Conversion of Solvent-Shared to Contact Ion Pairs in Sparingly Soluble MF <sub>2</sub> (M = Mg <sup>2+</sup> and Ca <sup>2+</sup> ) Aqueous Solutions: Implications for Understanding Supersaturated Behavior and Association Constant Determination. <i>Journal of Physical Chemistry B</i> , 2022, 126, 1566-1578.	1.2	0
5055	Mild Synthesis of a Dimethoxy-Terminated Siloxane through a Ring-Opening Reaction. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
5056	The Role of Through-Bond Stereoelectronic Effects in the Reactivity of 3-Azabicyclo[3.3.1]nonanes. <i>Journal of Organic Chemistry</i> , 2022, 87, 3378-3388.	1.7	3
5057	<sup>15</sup> N/ <sup>14</sup> N isotopic exchange in the dissociative adsorption of N <sub>2</sub> on tantalum nitride cluster anions Ta <sub>3</sub> N <sub>3</sub> <sup>+</sup> . <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 77-85.	0.6	4
5058	Understanding the catalysis by bis-selenonium cations as bidentate chalcogen bond donors. , 2022, 1, 100008.		7
5059	Iridium Dimer Anion-Mediated C≡C Triple Bond Cleavage and Successive Dehydrogenation of Acetylene in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1711-1717.	1.1	0
5060	Theoretical evidence for the formation of perfluorocarboxylic acids from atmospheric oxidation degradation of fluorotelomer acrylates. <i>Environmental Science and Pollution Research</i> , 2022, 29, 55092-55104.	2.7	1
5061	A Hierarchical Theoretical Study of the Hydrogen Abstraction Reactions of H <sub>2</sub> /C <sub>1</sub> -C <sub>4</sub> Molecules by the Methyl Peroxy Radical and Implications for Kinetic Modeling. <i>ACS Omega</i> , 2022, 7, 8675-8685.	1.6	2
5062	On the Origins of Stereo- and Regio-Selectivities in the Formation of Fullerene-Fluorene Dyads. <i>Journal of Organic Chemistry</i> , 2022, 87, 4702-4711.	1.7	2
5063	Mechanism, Stereoselectivity, and Role of O <sub>2</sub> in Aza-Diels-Alder Reactions Catalyzed by Dinuclear Molybdenum Complexes: A Theoretical Study. <i>Inorganic Chemistry</i> , 2022, 61, 4714-4724.	1.9	3
5064	Theoretical study of the substituent effect on the O-H insertion reaction of copper carbenoids. <i>Theoretical Chemistry Accounts</i> , 2022, 141, 1.	0.5	1
5065	Roads Not Taken: Mechanism and Origins of Regio- and Chemoselectivity of Directed Co <sup>III</sup> -Catalyzed Alkenylation of <i>N</i> -Pyridyl 2-Pyridone. <i>Organometallics</i> , 2022, 41, 937-947.	1.1	2
5066	Density functional theory study on the reductive elimination of ancillary ligand at PPC nickel complexes. <i>Bulletin of the Korean Chemical Society</i> , 0, , .	1.0	0
5067	Semiempirical Potential in Kinetics Calculations on the HC <sub>3</sub> N + CN Reaction. <i>Molecules</i> , 2022, 27, 2297.	1.7	3
5068	Experimental and theoretical studies on the conversion of biomass pyrolysis tar under the effect of steam. <i>Biomass Conversion and Biorefinery</i> , 2024, 14, 3917-3925.	2.9	0
5069	Decoding the reaction mechanism of the cyclocondensation of ethyl acetate ( $4\text{C}$ ) Tj ETQq1 1 0.784314 evolution theory. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	4

#	ARTICLE	IF	CITATIONS
5070	A Mixed-Ligand Strategy to Modulate P3HT Regioregularity for High-Efficiency Solar Cells. <i>Macromolecules</i> , 2022, 55, 3078-3086.	2.2	26
5071	Potential forensic markers from synthetic pathways to 1-phenyl-2-propanone from uncontrolled and controlled substances. <i>Forensic Chemistry</i> , 2022, 28, 100410.	1.7	4
5072	DFT study on mechanism of acetylene hydroamination catalyzed by metal chloride. <i>Chemical Engineering Science</i> , 2022, 253, 117559.	1.9	1
5073	Theoretical studies of the reactions of 1-Propanol, and 2-Propanol with hydrogen atom and methyl radical. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113688.	1.1	2
5074	A theoretical study on the mechanism and kinetics of the Dimeric TrimethylAluminum+O <sub>2</sub> reaction in the gas phase: A potential chain-initiation in the hypergolic combustion of TMA in air. <i>Computational and Theoretical Chemistry</i> , 2022, 1212, 113695.	1.1	0
5075	Microscopic mechanism and kinetics of NO heterogeneous reduction on char surface: A density functional theory study. <i>Energy</i> , 2022, 250, 123861.	4.5	7
5076	Fabrication of Novel Potentiometric Sensor for Lead Ion Detection in Blood Samples: Experimental and Theoretical Approaches. <i>Microchemical Journal</i> , 2022, 178, 107383.	2.3	1
5077	Gas Phase Reaction of Isocyanic Acid: Kinetics, Mechanisms, and Formation of Isopropyl Aminocarbonyl. <i>ACS Omega</i> , 2021, 6, 34661-34674.	1.6	0
5078	Acid-Catalyzed Esterification of Betaines: Theoretical Exploration of the Impact of the Carbon Chain Length on the Reaction Mechanism. <i>Physchem</i> , 2021, 1, 288-296.	0.5	0
5079	2- and 6-Purinylmagnesium Halides in Dichloromethane: Scope and New Insights into the Solvent Influence on the C-Mg Bond. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	1.2	1
5080	Theoretical Simulation and Experimental Optimization of Reaction Conditions and Product Composition of Ferrocene Acylation. <i>Russian Journal of Physical Chemistry A</i> , 2021, 95, S252-S258.	0.1	0
5081	Exploring the Effects of Water on the Mechanism of the Catalyst-Free Reaction between Isatin and 3-Methyl-2-pyrazolin-5-one from the Mixed Implicit/Explicit Multiple Types of Water Clusters. <i>Journal of Physical Chemistry B</i> , 2022, 126, 249-261.	1.2	1
5082	Synthesis and Application of Constrained Amidoboronic Acids Using Amphoteric Boron-Containing Building Blocks. <i>Journal of Organic Chemistry</i> , 2022, 87, 94-102.	1.7	4
5083	Hydroboration and Hydrosilylation of a Molybdenum-Nitride Complex Bearing a PNP-Type Pincer Ligand. <i>Organometallics</i> , 2022, 41, 366-373.	1.1	5
5084	Nature of C-H...X Halogen Bonding and its Role in Organocatalysis. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 6102-6110.	1.2	8
5085	Water-Assisted and Catalyst-Free Hetero-Michael Additions: Mechanistic Insights from DFT Investigations. <i>Asian Journal of Organic Chemistry</i> , 2022, 11, .	1.3	5
5086	Primary Amine Nucleophilic Addition to Nitrilium Closo-Dodecaborate [B <sub>12</sub> H <sub>11</sub> NCCH <sub>3</sub> ] <sup>+</sup> : A Simple and Effective Route to the New BNCT Drug Design. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13391.	1.8	25
5087	Effects of Axial Solvent Coordination to Dirhodium Complexes on the Reactivity and Selectivity in C-H Insertion Reactions: A Computational Study. <i>Organometallics</i> , 2021, 40, 4120-4132.	1.1	15

#	ARTICLE	IF	CITATIONS
5088	Al-Embedded C <sub>2</sub> N: a DFT study on a promising catalyst for CO oxidation. <i>New Journal of Chemistry</i> , 2022, 46, 9250-9257.	1.4	3
5089	A DFT study of NHC-catalyzed reactions between 2-bromo-2-enals and acylhydrazones: mechanisms, and chemo- and stereoselectivities. <i>New Journal of Chemistry</i> , 2022, 46, 9146-9154.	1.4	3
5090	Synthesis of an advanced metal-guided photochromic system for molecular keypad lock: detailed experimental findings and theoretical understanding. <i>New Journal of Chemistry</i> , 2022, 46, 8284-8302.	1.4	5
5091	Through-Space Interaction of Tetraphenylethylene: What, Where, and How. <i>Journal of the American Chemical Society</i> , 2022, 144, 7901-7910.	6.6	72
5092	Structures, Energetics, and Spectra of (NH) and (OH) Tautomers of 2-(2-Hydroxyphenyl)-1-azaazulene: A Density Functional Theory/Time-Dependent Density Functional Theory Study. <i>ACS Omega</i> , 2022, 7, 14222-14238.	1.6	4
5093	Protonation of Borylated Carboxonium Derivative [2,6-B10H8O2CCH3] <sup>+</sup> : Theoretical and Experimental Investigation. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4190.	1.8	8
5098	DFT Study on the Biosynthesis of Asperterpenol and Preasperterpenoid Sesterterpenoids: Exclusion of Secondary Carbocation Intermediates and Origin of Structural Diversification. <i>Journal of Organic Chemistry</i> , 2022, 87, 6432-6437.	1.7	7
5099	Computational insight into the mechanism and stereoselectivity of cycloaddition between donor-acceptor spirocyclopropane and aldehyde catalyzed by Brønsted acid TsOH. <i>Organic and Biomolecular Chemistry</i> , 2022, 20, 4006-4015.	1.5	3
5100	Reaction mechanism study on reactions of phenylacetylenes with HSnEt <sub>3</sub> promoted by B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> with and without DABCO. <i>Organic Chemistry Frontiers</i> , 0, , .	2.3	1
5101	The Sulfinylsulfonation of alkynes for $\beta$ -sulfinyl alkenylsulfone. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	12
5102	An efficient approach to angular tricyclic molecular architecture via Nazarov-like cyclization and double ring-expansion cascade. <i>Nature Communications</i> , 2022, 13, 2335.	5.8	12
5103	Quantum Chemical and Chemical Kinetic Investigation on Hydrogen Abstraction Reactions of CF <sub>3</sub> CF <sub>2</sub> C(O)OCH <sub>3</sub> and CHF <sub>2</sub> CF <sub>2</sub> C(O)OCH <sub>3</sub> with OH Radicals and Fate of Haloalkoxy Radicals. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 1596-1611.	1.2	4
5104	Computational study of the reaction of C <sub>3</sub> H <sub>3</sub> with HNCO and the decomposition of C <sub>4</sub> H <sub>4</sub> NO radicals. <i>International Journal of Chemical Kinetics</i> , 2022, 54, 447-460.	1.0	2
5105	Theoretical Insights into Enantioselective [3 + 2] Cycloaddition between Cinnamaldehyde and Cyclic <i>N</i> -Sulfonyl Trifluoromethylated Ketimine Catalyzed by <i>N</i> -Heterocyclic Carbene. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3124-3134.	1.1	1
5106	Water coordinated on Cu(I)-based catalysts is the oxygen source in CO <sub>2</sub> reduction to CO. <i>Nature Communications</i> , 2022, 13, 2577.	5.8	5
5107	Toward rational design of supported vanadia catalysts of lignin conversion to phenol. <i>Chemical Engineering Journal</i> , 2022, 446, 136965.	6.6	4
5108	Reaction mechanism of toluene decomposition in non-thermal plasma: How does it compare with benzene?. <i>Fundamental Research</i> , 2022, , .	1.6	5
5109	Mechanical Insights into Activation of Peroxides by Quinones: Formation of Oxygen-Centered Radicals or Singlet Oxygen. <i>Environmental Science &amp; Technology</i> , 2022, 56, 8776-8783.	4.6	20



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5110	NHC Catalyzed $\hat{\text{I}}^2$ -Carbon functionalization of carboxylic esters towards formation of $\hat{\text{I}}^1$ -Lactams: A mechanistic study. <i>Molecular Catalysis</i> , 2022, 524, 112311.	1.0	0
5111	Rate constant and mechanism of the OH-initiated degradation of 3-penten-2-one in the atmosphere. <i>Computational and Theoretical Chemistry</i> , 2022, 1213, 113737.	1.1	0
5112	Understanding the higher-order cycloaddition reactions of heptafulvene, tropone, and its nitrogen derivatives, with electrophilic and nucleophilic ethylenes inside the molecular electron density theory. <i>New Journal of Chemistry</i> , 2022, 46, 11520-11530.	1.4	4
5113	DFT Rationalization of Gold(I)-Catalyzed Couplings between Alkynyl Thioether and Nitrenoid Derivatives: Mechanism, Selectivity Patterns, and Effects of Substituents. <i>Journal of Organic Chemistry</i> , 2022, 87, 7193-7201.	1.7	4
5114	A Shuttle Catalysis: Elucidating a True Reaction Mechanism Involved in the Palladium Xantphos-Assisted Transposition of Aryl Chloride and Aryl Iodide Functional Groups. <i>Journal of Organic Chemistry</i> , 2022, 87, 12547-12557.	1.7	2
5115	A deeper analysis of the role of synchronicity on the Bell-Evans-Polanyi plot in multibond chemical reactions: a path-dependent reaction force constant. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14772-14779.	1.3	5
5116	Aqueous synthesis of 2-aryl-3-nitro-2H chromenes via l-prolinamide mediated tandem oxa-Michael Henry reactions. <i>Journal of Molecular Structure</i> , 2022, 1265, 133341.	1.8	3
5117	Diels-Alder Polar Reactions of Azaheterocycles: A Theoretical and Experimental Study. <i>Organics</i> , 2022, 3, 102-110.	0.6	1
5118	Activated carbon supported nitrogen-containing diheterocycle mercury-free catalyst for acetylene hydrochlorination. <i>Molecular Catalysis</i> , 2022, 525, 112366.	1.0	2
5119	Charge-regulated regioselective mechanism of bicobalt-catalyzed hydrogermylation of alkynes: DFT investigation. <i>Molecular Catalysis</i> , 2022, 526, 112379.	1.0	4
5120	Possible Skeletal Transformations of Cyclooctatetraene in Its Thermal Isomerization. <i>Russian Journal of Organic Chemistry</i> , 2022, 58, 488-498.	0.3	0
5121	Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction between Cyano Radicals and Cyanoethene ( $\text{C}_2\text{H}_3\text{CN}$ ). <i>Journal of Physical Chemistry A</i> , 2022, 126, 3569-3582.	1.1	13
5122	Theoretical Study of $\text{H}\ddot{\text{f}}$ -Bond Activation by Nickel(0) Complex: Reaction Mechanism, Electronic Processes, and Prediction of Better Ligand. <i>Inorganic Chemistry</i> , 2022, 61, 8715-8728.	1.9	2
5123	Microscopic mechanism of perfluorocarbon gas formation in aluminum electrolysis process. <i>Transactions of Nonferrous Metals Society of China</i> , 2022, 32, 1705-1717.	1.7	4
5124	Does an Enol Pathway Preclude High Stereoselectivity in Iron-Catalyzed Indole C-H Functionalization via Carbene Insertion?. <i>Journal of Organic Chemistry</i> , 2022, 87, 7919-7933.	1.7	10
5125	Elucidation of the molecular mechanisms of 1,2,3,5- and 1,2,4,5-tetrazines with strained and electron-rich alkynes. <i>Tetrahedron</i> , 2022, 119, 132860.	1.0	1
5126	Formation of persistent free radicals and reactive chlorine species during photochemical processes of Polychlorophenols: Effect of temperature, humidity and particles. <i>Chemical Engineering Journal</i> , 2022, 446, 137149.	6.6	4
5127	A molecular electron density theory study on the Chichibabin reaction: The origin of regioselectivity. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108240.	1.3	7

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5129	Quantum-chemical study of organic reaction mechanisms. XI.*1 <sup>1</sup> Biologically active 4-substituted 1,2,4-triazoles from diformylhydrazine and aminophenols. <i>Structural Chemistry</i> , 2022, 33, 2023-2032.	1.0	2
5130	Understanding of Photo-Induced Reversible Rearrangement from Borepin to Borirane. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4
5131	Rhodium-Catalyzed Ring Expansion Reactions for the Concise Construction of Densely Functionalized Oxathionines and Oxathiocines. <i>ACS Catalysis</i> , 2022, 12, 7524-7530.	5.5	5
5132	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of Pseudo(mono)radical Azomethine Ylides with Phenyl Vinyl Sulphone. <i>Organics</i> , 2022, 3, 122-136.	0.6	10
5133	Catalytic mechanism of the ruthenium-catalyzed benzonitrile hydrogenation: Insights from quantum mechanics calculations. <i>Chemical Physics Letters</i> , 2022, 803, 139803.	1.2	0
5134	Experimental and Computational Mechanistic Study of Carbonazidate-Initiated Cascade Reactions. <i>Journal of Organic Chemistry</i> , 2022, 87, 8983-9000.	1.7	1
5135	Synthesis of $\beta$ -Amino Acids by Stereoselective Alkylation of Isoleucine Derivatives Followed by Nucleophilic Ring Opening of Quaternary Sulfamidates. <i>Journal of Organic Chemistry</i> , 2022, 87, 8730-8743.	1.7	2
5136	Reaction of Ta <sub>3</sub> Clusters with Molecular Nitrogen: A Mechanism Investigation. <i>ACS Omega</i> , 2022, 7, 22682-22688.	1.6	3
5137	Connecting cation site location to alkane dehydrogenation activity in Ni/BEA catalysts. <i>Journal of Catalysis</i> , 2022, 413, 264-273.	3.1	3
5138	Experimental and Theoretical Study of N <sub>2</sub> Adsorption on Hydrogenated Y <sub>2</sub> C <sub>4</sub> H <sup>-</sup> and Dehydrogenated Y <sub>2</sub> C <sub>4</sub> <sup>-</sup> Cluster Anions at Room Temperature. <i>International Journal of Molecular Sciences</i> , 2022, 23, 6976.	1.8	2
5139	Quantum chemical and theoretical kinetics studies on the reactions of hydroperoxy radical with methanethiol and ethanethiol. <i>Computational and Theoretical Chemistry</i> , 2022, 1214, 113787.	1.1	0
5140	Should pyrolysis of diazotetranoic acid produce methylene ketene? A theoretical structural, thermochemical and kinetic study. <i>Chemical Physics Letters</i> , 2022, 802, 139770.	1.2	1
5141	Theoretical study on the quick thermal decomposition pathways for MTNI(1-Methyl-2,4,5-Trinitroimidazole). <i>Chemical Physics Letters</i> , 2022, 802, 139798.	1.2	1
5142	Multiple CO <sub>2</sub> reduction mediated by heteronuclear metal carbide cluster anions RhTaC <sub>2</sub> <sup>-</sup> . <i>Dalton Transactions</i> , 0, , .	1.6	3
5143	Controlled masking and targeted release of redox-cycling ortho-quinones via a C=C bond-cleaving 1,6-elimination. <i>Nature Chemistry</i> , 2022, 14, 754-765.	6.6	18
5144	Insights into the mechanism and stereoselectivity of the [3+2] cycloaddition reaction between N-methyl-C-(4-hydroxyphenyl) nitron and maleic anhydride with a molecular electron density theory perspective. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	7
5145	Deciphering the Molecular Mechanism of Intramolecular Reactions from the Perspective of Bonding Evolution Theory. <i>Physchem</i> , 2022, 2, 207-223.	0.5	4
5146	Not That DDT: A Databank of Dynamics Trajectories for Organic Reactions. <i>Journal of Chemical Education</i> , 2022, 99, 2721-2725.	1.1	4

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5147	Eco-Friendly Synthesis of 5-Hydroxymethylfurfural and Its Applications as a Starting Material to Synthesize Valuable Heterocyclic Compounds. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 8673-8684.	3.2	14
5148	Origin of Catalysis and Selectivity in Lewis Acid-Promoted Diels-Alder Reactions Involving Vinylarenes as Dienophiles. <i>Journal of Organic Chemistry</i> , 2022, 87, 9307-9315.	1.7	3
5149	Theoretical investigation for the reactions of triplet oxygen atom with dimethyl sulphide, ethyl methyl sulphide: mechanism and kinetics properties. <i>Molecular Physics</i> , 2022, 120, .	0.8	0
5150	Oxo-Rhenium-Mediated Allylation of Furanoside Derivatives: A Computational Study on the Mechanism and the Stereoselectivity. <i>Journal of Organic Chemistry</i> , 2022, 87, 9497-9506.	1.7	3
5151	Mechanistic aspects of the Diels-Alder reaction between (E)-N-benzylidene-2,2-difluoro-1-phenylethanamine and 2-vinyl pyridine: A molecular electron density theory study. <i>Computational and Theoretical Chemistry</i> , 2022, 1215, 113817.	1.1	4
5152	Quantum chemical hydrogenolysis strategy for elimination of heteroatoms in biomass homologous organic compounds based on oxolane and thiolane. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 116, 108268.	1.3	1
5153	The reaction of hydropersulfides (RSSH) with S-nitrosothiols (RS-NO) and the biological/physiological implications. <i>Free Radical Biology and Medicine</i> , 2022, 188, 459-467.	1.3	5
5154	Competing mechanisms of CO hydrogenation to ethanol over TM/Mo <sub>6</sub> S <sub>8</sub> catalysts. <i>Polyhedron</i> , 2022, 224, 116031.	1.0	0
5155	Mechanism and safety analysis of acetylene decomposition explosion: A combined ReaxFF MD with DFT study. <i>Fuel</i> , 2022, 327, 124996.	3.4	14
5156	Theoretical investigation on the mechanisms and kinetics of the reactions of hydroperoxy radical with dimethyl sulphide and ethyl methyl sulphide. <i>Molecular Physics</i> , 0, , .	0.8	0
5157	Theoretical survey of Diels-Alder between acrylic acid and isoprene catalyzed by the titanium tetrachloride and titanium tetrafluoride. <i>Journal of Molecular Structure</i> , 2022, 1269, 133630.	1.8	16
5158	Mechanism of the phosphine-catalyzed [3+3] annulation with MBH carbonates as the potential dipoles. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, .	0.9	1
5159	Portable Models for Entropy Effects on Kinetic Selectivity. <i>Journal of the American Chemical Society</i> , 2022, 144, 13996-14004.	6.6	9
5160	Theoretical study of the radical-radical reactions between HOCH <sub>2</sub> OO and OH. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	0
5161	Model Study on the Catalytic Cycle of Glutathione Peroxidase Utilizing Selenocysteine-Containing Tripeptides: Elucidation of the Protective Bypass Mechanism Involving Selenocysteine Selenenic Acids. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 1360-1379.	2.0	8
5162	Roles of CO <sub>2</sub> in Controlling the Chemoselectivity of [LCu-Fp] Heterobimetallic-Catalyzed CO <sub>2</sub> Hydroboration Reduction: A Computational Study. <i>Organometallics</i> , 2022, 41, 1922-1930.	1.1	3
5163	Unveiling the Chemistry of Higher-Order Cycloaddition Reactions within the Molecular Electron Density Theory. <i>Chemistry</i> , 2022, 4, 735-752.	0.9	6
5164	Theoretical study on the kinetics of the reactions of hydrogen atom, methyl radical with methanethiol and ethanethiol. <i>Molecular Physics</i> , 0, , .	0.8	0

#	ARTICLE	IF	CITATIONS
5165	Theoretical Investigations of the OH-Initialized Oxidation of 4-Methyl-3-Penten-2-One in the Atmosphere. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 2261-2273.	1.2	1
5166	Effect Mechanisms of Sodium on NO Heterogeneous Reduction by Nitrogen-Containing Char: Experimental and DFT Investigation. <i>Combustion Science and Technology</i> , 0, , 1-26.	1.2	1
5167	Investigation of the Gas-Phase Reaction of Nopinone with OH Radicals: Experimental and Theoretical Study. <i>Atmosphere</i> , 2022, 13, 1247.	1.0	3
5168	Ir and NHC Dual Chiral Synergetic Catalysis: Mechanism and Stereoselectivity in Î <sup>3</sup> -Butyrolactone Formation. <i>Journal of the American Chemical Society</i> , 2022, 144, 16171-16183.	6.6	14
5169	Theoretical Investigation of the Biogenetic Pathway for Formation of Antibacterial Indole Alkaloids from <i>Voacanga africana</i> . <i>ACS Omega</i> , 2022, 7, 31591-31596.	1.6	3
5170	Density Functional Theory Study on NiN <sub>x</sub> (x = 1, 2, 3, 4) Catalytic Hydrogenation of Acetylene. <i>Molecules</i> , 2022, 27, 5437.	1.7	1
5171	Distinctive Mechanistic Scenarios and Substituent Effects of Gold(I) versus Copper(I) Catalysis for Hydroacylation of Terminal Alkynes with Glyoxal Derivatives. <i>Journal of Organic Chemistry</i> , 2022, 87, 11681-11692.	1.7	5
5172	Comprehensive theoretical study of nickel-NHC-catalyzed enantioselective intramolecular indole C-H cyclization: Reaction mechanism, reactivity, regioselectivity, and electronic processes. <i>Applied Organometallic Chemistry</i> , 0, , .	1.7	0
5173	Formation of phosphorus monoxide through the $\mathbf{P}(\text{S})_4 + \mathbf{O}_2 \rightarrow \mathbf{O}_3\text{P} + \mathbf{PO}_2$ reaction. <i>Journal of Molecular Modeling</i> , 2022, 28, .	0.8	2
5174	Racemization Pathway for MoO <sub>2</sub> (acac) <sub>2</sub> Favored over Ray-Dutt, Bailar, and Conte-Hippler Twists. <i>Inorganic Chemistry</i> , 2022, 61, 14918-14923.	1.9	5
5175	Mechanistic aspects of the Pd(OAc) <sub>2</sub> (N <sub>3</sub> ) catalyzed ethylene acetoxylation: A density functional theory study. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	1
5176	NHC-catalyzed [3+4] annulation between 2-dromoenal and aryl 1,2-diamine: Insights into mechanisms, chemo and stereoselectivities. <i>Molecular Catalysis</i> , 2022, 530, 112604.	1.0	1
5177	Solvent-mediated selectivity control of furfural hydrogenation over a N-doped carbon-nanotube-supported Co/CoO <sub>x</sub> catalyst. <i>Applied Catalysis B: Environmental</i> , 2022, 318, 121838.	10.8	22
5178	Theoretical investigation on hydrolysis mechanism of cis-platin analogous Pt(II)/Pd(II) complex by DFT calculation and molecular docking approach for their interaction with DNA & HSA. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 117, 108314.	1.3	5
5179	Ortho-Phosphinoarenesulfonamide-Mediated Staudinger Reduction of Aryl and Alkyl Azides. <i>Molecules</i> , 2022, 27, 5707.	1.7	3
5180	Structure elucidation and risk assessment of degradation products in gamma irradiated rubber closures. <i>Polymer Degradation and Stability</i> , 2022, 204, 110126.	2.7	4
5181	Study on the activation mechanism of protactinium and NH <sub>3</sub> by density functional theory. <i>Chemical Physics Letters</i> , 2022, 806, 140072.	1.2	0
5182	Ultraviolet dechlorination of tetrachloro-p-benzoquinone by hydrogen sulfide: Theoretical confirmation of the significance of hydrosulfide radical. <i>Chemosphere</i> , 2022, 308, 136372.	4.2	0

#	ARTICLE	IF	CITATIONS
5183	Direct conversion of furfural to 1,5-pentanediol over a nickel-cobalt oxide-alumina trimetallic catalyt. Applied Catalysis B: Environmental, 2023, 320, 121971.	10.8	24
5184	Deciphering the Cooperative Effect of Base and N-Substituents on the Origin of Regioselectivity Switching for Mannich Reactions of Glycinate by Carbonyl Catalysts. SSRN Electronic Journal, 0, , .	0.4	0
5185	DFT studies on rhodium( <i>iii</i> )-catalyzed synthesis of indanones from <i>N</i> -methoxybenzamides via C-H activation reaction. New Journal of Chemistry, 2022, 46, 16576-16583.	1.4	0
5186	Suppression of reversible photocyclization reaction induced fluorescence enhancement: a theoretical study. Physical Chemistry Chemical Physics, 2022, 24, 25487-25494.	1.3	5
5187	Unveiling the non-polar [3+2] cycloaddition reactions of cyclic nitrones with strained alkylidene cyclopropanes within a molecular electron density theory study. RSC Advances, 2022, 12, 25354-25363.	1.7	2
5188	Unveiling the [3+2] cycloaddition between difluoromethyl diazomethane and 3-ylideneoxindole from the perspective of molecular electron density theory. New Journal of Chemistry, 0, , .	1.4	2
5189	Ultraviolet Dechlorination of Tetrachloro-P-Benzoquinone by Hydrogen Sulfide: Theoretical Confirmation of the Significance of Hydrosulfide Radical. SSRN Electronic Journal, 0, , .	0.4	0
5190	Theoretical Study of the Reaction O(3P)+1,2-Butadiene. Lecture Notes in Computer Science, 2022, , 249-263.	1.0	0
5191	The Si <sup>4+</sup> +SiH <sub>2</sub> Reaction: Toward the Synthesis of Interstellar SiS. Lecture Notes in Computer Science, 2022, , 233-245.	1.0	1
5192	Theoretical study on the reaction mechanism of Si <sub>2</sub> Cl <sub>6</sub> and HCl catalyzed by amine catalysts. New Journal of Chemistry, 2022, 46, 17977-17984.	1.4	2
5193	Theoretical insights into the mechanism and origin of chemoselectivity in the catalyst- and directing group-dependent oxidative cyclization of diynes with pyridine <i>N</i> -oxides. Organic Chemistry Frontiers, 2022, 9, 5168-5177.	2.3	2
5194	Computational exploration for possible reaction pathways, regioselectivity, and influence of substrate in gold-catalyzed cycloaddition of cyanamides with enynamides. RSC Advances, 2022, 12, 22939-22945.	1.7	0
5195	First-principles calculations for determining the mechanism of the photocatalytic selective oxidation of toluene to benzaldehyde on the g-C <sub>3</sub> N <sub>4</sub> catalyst. New Journal of Chemistry, 2022, 46, 16922-16931.	1.4	3
5196	Side-chain engineering for high degradation performance of mandrel materials in ICF target fabrication. Physical Chemistry Chemical Physics, 2022, 24, 25420-25425.	1.3	1
5197	Wavelength and Solvent Controlled Energy and Charge Transfer in Donor-Acceptor Substituted Platinum Acetylide Complexes. SSRN Electronic Journal, 0, , .	0.4	0
5198	Formation Routes of CO from O(1D)+Toluene: A Computational Study. Lecture Notes in Computer Science, 2022, , 260-269.	1.0	0
5199	A Theoretical Investigation of the Reactions of N <sub>2</sub> D and CN with Acrylonitrile and Implications for Prebiotic Chemistry of Titan. Lecture Notes in Computer Science, 2022, , 246-259.	1.0	0
5200	Hydride Relay Exchange Mechanism for the Heterocyclic C-H Arylation of Benzofuran and Benzothiophene Catalyzed by Pd Complexes. Journal of Organic Chemistry, 2022, 87, 12997-13010.	1.7	2

#	ARTICLE	IF	CITATIONS
5201	Unraveling origin of chemoselectivity and regioselectivity of iridium-catalyzed B(4)-H functionalization of <i>o</i> -carborane by alkyne. Journal of Physical Organic Chemistry, 0, , .	0.9	0
5202	Al-Decorated C <sub>2</sub> N Monolayer as a Potential Catalyst for NO Reduction with CO Molecules: A DFT Investigation. Molecules, 2022, 27, 5790.	1.7	3
5203	Wavelength and solvent controlled energy and charge transfer in donor-acceptor substituted platinum acetylide complexes. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 435, 114303.	2.0	6
5204	Reaction N( <sup>2</sup> D) + CH <sub>2</sub> CCH <sub>2</sub> (Allene): An Experimental and Theoretical Investigation and Implications for the Photochemical Models of Titan. ACS Earth and Space Chemistry, 2022, 6, 2305-2321.	1.2	6
5205	Temperature and Pressure-Dependent Rate Constants for the Reaction of the Propargyl Radical with Molecular Oxygen. ACS Omega, 2022, 7, 33470-33481.	1.6	5
5206	The N( <sup>2</sup> D) + CH <sub>2</sub> CHCN (Vinyl Cyanide) Reaction: A Combined Crossed Molecular Beam and Theoretical Study and Implications for the Atmosphere of Titan. Journal of Physical Chemistry A, 2022, 126, 6110-6123.	1.1	10
5207	Thorough Understanding of Bioluminophore Production in Bacterial Bioluminescence. Journal of Physical Chemistry A, 2022, 126, 6604-6616.	1.1	3
5208	Coupling of pseudoradical centers in the synthesis of oxazine fused-spiroindoline: a two-stage one-step double cyclization. Journal of Chemical Sciences, 2022, 134, .	0.7	2
5209	Promoting Catalytic Activity of Boron by Phosphor in Propane Oxidative Dehydrogenation. Journal of Physical Chemistry C, 2022, 126, 16672-16681.	1.5	2
5210	Mechanism and the Origins of Periselectivity in Cycloaddition Reactions of Benzyne with Dienes. Journal of Organic Chemistry, 2022, 87, 12954-12962.	1.7	4
5211	<b>Methane Activation by Vanadium Oxide Cluster Anions (V<sub>2</sub>O<sub>5</sub>)<sub>N</sub>O<sup>+</sup> (<i>i</i>N = 1<sup>18</sup>)</b> . Journal of Chemical Physics, 0, , .	1.2	4
5212	Role of monomolecular water and bimolecular water in IO <sub>2</sub> +CH <sub>2</sub> O reaction. Journal of Molecular Modeling, 2022, 28, .	0.8	0
5213	Advances on Understanding Coke Gasification Process with CO <sub>2</sub> : A Report from Density Functional Theory. ChemistrySelect, 2022, 7, .	0.7	0
5214	A comprehensive theoretical investigation on the thiophene hydrodesulphurisation mechanism over sulphided Co-Mo catalysts supported by ZSM-5, FAU, Beta and MCM-22 zeolites. Molecular Simulation, 0, , 1-24.	0.9	0
5216	Density Functional Study of Size-Dependent Hydrogen Adsorption on Ag <sub>n</sub> Cr ( <i>n</i> = 1-12) Clusters. ACS Omega, 2022, 7, 37379-37387.	1.6	2
5217	High-temperature mid-IR absorption spectra and reaction kinetics of 1,3-dioxolane. Proceedings of the Combustion Institute, 2023, 39, 621-631.	2.4	4
5218	Theoretical investigation for the reactions of hydrogen atom with dimethyl sulfide, ethyl methyl sulfide: Mechanism and kinetics properties. Computational and Theoretical Chemistry, 2022, 1217, 113893.	1.1	0
5219	Deciphering the cooperative effect of base and N-substituents on the origin of enantioselectivity switching for Mannich reactions of glycinate by carbonyl catalysts. Journal of Catalysis, 2022, 415, 1-11.	3.1	4

#	ARTICLE	IF	CITATIONS
5220	Mechanism of [3+2] Annulations between Indole-2-formaldehydes and Isatins Mediated by N-Heterocyclic Carbene: A DFT Study. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
5221	A Theoretical Study of the C=C Bond Cleavage Mediated by Cob(II)Aloxime. <i>Molecules</i> , 2022, 27, 7283.	1.7	0
5222	New Reactions for the Formation of Organic Nitrate in the Atmosphere. <i>ACS Omega</i> , 2022, 7, 39671-39679.	1.6	4
5223	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of an Azomethine Ylide with an Electrophilic Ethylene Linked to Triazole and Ferrocene Units. <i>Molecules</i> , 2022, 27, 6532.	1.7	3
5224	Theoretical kinetics studies on the temperature and pressure dependence of the reaction of ammonia with the Criegee intermediate CH <sub>2</sub> OO. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	2
5225	Toward efficient functionalization of polystyrene backbone through ketene chemistry: Synthesis, characterization, and <i>sc</i> DFT study. <i>Polymers for Advanced Technologies</i> , 0, , .	1.6	0
5226	Experimental and Theoretical Evidence for Relativistic Catalytic Activity in C-H Activation of <i>N</i> -Phenylbenzamide Using a Cationic Iridium Complex. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7627-7638.	1.1	1
5227	The hydrogen bond rotation of confined water affected by quantum resonance tunnelling. <i>Frontiers in Physics</i> , 0, 10, .	1.0	0
5228	Combining density functional theory and CFD-PBM model to predict TiO <sub>2</sub> nanoparticle evolution during chemical vapor deposition. <i>Chemical Engineering Journal</i> , 2023, 454, 140174.	6.6	7
5229	A Computational Study of the MoO <sub>2</sub> (acac) <sub>2</sub> Catalyzed Epoxidation of Ethylene with Hydrogen Peroxide and <i>t</i> -Butyl Hydroperoxid. <i>ChemCatChem</i> , 0, , .	1.8	3
5230	Computational studies on thermo-kinetics aspects of pyrolysis of isopropyl acetate and its methyl, bromide and hydroxyl derivatives. <i>Heliyon</i> , 2022, 8, e11274.	1.4	3
5231	Mechanistic insights into the self-esterification of lactic acid under neutral and acidic conditions. <i>Journal of Molecular Structure</i> , 2023, 1273, 134336.	1.8	1
5232	Hidden Intermediate Activation: A Concept to Elucidate the Reaction Mechanism of the Schmittel Cyclization of Enyne-Allenes. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	4
5233	Unveiling the role of indium and tin in Al-Ga based alloys for on-demand hydrogen supply from simulation to validation. <i>Journal of Power Sources</i> , 2023, 554, 232268.	4.0	12
5234	A Molecular Electron Density Theory Study of the Polar Diels-Alder Reaction of Naphtoquinone:Cr(CO) <sub>3</sub> Complex with Cyclic Dienes. <i>Polycyclic Aromatic Compounds</i> , 0, , 1-17.	1.4	1
5235	Direct Conversion of N <sub>2</sub> and O <sub>2</sub> to Nitric Oxide at Room Temperature Initiated by Double Aromaticity in the Y <sub>2</sub> BO <sup>+</sup> Cation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10697-10704.	2.1	3
5236	Unveiling the zwitterionic and stepwise mechanism for the domino reactions of amidine with 1,2,4,5-tetrazines and 1,2,3,5-tetrazines. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	0
5237	Computational investigation on mechanisms and kinetics of gas-phase reactions of 4-hydroxy-2-pentanone (4H2P) with hydroxyl radicals and subsequent reactions of CH <sub>3</sub> C(O)CH <sub>2</sub> C(OH)CH <sub>3</sub> radical. <i>Theoretical Chemistry Accounts</i> , 2022, 141, .	0.5	0

#	ARTICLE	IF	CITATIONS
5238	Combustion mechanism of fluorinated organic compound-modified nano-aluminum composite particles: Towards experimental and theoretical investigations. Chinese Journal of Aeronautics, 2023, 36, 334-349.	2.8	0
5239	Mechanistic insights into reductive deamination with hydrosilanes catalyzed by B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> : A DFT study. Frontiers in Chemistry, 0, 10, .	1.8	0
5240	Theoretical investigations on the reaction of ethenol with triplet oxygen atom. Molecular Physics, 2022, 120, .	0.8	1
5241	The influence of (H <sub>2</sub> O) <sub>2</sub> in the HOBr + HO <sub>2</sub> gas-phase reaction. RSC Advances, 2022, 12, 36028-36037.	1.7	1
5242	Unveiling the high reactivity of experimental pseudodiradical azomethine ylides within molecular electron density theory. Physical Chemistry Chemical Physics, 2022, 25, 314-325.	1.3	6
5243	A theoretical study on the methanol to propene mechanism catalyzed by a phosphorus-modified acidic FAU zeolite. New Journal of Chemistry, 2023, 47, 1740-1759.	1.4	2
5244	Theoretical investigations on reactivity influencing factors of $\dot{\text{E}}^{\text{TM}}\text{Mn}(\text{CO})_5$ catalyzed alkyne hydrosilylation and hydrogermylation. New Journal of Chemistry, 2023, 47, 2436-2443.	1.4	2
5245	Effects of steam and CO <sub>2</sub> on gasification tar composition and evolution of aromatic compounds. Waste Management, 2023, 157, 219-228.	3.7	3
5246	Photocatalytic degradation of phenol and its derivatives over ZnFe layered double hydroxide. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 438, 114509.	2.0	7
5247	A DFT study of the <i>endo</i> -selectivity mechanism of the Diels-Alder reaction in lindenane dimeric sesquiterpene synthesis promoted by pyridines. Physical Chemistry Chemical Physics, 2023, 25, 3772-3779.	1.3	1
5248	Unraveling the reaction mechanism of AlCl <sub>3</sub> Lewis acid catalyzed acylation reaction of pyrene from the perspective of the molecular electron density theory. New Journal of Chemistry, 2023, 47, 1925-1934.	1.4	3
5249	Destruction of phosphorus nitride through the $\text{N}(4\text{S}) + \text{PN}(1\text{E}) \rightarrow \text{N}_2(1\text{E}) + \text{P}(4\text{S})$ reaction. Monthly Notices of the Royal Astronomical Society, 2022, 518, 5991-5996.	1.6	0
5250	[EMmim][NTf <sub>2</sub> ] a Novel Ionic Liquid (IL) in Catalytic CO <sub>2</sub> Capture and ILs Applications. Advanced Science, 2023, 10, .	5.6	7
5251	Theoretical study on atmospheric gaseous reactions of glyoxal with sulfuric acid and ammonia. Computational and Theoretical Chemistry, 2023, 1219, 113950.	1.1	1
5252	Electronic and Steric Control of Rates and Selectivities in Rhodium-Catalyzed [2+2+2] Cycloadditions for Constructing Fused Tricyclic Hydronaphthofurans: A Density Functional Theory Study. Journal of Organic Chemistry, 2022, 87, 16328-16342.	1.7	1
5253	A de novo Stereocontrolled Synthetic Approach to a Functionalized Indolizidine Core. Synlett, 0, , .	1.0	0
5254	Concertedness and Activation Energy Control by Distal Methyl Group during Ring Contraction/Expansion in Scalarane-type Sesterterpenoid Biosynthesis. Chemistry - A European Journal, 0, , .	1.7	1
5256	Atmospheric degradation mechanisms and kinetics for OH-initiated oxidation of <i>trans</i> - $\beta$ -ocimene. Molecular Physics, 0, , .	0.8	0



#	ARTICLE	IF	CITATIONS
5257	A Density Functional Theory Study on the Cobalt-Mediated Intramolecular Pauson-Khand Reaction of Enynes Containing a Vinyl Fluoride Moiety. <i>Synthesis</i> , 2023, 55, 1139-1149.	1.2	1
5258	Mechanistic insight into the degradation of ciprofloxacin in water by hydroxyl radicals. <i>Journal of Hazardous Materials</i> , 2023, 446, 130676.	6.5	15
5259	Dramatic Size-dependence of $Rh_{n+1}$ Clusters in Reacting with Small Hydrocarbons: $Rh_3$ Cluster Catalysis for Dehydrogenation. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1
5260	How a Chromium Tricarbonyl Complex Catalyzes the [3 + 2] Cycloaddition Reaction of <i>N</i> -Substituted Phenyl Nitrones with Styrene: A Molecular Electron Density Theory Analysis. <i>Organometallics</i> , 2022, 41, 3809-3822.	1.1	3
5261	Structure and Spectroscopic Signatures of Interstellar Sodium Isocyanate Isomers. <i>Astrophysical Journal</i> , 2022, 941, 40.	1.6	2
5262	A Computational Perspective on the Chemical Reaction of HFO-1234zc with the OH Radical in the Gas Phase and in the Presence of Mineral Dust. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9564-9576.	1.1	2
5263	Visible Light-Induced Coupling Cyclization Reaction of $\hat{\pm}$ -Diazosulfonium Triflates with $\hat{\pm}$ -Oxocarboxylic Acids or Alkynes. <i>Journal of Organic Chemistry</i> , 2022, 87, 16604-16616.	1.7	8
5264	A Molecular Level Interpretation of the Underlying Chemical Phenomenon of Semi-coke and Coke Formation: A Treatise from <i>Ab Initio</i> Calculations. <i>ChemistrySelect</i> , 2022, 7, .	0.7	0
5265	Exploration of the mechanism of the condensation reaction of $Al(OH)_4^-$ with a D-gluconate using density functional theory. <i>Structural Chemistry</i> , 0, , .	1.0	0
5266	$\hat{\pm}$ -Metalated Aryl Iodides in Diels-Alder Cycloaddition Reactions: Mode of Activation and Catalysis. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	1
5267	Mechanistic insights into the challenges of organocatalytic Beckmann rearrangement reactions. <i>Organic and Biomolecular Chemistry</i> , 0, , .	1.5	0
5268	Revisiting the Burden Borne by Fumarase: Enzymatic Hydration of an Olefin. <i>Biochemistry</i> , 2023, 62, 476-493.	1.2	2
5269	A Mechanistic Study of HZSM-5-Catalyzed Guaiacol Amination Using Photoionization Time-of-Flight Mass Spectrometry. <i>Journal of Physical Chemistry A</i> , 2023, 127, 781-788.	1.1	1
5270	Research on oxidation decomposition mechanism of fluoroethane. <i>International Journal of Refrigeration</i> , 2023, 148, 35-44.	1.8	2
5271	Reactions $O_3 + HCCCN(X) \hat{\pm}$ (Cyanoacetylene): Crossed-Beam and Theoretical Studies and Implications for the Chemistry of Extraterrestrial Environments. <i>Journal of Physical Chemistry A</i> , 2023, 127, 685-703.	1.1	3
5272	Experimental and computational investigation of heteroatom substitution in nucleolytic $Cu_{ii}$ cyclen complexes for balancing stability and redox activity. <i>Dalton Transactions</i> , 2023, 52, 3176-3187.	1.6	1
5273	Unveiling the $Mg_{ii}$ promoted [3+2] cycloaddition reaction of mesitonitrile oxide to Baylis-Hilman adduct from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2023, 47, 2495-2506.	1.4	1
5274	Understanding the enhanced reactivity of strained intermolecular Frustrated Lewis Pairs. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 0, , .	0.6	0

#	ARTICLE	IF	CITATIONS
5275	Cooperative Asymmetric Dual Catalysis Involving a Chiral N-Heterocyclic Carbene Organocatalyst and Palladium in an Annulation Reaction: Mechanism and Origin of Stereoselectivity. <i>ACS Catalysis</i> , 0, , 1133-1148.	5.5	2
5276	Comprehensive Theoretical Study of Cp*Ir <sup>III</sup> -Catalyzed Intermolecular Enantioselective Allylic C-H Amidation: Reaction Mechanism, Electronic Processes, and Regioselectivity. <i>Journal of Organic Chemistry</i> , 2023, 88, 2493-2504.	1.7	1
5277	Degradation of Diethyl Phthalate by HO <sup>•</sup> and SO <sub>4</sub> <sup>•-</sup> in the Aqueous Phase: Mechanisms, Kinetics, and Toxicity. <i>ACS Earth and Space Chemistry</i> , 2023, 7, 460-470.	1.2	2
5278	Potential of Single Transition Metal Atom Embedded C <sub>2</sub> N as Efficient Catalysts for N <sub>2</sub> O Reduction: Theoretical Investigation. <i>Advanced Theory and Simulations</i> , 2023, 6, .	1.3	1
5279	A study of the thermodynamics and mechanisms of the atmospherically relevant reaction dimethyl sulphide (DMS) with atomic chlorine (Cl) in the absence and presence of water, using electronic structure methods. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4780-4793.	1.3	1
5280	An unexpected feasible route for the formation of organosulfates by the gas phase reaction of sulfuric acid with acetaldehyde catalyzed by dimethylamine in the atmosphere. <i>Environmental Science Atmospheres</i> , 2023, 3, 672-682.	0.9	2
5281	Understanding the mechanism and regio- and stereo selectivity of [3+2] cycloaddition reactions between substituted azomethine ylide and 3,3,3-trifluoro-1-nitroprop-1-ene, within the molecular electron density theory. <i>Journal of Computational Chemistry</i> , 0, , .	1.5	1
5282	Investigating the Mechanism of the Catalytic Intramolecular Aza-Wittig Reaction Involved in the Synthesis of 2-Methylbenzothiazole from the Perspective of Bonding Evolution Theory. <i>Synthesis</i> , 0, , .	1.2	1
5283	Role of Noncovalent Interactions in Inducing High Enantioselectivity in an Alcohol Reductive Deoxygenation Reaction Involving a Planar Carbocationic Intermediate. <i>Journal of the American Chemical Society</i> , 2023, 145, 2884-2900.	6.6	10
5284	Theoretical Study on the Formation of 2-Pyrone Derivatives from the Reaction of Alkynes with Carbon Dioxide in the Presence of Nickel Catalyst. <i>Organometallics</i> , 2023, 42, 197-210.	1.1	0
5285	Unveiling the Electrophilic Aromatic Substitution Reactions of Pyridine Derivatives with Nitronium Ion through Molecular Electron Density Theory. <i>New Journal of Chemistry</i> , 0, , .	1.4	0
5286	Polarity-Driven Isomerization of a Hydroxynaphthalimide-Containing Spiropyran at Room Temperature. <i>ACS Physical Chemistry Au</i> , 2023, 3, 290-298.	1.9	1
5287	Chlorination of trichlorosilane/chlorodimethylsilane using metal chlorides: experimental and mechanistic investigations. <i>RSC Advances</i> , 2023, 13, 7877-7885.	1.7	1
5288	Insights into the ruthenium-catalysed selective reduction of cardanol derivatives <i>via</i> transfer hydrogenation: a density functional theory study. <i>Catalysis Science and Technology</i> , 0, , .	2.1	0
5289	In Silico Design of Dihydroazulene/Vinylheptafulvene Photoswitches for Solar Energy Storage Guided by an All-Around Performance Descriptor**. <i>Chemistry Methods</i> , 2023, 3, .	1.8	5
5290	Kinetics, Products, and Mechanisms Study of the Atmospheric Degradation of ( <i>E</i> )-4-Methoxy-3-buten-2-one with Hydroxyl Radicals. <i>ACS Earth and Space Chemistry</i> , 0, , .	1.2	0
5291	Electrostatic interactions, binding energies and structures of the $B_2$ $\rightarrow$ $B_2^+$ $\rightarrow$ $B_2^{2+}$ $\rightarrow$ $B_2^{3+}$ $\rightarrow$ $B_2^{4+}$ $\rightarrow$ $B_2^{5+}$ $\rightarrow$ $B_2^{6+}$ $\rightarrow$ $B_2^{7+}$ $\rightarrow$ $B_2^{8+}$ $\rightarrow$ $B_2^{9+}$ $\rightarrow$ $B_2^{10+}$ $\rightarrow$ $B_2^{11+}$ $\rightarrow$ $B_2^{12+}$ $\rightarrow$ $B_2^{13+}$ $\rightarrow$ $B_2^{14+}$ $\rightarrow$ $B_2^{15+}$ $\rightarrow$ $B_2^{16+}$ $\rightarrow$ $B_2^{17+}$ $\rightarrow$ $B_2^{18+}$ $\rightarrow$ $B_2^{19+}$ $\rightarrow$ $B_2^{20+}$ $\rightarrow$ $B_2^{21+}$ $\rightarrow$ $B_2^{22+}$ $\rightarrow$ $B_2^{23+}$ $\rightarrow$ $B_2^{24+}$ $\rightarrow$ $B_2^{25+}$ $\rightarrow$ $B_2^{26+}$ $\rightarrow$ $B_2^{27+}$ $\rightarrow$ $B_2^{28+}$ $\rightarrow$ $B_2^{29+}$ $\rightarrow$ $B_2^{30+}$ $\rightarrow$ $B_2^{31+}$ $\rightarrow$ $B_2^{32+}$ $\rightarrow$ $B_2^{33+}$ $\rightarrow$ $B_2^{34+}$ $\rightarrow$ $B_2^{35+}$ $\rightarrow$ 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#	ARTICLE	IF	CITATIONS
5293	Theoretical Investigation on Hydrogen Abstraction Reactions of Sulfur Compounds HSX( <i>O</i> )H and CH <sub>3</sub> SX( <i>O</i> )H (X = C, S) by OH Radicals. ACS Earth and Space Chemistry, 0, , .	1.2	0
5294	Chemo- and regioselectivities of the TBAF-catalyzed C F bond allylation of trifluoromethylalkenes: A theoretical view. Molecular Catalysis, 2023, 542, 113111.	1.0	0
5295	Reaction mechanism and kinetics of H and Cl atom abstraction in Dichloromethane with OH radical. Computational and Theoretical Chemistry, 2023, 1223, 114082.	1.1	1
5296	Mechanisms and origins of stereoselectivity involved in NHC-catalyzed [3+3] Annulation of 2-bromoenals and $\beta^2$ -ketothioamides: A DFT study. Molecular Catalysis, 2023, 542, 113135.	1.0	0
5297	Theoretical investigation into activation of hydroperoxides by excited quinones under ultraviolet irradiation. Chemical Engineering Journal, 2023, 463, 142423.	6.6	0
5298	Theoretical insights into the synthesis reaction mechanism of HMX based on TAT nitration reaction. Chemical Physics Letters, 2023, 820, 140448.	1.2	2
5299	An experimental and kinetic modeling study on the high-temperature ignition and pyrolysis characteristics of cyclohexylamine. Combustion and Flame, 2023, 252, 112769.	2.8	3
5300	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. Scientific Reports, 2023, 13, .	1.6	3
5301	C <sup>+</sup> H Activation by Iron-Vanadium Bimetallic Oxide Cluster Anions FeV <sub>3</sub> O <sub>10</sub> <sup>+</sup> and FeV <sub>5</sub> O <sub>15</sub> <sup>+</sup> : A Comparison with Scandium-Vanadium Oxide Clusters. ChemPhysChem, 0, , .	1.0	0
5302	High-temperature mid-IR absorption and reaction kinetics of 2-methyl-1,3-dioxolane: An experimental and theoretical study. Journal of Photochemistry and Photobiology, 2023, 13, 100165.	1.1	2
5303	The structure-based optimization of 3-substituted indolin-2-one derivatives as potent and isoform-selective c-Jun N-terminal kinase 3 (JNK3) inhibitors and biological evaluation. European Journal of Medicinal Chemistry, 2023, 250, 115167.	2.6	2
5304	Theoretical insights into the reaction mechanism and kinetics of ampicillin degradation with hydroxyl radical. Journal of Molecular Modeling, 2023, 29, .	0.8	4
5305	Computational Evidence of the Incipient Oxocarbenium Ion as a "Hidden Intermediate" During the Cyclization of Hydroxyenol Ether into Spiroketal Under Mild Acidic Condition. Chemistry - A European Journal, 0, , .	1.7	0
5306	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5] <sup>+</sup> : Theoretical and Experimental Study. Molecules, 2023, 28, 1757.	1.7	1
5307	A Silver-Based Integrated System Showing Mutually Inclusive Super Protonic Conductivity and Photoswitching Behavior. Inorganic Chemistry, 2023, 62, 3485-3497.	1.9	5
5308	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s] Sigmatropic Shift through Transition State Complexation and Stereoelectronic Effects. Angewandte Chemie - International Edition, 2023, 62, .	7.2	2
5309	Designing an Apparently Orbital-Symmetry-Forbidden [3s,5s] Sigmatropic Shift through Transition State Complexation and Stereoelectronic Effects. Angewandte Chemie, 2023, 135, .	1.6	0
5310	Thermal Methane Conversion to Formaldehyde Mediated by NiAlO <sub>3</sub> <sup>+</sup> in the Gas Phase. Journal of Physical Chemistry A, 2023, 127, 1636-1641.	1.1	2

#	ARTICLE	IF	CITATIONS
5311	A theoretical study on the photochemical generation of phenylborylene from phenyldiazidoborane. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8074-8081.	1.3	4
5312	Tailoring the mechanistic pathways and kinetics of OH-addition reaction of sulfoxaflor and its ecotoxicity assessment. <i>Environmental Science and Pollution Research</i> , 2023, 30, 50209-50224.	2.7	0
5313	Oxidopyridinium Cycloadditions Revisited: A Combined Computational and Experimental Study on the Reactivity of 1-(2-Pyrimidyl)-3-oxidopyridinium Betaine. <i>Journal of Organic Chemistry</i> , 2023, 88, 3193-3207.	1.7	3
5314	C <sub>(sp3)</sub> -H Oxidative Addition at Tantalocene Hydrides. <i>Organometallics</i> , 0, , .	1.1	0
5315	Coordination of sorbitol to Ga(OTf) <sub>3</sub> in the liquid phase: an experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8507-8514.	1.3	0
5316	The study on gas phase dehydrogenation reactions of transition metal cation and ethylene. <i>Molecular Physics</i> , 2023, 121, .	0.8	1
5317	Mechanism Investigation on Direct Conversion of Methane over a Mononuclear Rh-ZSM-5 Catalyst: Multiple Roles of CO. <i>Journal of Physical Chemistry C</i> , 2023, 127, 4887-4895.	1.5	0
5318	A DFT study of Ni-catalyzed (3 + 3)-annulation between donor-acceptor cyclopropanes and diaziridines. <i>Organic Chemistry Frontiers</i> , 2023, 10, 1948-1958.	2.3	4
5319	Tautomerization reactions of thiobarbituric acid: A detailed kinetic study using combined canonical variational transition state theory and QTAIM approach. <i>International Journal of Chemical Kinetics</i> , 2023, 55, 247-260.	1.0	1
5320	DFT Studies on Ligand Controlled Highly Selective Copper-Catalyzed Borylations of Allenes. <i>Asian Journal of Organic Chemistry</i> , 0, , .	1.3	0
5321	Theoretical study on the kinetics of hydrogen cyanide and hydrogen isocyanide reactions with the methyl radical. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10121-10128.	1.3	0
5322	Reciprocity of C <sup>+</sup> -π interactions with the dominant anion-π on fullerene (C <sub>60</sub> )-amine-based organocatalysts: a mechanistic elucidation for addition vs. decarboxylation reaction. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 10647-10660.	1.3	1
5324	Excited-State Intramolecular Proton Transfer in Salicylidene-1-Hydroxy Carboxylate Derivatives: Direct Detection of the Triplet Excited State of the <i>cis</i> -Keto Tautomer. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2765-2778.	1.1	0
5325	Interactive Organic Reaction Trajectory Animation iPhone Application (iORA) and Web Site (webORA). <i>Journal of Chemical Education</i> , 2023, 100, 1659-1663.	1.1	1
5326	Propane Oxidative Dehydrogenation on Nanosized Boron Carbide: Effect of Boron Content and Its Oxidation Implicated by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2023, 127, 6280-6293.	1.5	0
5327	Ligand Control in Co-Catalyzed Regio- and Enantioselective Hydroboration: Homoallyl Secondary Boronates via Uncommon 4,3-Hydroboration of 1,3-Dienes. <i>Journal of the American Chemical Society</i> , 2023, 145, 7462-7481.	6.6	5
5328	Mechanistic insights and computational design of Cu/M bimetallic synergistic catalysts for Suzuki-Miyaura coupling of arylboronic esters with alkyl halides. <i>Molecular Catalysis</i> , 2023, 541, 113098.	1.0	2
5329	A DFT study of the catalytic ODH of n-hexane over a cluster model of vanadium oxide. <i>Molecular Catalysis</i> , 2023, 541, 113078.	1.0	0

#	ARTICLE	IF	CITATIONS
5330	Two Carbon Dioxide Molecules Consecutively Reduced by Metal-Free $B_{2}O_{2}^{-}$ Anions. <i>Journal of Physical Chemistry A</i> , 2023, 127, 3082-3087.	1.1	0
5331	Understanding the Reactivity of Diazaborinines towards the Activation of $\pi$ -Bonds. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	1
5332	Conversion of Dinitrogen and Oxygen to Nitric Oxide Mediated by Triatomic Yttrium Cations: Reversible $N \rightleftharpoons N$ Bond Switching. <i>Inorganic Chemistry</i> , 2023, 62, 6102-6108.	1.9	3
5333	Infrared Photodissociation Spectroscopy of Mass-Selected $[TaO_3(CO_2)_n]^+$ ( $n = 2-5$ ) Complexes in the Gas Phase. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	2
5334	Understanding the insight into the mechanisms and dynamics of the OH-initiated oxidation of $CHF_2CF_2OCHF_2$ and the subsequent reactions in the presence of NO and $O_2$ . <i>Journal of Molecular Graphics and Modelling</i> , 2023, 122, 108489.	1.3	0
5335	Thermochemistry of the Smallest Hyperbolic Paraboloid Hydrocarbon: A High-Level Quantum Chemical Perspective. <i>Journal of Carbon Research</i> , 2023, 9, 41.	1.4	0
5336	Unveiling the exclusive stereo and site selectivity in [3+2] cycloaddition reactions of a tricyclic strained alkene with nitrile oxides from the molecular electron density theory perspective. <i>Chemistry of Heterocyclic Compounds</i> , 0, , .	0.6	2
5337	An experimental and theoretical investigation of the $N_2^+ + C_6H_6$ (benzene) reaction with implications for the photochemical models of Titan. <i>Faraday Discussions</i> , 0, 245, 327-351.	1.6	4
5385	A Computational Study of the Reaction Between $N(2D)$ and Simple Aromatic Hydrocarbons. <i>Lecture Notes in Computer Science</i> , 2023, , 718-734.	1.0	0
5479	Theoretical and Experimental Study of the Chemical Modification of Poly(epichlorohydrin) by Grafting Menthol. , 0, , .		0