

A complete basis set model chemistry. VI. Use of density frequencies

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Citation Report

#	ARTICLE	IF	CITATIONS
18	Heat of atomization of sulfur trioxide, SO ₃ : a benchmark for computational thermochemistry. Chemical Physics Letters, 1999, 310, 271-276.	2.6	53
19	Gaussian-3 theory using coupled cluster energies. Chemical Physics Letters, 1999, 314, 101-107.	2.6	217
20	Towards standard methods for benchmark quality ab initio thermochemistry—W1 and W2 theory. Journal of Chemical Physics, 1999, 111, 1843-1856.	3.0	947
21	An assessment of theoretical procedures for the calculation of reliable radical stabilization energies—W1 and W2 theory. Journal of the Chemical Society Perkin Transactions II, 1999, , 2305-2313.	0.9	121
22	Gaussian-3 theory using density functional geometries and zero-point energies. Journal of Chemical Physics, 1999, 110, 7650-7657.	3.0	1,606
23	Dissociation Pathways of Peroxyacetyl Nitrate (PAN). Journal of Physical Chemistry A, 1999, 103, 11451-11459.	2.5	38
24	A Quantum-Chemical Study of the C ₂ H ₃ F ₂ and C ₂ H ₃ Cl ₂ Isomers and Their Interconversion. CBS-QB3 Proton Affinities of Difluoroethenes and Dichloroethenes. Journal of Physical Chemistry A, 1999, 103, 7872-7882.	2.5	3
25	A Definitive Heat of Vaporization of Silicon through Benchmark ab Initio Calculations on SiF ₄ . Journal of Physical Chemistry A, 1999, 103, 4427-4431.	2.5	30
26	Theoretical study of synthetic reaction of tetrazole and tetrazolate anion. International Journal of Quantum Chemistry, 2000, 80, 27-37.	2.0	24
27	Conformational Equilibrium and Potential Energy Surface of 1-Fluorobutane by Microwave Spectroscopy and Ab Initio Calculations. Chemistry - A European Journal, 2000, 6, 3018-3025.	3.3	10
28	Ab initio and RRKM calculations on the dissociation of the propionyl radical. Journal of Molecular Structure, 2000, 556, 123-129.	3.6	3
29	Characterization of iminothiosulfine-type ions [HNCS ₂] ⁺ and their neutral counterparts by mass spectrometry and computational chemistry. Chemical Physics Letters, 2000, 332, 251-258.	2.6	5
30	CBS-QB3 determination of enthalpy and free energy changes at normal and elevated temperatures. Computational and Theoretical Chemistry, 2000, 529, 41-45.	1.5	7
31	Theoretical Study of the Heats of Formation of SF, FSO, FSO ₂ and HSO Radicals. Zeitschrift Fur Physikalische Chemie, 2000, 214, .	2.8	9
32	The HCO[_{sub 2}] potential energy surface: Stationary point energetics and the HOCO heat of formation. Journal of Chemical Physics, 2000, 113, 5138.	3.0	71
33	A new complete basis set model (CBS-QB3) study on the possible intermediates in chemiluminescence. Journal of Chemical Physics, 2000, 113, 7731-7734.	3.0	12
34	Complexes of Hydroxyl and Hydroperoxyl Radical with Formaldehyde, Acetaldehyde, and Acetone. Journal of Physical Chemistry A, 2000, 104, 3211-3224.	2.5	69
35	Computational Study of the Electronic Structure of Substituted Phenylcarbene in the Gas Phase. Journal of Organic Chemistry, 2000, 65, 8348-8356.	3.2	72

#	ARTICLE	IF	CITATIONS
36	A Theoretical Study of the P++ SH2Reaction:Â Potential Energy Surfaces and Reaction Dynamics. Journal of Physical Chemistry A, 2000, 104, 11095-11105.	2.5	2
37	Thermochemical Database of Halomethanes, Halosilanes, Halophosphines, and Haloamines. Journal of Chemical Information and Computer Sciences, 2000, 40, 358-360.	2.8	9
38	Assessment of Gaussian-3 and density functional theories for a larger experimental test set. Journal of Chemical Physics, 2000, 112, 7374-7383.	3.0	711
40	Can Hydrocarbon Chains Be Disrupted by Fast O(3P) Atoms?. Journal of Physical Chemistry A, 2000, 104, 9976-9982.	2.5	28
41	A complete basis set model chemistry. VII. Use of the minimum population localization method. Journal of Chemical Physics, 2000, 112, 6532-6542.	3.0	1,716
42	Computational Analysis of the Potential Energy Surfaces of Glycerol in the Gas and Aqueous Phases:Â Effects of Level of Theory, Basis Set, and Solvation on Strongly Intramolecularly Hydrogen-Bonded Systems. Journal of the American Chemical Society, 2001, 123, 11743-11754.	13.7	133
43	Dream or Reality: Complete Basis Set Full Configuration Interaction Potential Energy Hypersurfaces. , 2001, , 317-339.		51
44	Assessment of W1 and W2 theories for the computation of electron affinities, ionization potentials, heats of formation, and proton affinities. Journal of Chemical Physics, 2001, 114, 6014-6029.	3.0	444
45	Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data. Journal of Physical Chemistry A, 2001, 105, 10483-10487.	2.5	131
46	Energetics of Aluminum Combustion. Journal of Physical Chemistry A, 2001, 105, 7473-7480.	2.5	56
47	Corannulene as a Lewis Base:â€‰ Computational Modeling of Protonation and Lithium Cation Binding. Journal of the American Chemical Society, 2001, 123, 6687-6695.	13.7	67
48	Stereochemistry of Radical Halogenation Reactions. An ab Initio Molecular Orbital Study. Journal of Physical Chemistry A, 2001, 105, 10890-10898.	2.5	10
49	Gaussian-3X (G3X) theory: Use of improved geometries, zero-point energies, and Hartreeâ€‰Fock basis sets. Journal of Chemical Physics, 2001, 114, 108.	3.0	477
50	A Mechanistic Study of the Reactions of H, O (3P), and OH with Monocyclic Aromatic Hydrocarbons by Density Functional Theory. Journal of Physical Chemistry A, 2001, 105, 140-152.	2.5	66
51	Accurate relative pK[sub a] calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. Journal of Chemical Physics, 2001, 114, 4595.	3.0	145
52	Accurate pKaCalculations for Carboxylic Acids Using Complete Basis Set and Gaussian-n Models Combined with CPCM Continuum Solvation Methods. Journal of the American Chemical Society, 2001, 123, 7314-7319.	13.7	544
53	Quantum Chemical and RRKM Investigation of the Elementary Channels of the Reaction C6H6 + O (3P). Journal of Physical Chemistry A, 2001, 105, 4316-4327.	2.5	34
54	The reactivity of aminoxyls towards peroxy radicals: an ab initio thermochemical studyâ€‰. Perkin Transactions II RSC, 2001, , 1793-1797.	1.1	14

#	ARTICLE	IF	CITATIONS
55	Theoretical studies of the thermal and chemically activated decomposition of CF ₃ CY ₂ O (Y = F, H) radicals. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 2352-2364.	2.8	28
56	S ⁺ N Dissociation Energies of S-Nitrosothiols: On the Origins of Nitrosothiol Decomposition Rates. <i>Journal of the American Chemical Society</i> , 2001, 123, 8868-8869.	13.7	126
57	Multi-coefficient Correlation Method: A Comparison of Specific-Range Reaction Parameters to General Parameters for C _n H _x O _y Compounds. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4143-4149.	2.5	15
58	On Comparison of Experimental Thermochemical Data with G3 Theory. <i>Journal of Physical Chemistry A</i> , 2001, 105, 227-228.	2.5	31
59	Symmetry Breaking and the Molecular Structure of NO ₃ ⁺ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 1662-1668.	2.5	8
60	A Theoretical Investigation of the Triplet Carbon Atom C(3P) + Vinyl Radical C ₂ H ₃ (2A ⁺) Reaction and Thermochemistry of C ₃ H _n (n = 1-4) Species. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3284-3299.	2.5	55
61	Enzyme Catalysis of 1,2-Amino Shifts: The Cooperative Action of B6, B12, and Aminomutases. <i>Journal of the American Chemical Society</i> , 2001, 123, 8678-8689.	13.7	67
62	Benchmark ab Initio Energy Profiles for the Gas-Phase S _N 2 Reactions Y ⁻ + CH ₃ X → CH ₃ Y + X ⁻ (X, Y = F, Cl, Br). Validation of Hybrid DFT Methods. <i>Journal of Physical Chemistry A</i> , 2001, 105, 895-904.	2.5	199
63	Theoretical studies of coenzyme B12-dependent carbon-skeleton rearrangements. <i>Theoretical and Computational Chemistry</i> , 2001, , 183-214.	0.4	1
64	Computational studies of the reaction of the hydroxyl radical with hydrofluorocarbons (HFCs) and hydrofluoroethers (HFEs). <i>Journal of Fluorine Chemistry</i> , 2001, 109, 113-121.	1.7	25
65	The chemistry of some low energy C ₅ H ₉ O ⁺ oxonium ions. <i>International Journal of Mass Spectrometry</i> , 2001, 209, 153-169.	1.5	4
66	Energetics of the 2+2 cyclization of limonene. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2001, 139, 17-21.	3.9	5
67	Experimentation with different thermodynamic cycles used for pK _a calculations on carboxylic acids using complete basis set and Gaussian-n models combined with CPCM continuum solvation methods. <i>International Journal of Quantum Chemistry</i> , 2001, 85, 727-741.	2.0	176
68	Computational chemistry: A useful (sometimes mandatory) tool in mass spectrometry studies. <i>Mass Spectrometry Reviews</i> , 2001, 20, 195-245.	5.4	160
69	Benzdiynes revisited: ab initio and density functional theory. <i>Journal of Computational Chemistry</i> , 2001, 22, 923-930.	3.3	17
71	Factors Controlling the Addition of Carbon-Centered Radicals to Alkenes: An Experimental and Theoretical Perspective. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1340-1371.	13.8	640
72	Double charge transfer spectroscopy of acetylene dication C ₂ H ₂ ²⁺ at vibrational resolution. <i>Chemical Physics Letters</i> , 2001, 342, 625-630.	2.6	16
73	Polarization consistent basis sets: Principles. <i>Journal of Chemical Physics</i> , 2001, 115, 9113-9125.	3.0	571

#	ARTICLE	IF	CITATIONS
74	Stability of XSO ₂ (X=F, Cl, and Br) radical: impact of the basis set on X-S bonding energy in ab initio and DFT calculations. Chemical Physics Letters, 2001, 350, 173-180.	2.6	5
75	The heat of formation of sulfine, CH ₂ =S=O, revisited: a CBS-QB3 study. Chemical Physics Letters, 2001, 342, 447-451.	2.6	12
76	Thermochemical analysis of the OH+C ₂ H ₄ →C ₂ H ₄ OH reaction using accurate theoretical methods. Computational and Theoretical Chemistry, 2001, 537, 199-212.	1.5	17
77	Influence of the basis set and correlation method on the calculation of molecular structures: thiadiazoles revisited. Computational and Theoretical Chemistry, 2001, 548, 153-163.	1.5	23
78	Computational characterization of energetic materials. Computational and Theoretical Chemistry, 2001, 573, 1-10.	1.5	93
79	Calculation of electron affinities for small homonuclear and heteronuclear diatomic molecules with the CBS-QB3 and G3B3 method: basis set effects, and need for further development. Computational and Theoretical Chemistry, 2001, 574, 141-143.	1.5	5
80	A direct dynamics study of the H ₂ elimination from 2,5-dihydrofuran. Journal of Chemical Physics, 2001, 115, 7872-7880.	3.0	6
81	Fully ab initio atomization energy of benzene via Weizmann-2 theory. Journal of Chemical Physics, 2001, 115, 2051-2054.	3.0	39
82	Scaled higher-order correlation energies: In pursuit of the complete basis set full configuration interaction limit. Journal of Chemical Physics, 2001, 114, 5491-5496.	3.0	18
83	Complete Basis Set Models for Chemical Reactivity: from the Helium Atom to Enzyme Kinetics. , 2001, , 99-130.		19
84	Photoelectron spectroscopy of HCCN ⁺ and HCNC ⁺ reveals the quasilinear triplet carbenes, HCCN and HCNC. Journal of Chemical Physics, 2002, 117, 4323-4339.	3.0	52
85	Atom-radical reaction dynamics of O(3P)+C ₃ H ₅ →C ₃ H ₄ +OH: Nascent rovibrational state distributions of product OH. Journal of Chemical Physics, 2002, 117, 2017-2029.	3.0	35
86	The reduction potential of nitric oxide (NO) and its importance to NO biochemistry. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10958-10963.	7.1	339
87	The heats of formation of the haloacetylenes XCCY [X, Y = H, F, Cl]: basis set limit ab initio results and thermochemical analysis. Molecular Physics, 2002, 100, 453-464.	1.7	21
88	Crossed beam investigations of the reaction dynamics of O(3P) with allyl radical, C ₃ H ₅ . Journal of Chemical Physics, 2002, 116, 2675-2679.	3.0	30
89	Missing Thermochemical Groups for Large Unsaturated Hydrocarbons: A Contrasting Predictions of G2 and CBS-Q. Journal of Physical Chemistry A, 2002, 106, 11141-11149.	2.5	34
90	The Hydration of Formic Acid. Journal of Physical Chemistry A, 2002, 106, 363-370.	2.5	101
91	Computational and Experimental Studies of the Effect of Substituents on the Singlet-Triplet Energy Gap in Phenyl(carbomethoxy)carbene. Journal of Organic Chemistry, 2002, 67, 3079-3088.	3.2	39

#	ARTICLE	IF	CITATIONS
92	Transition State Structure and Energetics of the N ₂ O + X (X = Cl, Br) Reactions. Journal of Chemical Information and Computer Sciences, 2002, 42, 706-711.	2.8	11
93	Solvation of Sulfur-Centered Cations and Anions in Acetonitrile. Journal of Physical Chemistry A, 2002, 106, 8827-8833.	2.5	23
94	Rearrangement Pathways of 2-Hydroxy-2-methylpropylidene: An Experimental and Computational Study. Journal of Organic Chemistry, 2002, 67, 3257-3265.	3.2	14
95	Experimental and Theoretical Dissection of Sodium Cation/Glycine Interactions. Journal of Physical Chemistry A, 2002, 106, 10350-10362.	2.5	134
96	Enthalpy of the Gas-Phase CO ₂ + Mg Reaction from ab Initio Total Energies. Journal of Chemical Information and Computer Sciences, 2002, 42, 853-857.	2.8	2
97	Methyl Radical Addition to CS Double Bonds: Kinetic versus Thermodynamic Preferences. Journal of Physical Chemistry A, 2002, 106, 12124-12138.	2.5	82
98	Anchoring the Gas-Phase Acidity Scale. Journal of Physical Chemistry A, 2002, 106, 9947-9956.	2.5	190
99	Absolute pK _a Determinations for Substituted Phenols. Journal of the American Chemical Society, 2002, 124, 6421-6427.	13.7	519
100	Nitro derivatives of pyrrole, furan and 1H-tetrazole: ring or nitro bases?. New Journal of Chemistry, 2002, 26, 1567-1574.	2.8	14
101	Conformation-Dependent State Selectivity in O-O Cleavage of ONOONO: An Inorganic Cope Rearrangement Helps Explain the Observed Negative Activation Energy in the Oxidation of Nitric Oxide by Dioxygen. Journal of the American Chemical Society, 2002, 124, 9469-9475.	13.7	53
102	An Assessment of the Performance of High-Level Theoretical Procedures in the Computation of the Heats of Formation of Small Open-Shell Molecules. Journal of Physical Chemistry A, 2002, 106, 7927-7936.	2.5	109
103	On the thermochemical stability of the sextet CO ₂ anion: results from density functional theory. Molecular Physics, 2002, 100, 3691-3697.	1.7	0
104	1,8-Chalcogen-bridged naphthalenes. Strong carbon bases in the gas phase. New Journal of Chemistry, 2002, 26, 1747-1752.	2.8	33
105	Computational determination of the enthalpy of formation of alkylthial S-oxides and alkylthione S-oxides: a study of (Z)-propanethial-S-oxide, the lachrymatory factor of the onion (Allium cepa). Physical Chemistry Chemical Physics, 2002, 4, 4328-4333.	2.8	3
106	Electron-spin conservation and methyl-substitution effects on bonds in closed- and open-shell systems: A G3 ab initio study of small boron-containing molecules and radicals. Canadian Journal of Chemistry, 2002, 80, 25-30.	1.1	11
107	Triaziridine and tetrazetidine vs. cyclic water trimer and tetramer: A computational approach to the relationship between molecular and supramolecular conformational analysis. Physical Chemistry Chemical Physics, 2002, 4, 2123-2129.	2.8	10
108	Rotational Spectrum, Hyperfine Structure, and Internal Rotation of Methyl Carbamate. Journal of Molecular Spectroscopy, 2002, 215, 312-316.	1.2	26
109	Ab initio conformational studies on diols and binary diol-water systems using DFT methods. Intramolecular hydrogen bonding and 1:1 complex formation with water. Journal of Computational Chemistry, 2002, 23, 585-599.	3.3	104

#	ARTICLE	IF	CITATIONS
110	Gas phase nucleophilic substitution. International Journal of Mass Spectrometry, 2002, 214, 277-314.	1.5	211
111	Hydrogen-shift isomers of ionic and neutral hydroxypyridines: a combined experimental and computational investigation. International Journal of Mass Spectrometry, 2002, 217, 1-22.	1.5	25
112	Generation and characterization of protonated silicic acid $\text{Si}(\text{OH})_3^+$ and its neutral counterpart by tandem mass spectrometry and computational chemistry. International Journal of Mass Spectrometry, 2002, 221, 219-227.	1.5	4
113	Heats of formation for AlH , AlOH , OAlH and OAlOH and their monocations. Computational and Theoretical Chemistry, 2002, 581, 17-29.	1.5	39
114	Part I. High level ab initio approximations of the atomization energies of C_n ($n = 2\text{--}6$) neutral carbon clusters. Computational and Theoretical Chemistry, 2002, 584, 143-147.	1.5	5
115	The $\text{CH}_2\text{OH}+\text{CHO} \rightarrow \text{H}_2$ decomposition mechanism: a G3, G3B3, CBS-Q, CBS-QB3 versus pure DFT comparison: interesting variations. Computational and Theoretical Chemistry, 2002, 594, 129-133.	1.5	6
116	On the $\text{HNO} \rightarrow \text{HON}$ isomerization mechanism: high level ab initio and density functional theory study. Computational and Theoretical Chemistry, 2002, 585, 199-203.	1.5	7
117	Part II. Ionization energies, hardness, softness, and absolute electronegativity of heteronuclear and homonuclear diatomic molecules by the CBS-QB3 and G3B3 methods. Computational and Theoretical Chemistry, 2002, 585, 205-208.	1.5	10
118	Physical characterization of C3B2 isomers: a combined density functional theory and advanced ab initio analysis. Computational and Theoretical Chemistry, 2002, 593, 49-54.	1.5	1
119	The isomerization of CLOOCl : high level ab initio and density functional theory analysis. Computational and Theoretical Chemistry, 2002, 594, 1-7.	1.5	6
120	A communication on Mg_2 thermochemical stability. Computational and Theoretical Chemistry, 2002, 589-590, 75-78.	1.5	1
121	CLOOCl : theoretical insights into its torsional potentials. Computational and Theoretical Chemistry, 2002, 592, 123-135.	1.5	7
122	DFT/B3-LYP and ab initio analysis of the ozone potential energy surface. Computational and Theoretical Chemistry, 2002, 617, 5-8.	1.5	6
123	H-atom product channels in the photodissociation of CH_3F and CH_3Cl : a density functional theory and high level ab initio study. Computational and Theoretical Chemistry, 2002, 618, 35-40.	1.5	3
124	MgO internuclear interactions. A theoretical study. Computational and Theoretical Chemistry, 2002, 618, 85-92.	1.5	3
125	Ab initio and density functional theory study of the enthalpies of formation of F_2SO_x and FCISO_x ($x=1, 2$). Journal of Fluorine Chemistry, 2002, 116, 135-141.	1.7	15
126	Density functional computational thermochemistry: solving the discrepancy between MO and DFT calculations on the enthalpy of formation of sulfine, $\text{CH}_2\text{S} \rightarrow \text{S} \rightarrow \text{O}$. Chemical Physics Letters, 2002, 355, 207-213.	2.6	19
127	Gaussian-3X (G3X) theory using coupled cluster and Brueckner energies. Chemical Physics Letters, 2002, 359, 390-396.	2.6	43

#	ARTICLE	IF	CITATIONS
128	A quadratic configuration interaction study of the proton affinity of acetic acid. Chemical Physics Letters, 2002, 364, 427-431.	2.6	7
129	Complete basis set and density functional determination of the enthalpy of formation of the controversial HO3 radical: a discrepancy between theory and experiment. Chemical Physics Letters, 2002, 365, 440-449.	2.6	39
130	Title is missing!. Structural Chemistry, 2002, 13, 479-490.	2.0	6
131	A Standard Set of Pericyclic Reactions of Hydrocarbons for the Benchmarking of Computational Methods: The Performance of ab Initio, Density Functional, CASSCF, CASPT2, and CBS-QB3 Methods for the Prediction of Activation Barriers, Reaction Energetics, and Transition State Geometries. Journal of Physical Chemistry A, 2003, 107, 11445-11459.	2.5	342
132	Title is missing!. Russian Chemical Bulletin, 2003, 52, 837-845.	1.5	8
133	Ab Initio Calculations for Hydrocarbons: Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. Journal of Physical Chemistry A, 2003, 107, 9147-9159.	2.5	170
134	Radical-radical reaction dynamics: The OH formation in the reaction of O(3P) with propargyl radical, C3H3. Journal of Chemical Physics, 2003, 119, 9337-9340.	3.0	18
135	Hydrogen bonding in diols and binary diol-water systems investigated using DFT methods. II. Calculated infrared OH-stretch frequencies, force constants, and NMR chemical shifts correlate with hydrogen bond geometry and electron density topology. A reevaluation of geometrical criteria for hydrogen bonding. Journal of Computational Chemistry, 2003, 24, 1120-1131.	3.3	79
136	Solvent effects on glycine. I. A supermolecule modeling of tautomerization via intramolecular proton transfer. Journal of Computational Chemistry, 2003, 24, 1789-1802.	3.3	65
138	Resonance-Assisted Intramolecular Chalcogen-Chalcogen Interactions?. Chemistry - A European Journal, 2003, 9, 4548-4555.	3.3	79
139	Binding Affinities of Host-Guest, Protein-Ligand, and Protein-Transition-State Complexes. Angewandte Chemie - International Edition, 2003, 42, 4872-4897.	13.8	511
140	A curious regularity in the dissociative photoionization of fluorinated benzenes: why do C6F6+ and C6H6+ dissociate so differently?. Chemical Physics Letters, 2003, 368, 276-281.	2.6	3
141	Generation of the elusive methyl dioxophosphorane molecule, CH3P(=O)2, by delayed dissociation of selected precursors. Chemical Physics Letters, 2003, 368, 584-588.	2.6	11
142	Theoretical calculations of product percentage yields for the thermal decomposition of 2-chloro-1,1-difluoroethane. Tetrahedron Letters, 2003, 44, 7265-7268.	1.4	21
143	Enhancement of 1,2-dehydration of alcohols by alkali cations and protons: a model for dehydration of carbohydrates. Journal of Analytical and Applied Pyrolysis, 2003, 66, 3-27.	5.5	55
144	Does Mg4 exist? A combined Gaussian, complete basis set and density functional theory study. Computational and Theoretical Chemistry, 2003, 629, 7-10.	1.5	3
145	Influence of the basis set and correlation method on the calculation of the dipole moments of isomeric thiadiazoles. Computational and Theoretical Chemistry, 2003, 634, 77-81.	1.5	7
146	A high-level calculation of the proton affinity of diborane. Computational and Theoretical Chemistry, 2003, 638, 189-195.	1.5	9

#	ARTICLE	IF	CITATIONS
147	The isobaric ions $\text{CH}_3\text{O}^-\text{P}^+\dots\text{O}^+$ and $\text{CH}_3\text{O}^-\text{P}^+\text{NH}_2^+$ and their neutral counterparts: a tandem mass spectrometry and CBS-QB3 computational study. International Journal of Mass Spectrometry, 2003, 225, 11-23.	1.5	15
148	Binding energies of Cu^+ to saturated and $\hat{1}\pm, \hat{1}^2$ -unsaturated alkanes, silanes and germanes. International Journal of Mass Spectrometry, 2003, 227, 401-412.	1.5	26
149	Proton affinities and gas-phase basicities: theoretical methods and structural effects. International Journal of Mass Spectrometry, 2003, 227, 601-616.	1.5	104
150	Tautomerization and dissociation of ethylene phosphonate ions $[\text{i}-\text{OCH}_2\text{CH}_2\text{O}^-\text{P}^+(\text{H})\dots\text{O}^+]$: an experimental and CBS-QB3 computational study. International Journal of Mass Spectrometry, 2003, 227, 453-469.	1.5	8
151	The remarkable decarbonylation of $\text{CH}_3\text{O}^-\text{P}^+\dots\text{O}^+$ and its distonic isomer $\text{CH}_2\text{O}^-\text{P}^+\text{OH}^+$: an experimental and CBS-QB3 computational study. International Journal of Mass Spectrometry, 2003, 228, 759-777.	1.5	9
152	Theoretical Study of Molecular Structure and Gas-Phase Acidity of Some Biologically Active Sulfonamides. Journal of Physical Chemistry A, 2003, 107, 720-725.	2.5	38
153	Estimates of quantum chemical molecular characteristics for complete basis sets. Israel Journal of Chemistry, 2003, 43, 243-265.	2.3	6
154	Coupled Cluster Theory Determination of the Heats of Formation of Combustion-Related Compounds: $\hat{\text{A}}$ CO, HCO, CO ₂ , HOCO, HC(O)OH, and HC(O)OOH. Journal of Physical Chemistry A, 2003, 107, 1604-1617.	2.5	94
155	Assessment of the suitability of using the composite G2, G3, and CBS-RAD methods for predicting activation energies. Chemical Engineering Communications, 2003, 190, 1233-1248.	2.6	5
156	Agostic vs $\hat{\text{I}}\text{C}$ -Interactions in Complexes of Ethynylsilanes and Ethynylgermanes with Cu^+ in the Gas Phase. Journal of Physical Chemistry A, 2003, 107, 1370-1376.	2.5	37
157	Computational Study of the Halogen Atom $\hat{\text{A}}$ Benzene Complexes. Journal of the American Chemical Society, 2003, 125, 8390-8399.	13.7	43
158	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for $\hat{\text{A}}$ C^-NHX Radicals. Journal of Physical Chemistry A, 2003, 107, 7985-7990.	2.5	37
159	Substituent Effects on Benzdiyne: $\hat{\text{A}}$ A Density Functional Theory Study. Journal of Organic Chemistry, 2003, 68, 5084-5090.	3.2	10
160	Low-Temperature Kinetics of Reactions of OH Radical with Ethene, Propene, and 1-Butene. Journal of Physical Chemistry A, 2003, 107, 10055-10062.	2.5	77
161	Nitroxyl Disulfides, Novel Intermediates in Transnitrosation Reactions. Journal of the American Chemical Society, 2003, 125, 6972-6976.	13.7	72
162	Peroxynitrate and Peroxynitrite: $\hat{\text{A}}$ A Complete Basis Set Investigation of Similarities and Differences between These NO _x Species. Journal of the American Chemical Society, 2003, 125, 3999-4006.	13.7	42
163	Structure, Intramolecular Rotation Barrier, and Thermochemical Properties of Hydroxycyclohexadienyl Radical. Journal of Physical Chemistry A, 2003, 107, 6451-6456.	2.5	7
164	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Methyl Ethyl, Methyl Isopropyl, and Methyl tert-Butyl Ethers and the Corresponding Radicals. Journal of Physical Chemistry A, 2003, 107, 4531-4546.	2.5	40

#	ARTICLE	IF	CITATIONS
165	Density Functional Computational Thermochemistry: Determination of the Enthalpy of Formation of Methanethial-S,S-dioxide (Sulfene). Journal of Physical Chemistry A, 2003, 107, 518-521.	2.5	11
166	Theoretical Studies of the O(3P) + Ethane Reaction. Journal of Physical Chemistry A, 2003, 107, 7161-7169.	2.5	47
167	Reactions of Silylene with Unreactive Molecules. 2. Nitrogen: Gas-Phase Kinetic and Theoretical Studies. Journal of Physical Chemistry A, 2003, 107, 9588-9593.	2.5	8
168	Computational Studies of the Chemistry of Syn Acetaldehyde Oxide. Journal of Physical Chemistry A, 2003, 107, 11525-11532.	2.5	37
169	Complexes of Hydroperoxyl Radical with Glyoxal, Methylglyoxal, Methylvinyl Ketone, Acrolein, and Methacrolein: Possible New Sinks for HO ₂ in the Atmosphere?. Journal of Physical Chemistry A, 2003, 107, 2492-2496.	2.5	29
170	Ab Initio Heat of Formation and Singlet-Triplet Splitting for Cyanocarbene (HCCN) and Isocyanocarbene (HCNC). Journal of Physical Chemistry A, 2003, 107, 4717-4723.	2.5	20
171	Reaction of Criegee Intermediates with Water Vapor: An Additional Source of OH Radicals in Alkene Ozonolysis?. Journal of Physical Chemistry A, 2003, 107, 6176-6182.	2.5	103
172	Kinetics and Thermochemistry for the Gas-Phase Keto-Enol Tautomerism of Phenol and 2,4-Cyclohexadienone. Journal of Physical Chemistry A, 2003, 107, 3696-3703.	2.5	70
173	An Assessment of Theoretical Methods for the Calculation of Accurate Structures and SN Bond Dissociation Energies of S-Nitrosothiols (RSNOs). Journal of Physical Chemistry A, 2003, 107, 9946-9952.	2.5	57
174	Experimental and theoretical studies of gas phase NO ₃ and OH radical reactions with formaldehyde, acetaldehyde and their isotopomers. Electronic supplementary information (ESI) available: program package FACSIMILE for simulation of the complex set of reactions and the kinetics of the reactor system. Kinetic data from the acetaldehyde studies, the spectral ranges and the compounds included in the subtraction procedures, and a full report of the statistical analyses. Calculated energies of the reactants, intermediates. Physical Chemistry Chemical Physics, 2003, 5, 1790-1805.	2.8	77
175	Extension of complete basis set model chemistries to molecules containing third row atoms Ga-Kr. Journal of Chemical Physics, 2003, 118, 6137-6143.	3.0	12
176	The standard enthalpy of formation of CH ₂ . Journal of Chemical Physics, 2003, 118, 10631-10642.	3.0	82
177	The reaction of OH with acetone and acetone-d ₆ from 298 to 832 K: Rate coefficients and mechanism. Journal of Chemical Physics, 2003, 119, 10600-10606.	3.0	46
178	A theoretical study of the reaction of O(3P) with an allyl radical C ₃ H ₅ . Journal of Chemical Physics, 2003, 119, 8966-8978.	3.0	31
179	Computational approaches to heats of formation. Theoretical and Computational Chemistry, 2003, 12, 247-277.	0.4	4
180	Gas-phase reactivity of lactones: structure and stability of their Cu ⁺ complexes. Molecular Physics, 2003, 101, 1249-1258.	1.7	7
181	Reactions of the Ionised Enol Tautomer of Acetanilide: Elimination of HNCO via a Novel Rearrangement. European Journal of Mass Spectrometry, 2003, 9, 343-350.	1.0	4
182	Is Allylphosphine a Carbon or a Phosphorus Base in the Gas Phase?. European Journal of Mass Spectrometry, 2003, 9, 245-255.	1.0	5

#	ARTICLE	IF	CITATIONS
183	A combined crossed beam and theoretical investigation of $O(3P)+C_3H_3\rightarrow C_3H_2+OH$. Journal of Chemical Physics, 2004, 120, 2215-2224.	3.0	20
184	Accurate energetics of small molecules containing third-row atoms Ga–Kr: A comparison of advanced ab initio and density functional theory. Journal of Chemical Physics, 2004, 121, 60.	3.0	18
185	O–H Bond Dissociation Enthalpies in Oximes: Δ Order Restored. Journal of the American Chemical Society, 2004, 126, 10667-10675.	13.7	61
186	Theoretical Study of Molecular Structure, Reactivity, Lipophilicity, and Solubility of N-Hydroxyurea, N-Hydroxythiourea, and N-Hydroxysilaurea. Structural Chemistry, 2004, 15, 285-294.	2.0	8
187	Computational Determination of Nitroaromatic Solid Phase Heats of Formation. Structural Chemistry, 2004, 15, 469-478.	2.0	32
188	Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbon–Carbon Double and Triple Bonds. Journal of Physical Chemistry A, 2004, 108, 2874-2883.	2.5	122
189	Reactions of ionised pyridazine, aminopyrazine and aminopyridine and their isomeric $\hat{\pm}$ -distonic ions. International Journal of Mass Spectrometry, 2004, 236, 1-9.	1.5	9
190	The ability of the Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO model chemistries to model the geometries of small water clusters. International Journal of Quantum Chemistry, 2004, 100, 1065-1070.	2.0	33
191	Ab initio group contribution method for activation energies for radical additions. AIChE Journal, 2004, 50, 426-444.	3.6	88
192	Association of Cu^{2+} with Uracil and Its Thio Derivatives: A Theoretical Study. ChemPhysChem, 2004, 5, 1871-1878.	2.1	66
193	Enthalpies of formation from B3LYP calculations. Journal of Computational Chemistry, 2004, 25, 725-733.	3.3	61
194	Solvent effects on glycine II. Water-assisted tautomerization. Journal of Computational Chemistry, 2004, 25, 690-703.	3.3	60
195	Protonated silanoic acid $HSi(OH)_2^+$ and its neutral counterpart: a tandem mass spectrometric and CBS-QB3 computational study. Journal of Mass Spectrometry, 2004, 39, 303-311.	1.6	4
196	Improved Reaction and Activation Energies of [4+2] Cycloadditions, [3,3] Sigmatropic Rearrangements and Electrocyclizations with the Spin-Component-Scaled MP2 Method. Chemistry - A European Journal, 2004, 10, 6468-6475.	3.3	64
197	Electron impact ionization of C_2H_6 : ionization energies and temperature effects. International Journal of Mass Spectrometry, 2004, 235, 155-162.	1.5	16
198	Heats of formation and vibrational spectra of two isomers of S_2F_2 . G2, G3, and CBS-QB3 calculations. Computational and Theoretical Chemistry, 2004, 676, 15-18.	1.5	8
199	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the flavonoid quercetin. Computational and Theoretical Chemistry, 2004, 681, 71-76.	1.5	55
200	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of the antiparasitic drug meglumine. Computational and Theoretical Chemistry, 2004, 681, 77-82.	1.5	20

#	ARTICLE	IF	CITATIONS
201	CHIH-DFT determination of the molecular structure, infrared and ultraviolet spectra of potentially organic corrosion inhibitors. Computational and Theoretical Chemistry, 2004, 681, 83-88.	1.5	35
202	Basis set effects on the energy of intramolecular Oâ€“Hâ€“halogen hydrogen bridges in ortho-halophenols and 2,4-dihalo-malonaldehyde. Chemical Physics, 2004, 300, 107-117.	1.9	9
203	The ionic isomerization [HCOH]+â†’[CH2â€“...O]+: proton-transport catalysis by CO and CO2. Chemical Physics Letters, 2004, 387, 204-208.	2.6	19
204	Fragmentation Pathways in a Series of CH3COX Molecules in the Strong Field Regimeâ€“. Journal of Physical Chemistry A, 2004, 108, 3162-3165.	2.5	17
205	Theoretical Analysis of Lewis Basicity Based on Local Electron-Donating Ability. Origin of Basic Strength of Cyclic Amines. Journal of Organic Chemistry, 2004, 69, 7486-7494.	3.2	61
206	An experimental and theoretical dissection of potassium cation-glycine interactionsElectronic supplementary information (ESI) available: Fig. S1 shows a complete set of figures for collision-induced dissociation of six potassiated complexes with Xe. Table S1 lists vibrational frequencies and average vibrational energies at 298 K of the neutral molecules and potassiated complexes determined from vibrational analysis at the MP2(full)/6-31G(d) level. Table S2 lists rotational constants for the potassiated comp. Physical Chemistry Chemical Physics, 2004, 6, 2588.	2.8	73
207	Reaction kinetics of the addition of atomic sulfur to nitric oxide. Journal of Chemical Physics, 2004, 121, 9999-10005.	3.0	17
208	Computational Study of the Oxygen Initiated Decomposition of 2-Oxepinoxy Radical:â€“ A Key Intermediate in the Oxidation of Benzene. Journal of Physical Chemistry A, 2004, 108, 8419-8433.	2.5	20
209	Mechanisms of Peroxynitrous Acid and Methyl Peroxynitrite, ROONO (R = H, Me), Rearrangements:â€“ A Conformation-Dependent Homolytic Dissociation. Journal of Physical Chemistry A, 2004, 108, 5864-5871.	2.5	77
210	Reliable Theoretical Procedures for the Calculation of Electronic-Structure Information in Hydrogen Abstraction Reactions. Journal of Physical Chemistry A, 2004, 108, 3865-3872.	2.5	148
211	Low Energy Dissociation Processes of Ionized Cyclohexene:â€“ A Theoretical Insightâ€“,â€“. Journal of Physical Chemistry A, 2004, 108, 9853-9862.	2.5	10
212	Nitroacetylene:â€“ Computed Heats of Formation and Analysis of Reaction Mechanisms with Vinyl Ethers. Journal of Physical Chemistry A, 2004, 108, 3493-3498.	2.5	2
213	An Assessment of Theoretical Protocols for Calculation of the pKa Values of the Prototype Imidazolium Cation. Australian Journal of Chemistry, 2004, 57, 1205.	0.9	85
214	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.	3.2	84
215	Thermodynamics of Forming Water Clusters at Various Temperatures and Pressures by Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO Model Chemistries; Implications for Atmospheric Chemistry. Journal of the American Chemical Society, 2004, 126, 2647-2653.	13.7	155
216	Thermochemistry of Siliconâ€“Hydrogen Compounds Generalized from Quantum Chemical Calculations. Journal of Physical Chemistry A, 2004, 108, 874-897.	2.5	51
217	Accurate Experimental Values for the Free Energies of Hydration of H+, OH-, and H3O+. Journal of Physical Chemistry A, 2004, 108, 3692-3694.	2.5	135
218	Energetics of Intramolecular Hydrogen Bonding in Di-substituted Benzenes by the orthoâ€“para Method. Journal of Physical Chemistry A, 2004, 108, 10834-10843.	2.5	94

#	ARTICLE	IF	CITATIONS
219	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2475-2486.	2.5	70
220	Thermochemical Properties, Pathway, and Kinetic Analysis on the Reactions of Benzene with OH: An Elementary Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4632-4652.	2.5	49
221	Steric Retardation of SN2 Reactions in the Gas Phase and Solution. <i>Journal of the American Chemical Society</i> , 2004, 126, 9054-9058.	13.7	174
222	Basicity of Nucleophilic Carbenes in Aqueous and Nonaqueous Solvents Theoretical Predictions. <i>Journal of the American Chemical Society</i> , 2004, 126, 8717-8724.	13.7	426
223	The isomerization of $[H_2O \cdots C\tilde{} \cdots O]^+$ and $[HC(\tilde{} \cdots O)OH]^+$ into $[HO \cdots C \cdots OH]^+$: proton-transport catalysis by CO. <i>Chemical Physics Letters</i> , 2004, 390, 176-180.	2.6	16
224	Energy and Stability of Protonated Ketenes: Inductive and Resonance Effects. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 791-799.	1.0	2
225	The Formation and Heats of Formation of Simple $\hat{\pm}$ -Distonic Ions. <i>European Journal of Mass Spectrometry</i> , 2004, 10, 775-782.	1.0	4
226	Differentiation of Ionised Benzimidazole from its Isomeric $\hat{\pm}$ -Distonic Ion by Collision-Induced Dissociation and Neutralisation-Reionisation Mass Spectrometry. <i>European Journal of Mass Spectrometry</i> , 2005, 11, 381-387.	1.0	3
227	Rate constants for the abstraction reactions $RO_2 + C_2H_6$; $R = H, CH_3$, and C_2H_5 . <i>Proceedings of the Combustion Institute</i> , 2005, 30, 995-1003.	3.9	41
228	Theoretical studies of the reaction of hydroperoxy radicals (HO_2) with ethyl peroxy ($CH_3CH_2O_2$), acetyl peroxy ($CH_3C(O)O_2$), and acetonyl peroxy ($CH_3C(O)CH_2O_2$) radicals. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2005, 176, 218-230.	3.9	57
229	A computational study of alkane hydrogen-exchange reactions on zeolites. <i>Journal of Molecular Catalysis A</i> , 2005, 242, 18-25.	4.8	20
230	Ab initio studies of isomerization and dissociation reactions of peroxyacetyl nitrate (PAN). <i>Chemical Physics</i> , 2005, 312, 241-259.	1.9	6
231	DFT study of the thermochemistry of gas-phase 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (\hat{i}^2 -HMX). <i>Computational and Theoretical Chemistry</i> , 2005, 714, 147-152.	1.5	26
232	CHIH-DFT study of the electronic properties and chemical reactivity of quercetin. <i>Computational and Theoretical Chemistry</i> , 2005, 716, 67-72.	1.5	67
233	CHIH-DFT determination of the electrical, optical, and magnetic properties and NICS aromaticity of megazol. <i>Computational and Theoretical Chemistry</i> , 2005, 717, 1-3.	1.5	19
234	High-level calculations of the enthalpy of formation of diazomethane. <i>Computational and Theoretical Chemistry</i> , 2005, 722, 213-215.	1.5	5
235	DFT and ab initio direct dynamics study on the reaction of H_2 loss reaction from H_2BNH_2 . <i>Computational and Theoretical Chemistry</i> , 2005, 717, 33-39.	1.5	14
236	New potential high-energy materials: Oxadiaziridine, N_2H_2O . High-level calculations. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 19-23.	1.5	14

#	ARTICLE	IF	CITATIONS
237	Oxygenâ€“oxygen bond dissociation enthalpies of di-tert-butyl peroxide and di-trifluoromethyl peroxide. Computational and Theoretical Chemistry, 2005, 729, 223-227.	1.5	14
238	Cyclic diamines as potential high energy materials. Thermochemical properties of diaziridine, 1,2-diazetidione, and 1,3-diazetidione. Computational and Theoretical Chemistry, 2005, 730, 95-103.	1.5	19
239	Cyclic triamines as potential high energy materials. Thermochemical properties of triaziridine and triazirine. Computational and Theoretical Chemistry, 2005, 732, 47-53.	1.5	11
240	Potential energy surface survey towards prediction of a new radical [H2,Si,C,N]. Chemical Physics, 2005, 316, 205-216.	1.9	5
241	Electron impact ionization of C3H8: appearance energies and temperature effects. Chemical Physics Letters, 2005, 402, 80-87.	2.6	15
242	Thermochemistry of reactive nitrogen oxide species and reaction enthalpies for decomposition of ONOOâ€” and ONOOH. Chemical Physics Letters, 2005, 403, 192-197.	2.6	9
243	Linear regression correction to first principle theoretical calculations â€“ Improved descriptors and enlarged training set. Chemical Physics Letters, 2005, 409, 315-321.	2.6	9
244	Neural network correction for heats of formation with a larger experimental training set and new descriptors. Chemical Physics Letters, 2005, 410, 125-130.	2.6	34
245	Density functional characterization of the potential energy surface of the NO2+Br reaction. Chemical Physics Letters, 2005, 413, 36-41.	2.6	5
246	A â€“universalâ€” B3LYP-based method for gas-phase molecular properties: bond dissociation enthalpy, ionization potential, electron and proton affinity and gas-phase acidity. Molecular Physics, 2005, 103, 815-823.	1.7	69
247	Silanes/Oxygen/(Water): Green High-Energy-Density Materials. European Journal of Inorganic Chemistry, 2005, 2005, 3131-3134.	2.0	9
248	Activation Energies and Reaction Energetics for 1,3-Dipolar Cycloadditions of Hydrazoic Acid with CÎ£;C and CÎ£;N Multiple Bonds from High-Accuracy and Density Functional Quantum Mechanical Calculations. Helvetica Chimica Acta, 2005, 88, 1702-1710.	1.6	28
249	Assessment of Performance of G3B3 and CBS-QB3 Methods in Calculation of Bond Dissociation Energies. Chinese Journal of Chemistry, 2005, 23, 194-199.	4.9	37
250	C5H4?BR2 Bending in Ferrocenylboranes: A Delocalized Through-Space Interaction Between Iron and Boron. Chemistry - A European Journal, 2005, 11, 584-603.	3.3	131
251	An ab initio study of ethane conversion reactions on zeolites using the complete basis set composite energy method. Journal of Molecular Catalysis A, 2005, 229, 77-85.	4.8	34
252	The acid-catalyzed rearrangement CH3Oâ†’CH2OH and its involvement in the dissociation of the methanol dimer radical cation. International Journal of Mass Spectrometry, 2005, 242, 49-56.	1.5	14
253	Structural Nonrigidity of the 1,2,3-Trifluorobenzene Radical Anion as Probed by Quantum-Chemical Methods and OD ESR. Doklady Physical Chemistry, 2005, 403, 142-145.	0.9	0
254	The FC(O)OF torsional potential: thermochemistry and kinetics. Journal of Molecular Structure, 2005, 737, 83-89.	3.6	1

#	ARTICLE	IF	CITATIONS
255	Pople's Gaussian-3 model chemistry applied to an investigation of (H ₂ O) ₈ water clusters. International Journal of Quantum Chemistry, 2005, 102, 565-572.	2.0	38
256	Theoretical study of reaction channels for the weakly bound complex systems created with HF, CO ₂ , and various amines. International Journal of Quantum Chemistry, 2005, 103, 198-214.	2.0	0
257	Comparison of density functional theory predictions of gas-phase deprotonation data. International Journal of Quantum Chemistry, 2005, 105, 580-587.	2.0	43
258	Computational prediction of standard gas, liquid, and solid-phase heats of formation and heats of vaporization and sublimation. International Journal of Quantum Chemistry, 2005, 105, 341-347.	2.0	119
259	G2, G3 and associated quantum chemical models for accurate theoretical thermochemistry. , 2005, , 785-812.		5
260	Structures of alateborane(10) and gallatetraalane(10) isomers. Molecular Physics, 2005, 103, 1139-1149.	1.7	2
261	Ab Initio MO Study on the Reaction Mechanism of Reduction of Hypophosphorous Acid. Journal of the Electrochemical Society, 2005, 152, C861.	2.9	3
262	The Gas-Phase Acidity of 2(3H)-Oxepinone: A Step toward an Experimental Heat of Formation for the 2-Oxepinoxy Radical. Journal of the American Chemical Society, 2005, 127, 7466-7473.	13.7	15
263	Chapter 3 Computational Thermochemistry: A Brief Overview of Quantum Mechanical Approaches. Annual Reports in Computational Chemistry, 2005, 1, 31-43.	1.7	46
264	Protonation Thermochemistry of Selected Hydroxy- and Methoxycarbonyl Molecules. Journal of Physical Chemistry A, 2005, 109, 11851-11859.	2.5	9
265	Intramolecular Hydrogen Bonding and Hydrogen Atom Abstraction in Gas-Phase Aliphatic Amine Radical Cations. Journal of Physical Chemistry A, 2005, 109, 12046-12053.	2.5	22
266	Nitrosonium-Catalyzed Decomposition of S-Nitrosothiols in Solution: A Theoretical and Experimental Study. Journal of the American Chemical Society, 2005, 127, 10917-10924.	13.7	27
267	Synchrotron photoionization measurements of combustion intermediates: Photoionization efficiency and identification of C ₃ H ₂ isomers. Physical Chemistry Chemical Physics, 2005, 7, 806.	2.8	113
268	The investigation of hydrocarbon cracking reaction energetics with composite energy methods. Molecular Simulation, 2005, 31, 979-986.	2.0	4
269	Application of compound models for estimating rate constants of hydrocarbon thermal cracking reactions: The neopentyl radical β -scission reaction. Molecular Simulation, 2005, 31, 615-621.	2.0	7
270	Energetics of Hydroxybenzoic Acids and of the Corresponding Carboxyphenoxy Radicals. Intramolecular Hydrogen Bonding in 2-Hydroxybenzoic Acid. Journal of Physical Chemistry A, 2005, 109, 9700-9708.	2.5	33
271	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide (DMPO). 1. The Thermodynamics of Formation and Its Acidity. Journal of Physical Chemistry A, 2005, 109, 6083-6088.	2.5	53
272	Dissociation of Benzene Dication [C ₆ H ₆] ²⁺ : Exploring the Potential Energy Surface. Journal of Physical Chemistry A, 2005, 109, 11551-11559.	2.5	27

#	ARTICLE	IF	CITATIONS
273	Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrrolineN-Oxide (DMPO). 2. The Thermodynamics of Decay and EPR Spectral Properties. Journal of Physical Chemistry A, 2005, 109, 6089-6098.	2.5	58
274	Detailed Modeling of the Reaction of C ₂ H ₅ + O ₂ . Journal of Physical Chemistry A, 2005, 109, 2264-2281.	2.5	65
275	Experimental and Theoretical Studies of the C ₂ F ₄ + O Reaction:â€‰ Nonadiabatic Reaction Mechanism. Journal of Physical Chemistry A, 2005, 109, 9786-9794.	2.5	7
276	Metal Ion Binding by a Bicyclic Diamide:â€‰ Deep UV Raman Spectroscopic Characterization. Journal of Physical Chemistry A, 2005, 109, 7094-7098.	2.5	5
277	Benchmark Calculations of Reaction Energies, Barrier Heights, and Transition-State Geometries for Hydrogen Abstraction from Methanol by a Hydrogen Atom. Journal of Physical Chemistry A, 2005, 109, 773-778.	2.5	57
278	pK _a of Acetate in Water:â€‰ A Computational Study. Journal of Physical Chemistry A, 2005, 109, 10776-10785.	2.5	56
279	Comparison of Model Chemistry and Density Functional Theory Thermochemical Predictions with Experiment for Formation of Ionic Clusters of the Ammonium Cation Complexed with Water and Ammonia; Atmospheric Implications. Journal of Physical Chemistry A, 2005, 109, 4905-4910.	2.5	54
280	Thermochemical and Kinetic Analyses on Oxidation of Isobutenyl Radical and 2-Hydroperoxymethyl-2-propenyl Radical. Journal of Physical Chemistry A, 2005, 109, 9044-9053.	2.5	21
281	Quantum Chemical and Master Equation Simulations of the Oxidation and Isomerization of Vinyloxy Radicals. Journal of Physical Chemistry A, 2005, 109, 2514-2524.	2.5	43
282	Structures and Thermochemistry of Calcium-Containing Molecules. Journal of Physical Chemistry A, 2005, 109, 9156-9168.	2.5	17
283	Theoretical Determinations of the Ambient Conformational Distribution and Unimolecular Decomposition of n-Propylperoxy Radical. Journal of Physical Chemistry A, 2005, 109, 3637-3646.	2.5	36
284	Theoretical Study on the Reaction Mechanism of Vinyl Radical with Formaldehyde. Journal of Physical Chemistry A, 2005, 109, 8419-8423.	2.5	11
285	The Reaction of Triplet Nitrenes with Oxygen:â€‰ A Computational Study. Organic Letters, 2005, 7, 549-552.	4.6	38
286	Mechanistic Studies on the Cyclization of (Z)-1,2,4-Heptatrien-6-yne in Methanol:â€‰ A Possible Nonadiabatic Thermal Reaction. Journal of the American Chemical Society, 2005, 127, 6652-6661.	13.7	34
287	Infrared Spectra of a Species of Astrochemical Interest:â€‰ Aminoacrylonitrile (3-Amino-2-propenenitrile). Journal of Physical Chemistry A, 2005, 109, 4705-4712.	2.5	22
288	Mechanistic Insights into the Bazarov Synthesis of Urea from NH ₃ and CO ₂ Using Electronic Structure Calculation Methods. Journal of Physical Chemistry A, 2005, 109, 8560-8567.	2.5	43
289	CH ₂ CHOH ₂ ⁺⁺ + PN:â€‰ A Proton-Transfer Triple Play. Journal of Physical Chemistry A, 2005, 109, 6326-6334.	2.5	11
290	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	2.5	72

#	ARTICLE	IF	CITATIONS
291	Observation of the $\tilde{\sigma} \rightarrow \pi^*$ Electronic Transition of the 1-C ₃ H ₇ O ₂ and 2-C ₃ H ₇ O ₂ Radicals Using Cavity Ringdown Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1308-1315.	2.5	34
292	Multicoefficient Extrapolated Density Functional Theory Studies of π - π Interactions: The Benzene Dimer. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4209-4212.	2.5	99
293	Modeling β -Scission Reactions of Peptide Backbone Alkoxy Radicals: Backbone C-C Bond Fission. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 889-899.	5.3	6
294	Activation Energies of Pericyclic Reactions: Performance of DFT, MP2, and CBS-QB3 Methods for the Prediction of Activation Barriers and Reaction Energetics of 1,3-Dipolar Cycloadditions, and Revised Activation Enthalpies for a Standard Set of Hydrocarbon Pericyclic Reactions. <i>Journal of Physical Chemistry A</i> , 2005, 109, 9542-9553.	2.5	233
295	π -Aromaticity and π -Antiaromaticity in Saturated Inorganic Rings. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3711-3716.	2.5	60
296	Potential Energy Surfaces, Product Distributions and Thermal Rate Coefficients of the Reaction of O(3P) with C ₂ H ₄ (X1Ag): A Comprehensive Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7489-7499.	2.5	91
297	Boric acid, α -carbonic acid, and N-containing oxyacids in aqueous solution: Ab initio studies of structure, pKa, NMR shifts, and isotopic fractionations. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 5647-5658.	3.9	52
298	Benchmark calculations of proton affinities and gas-phase basicities of molecules important in the study of biological phosphoryl transfer. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 3070.	2.8	76
299	Generation of peroxyxynitrite from reaction of N-acetyl-N-nitrosotryptophan with hydrogen peroxide over a wide range of pH values. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 2085.	2.8	18
300	Mechanisms of Thermal Decompositions of Polysulfones: A DFT and CBS-QB3 Study. <i>Macromolecules</i> , 2005, 38, 10279-10285.	4.8	24
301	Absolute Calculations of Acidity of C-Substituted Tetrazoles in Solution. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5590-5595.	2.5	43
302	Accurate ab initio predictions of ionization energies of hydrocarbon radicals: CH ₂ , CH ₃ , C ₂ H, C ₂ H ₃ , C ₂ H ₅ , C ₃ H ₃ , and C ₃ H ₅ . <i>Journal of Chemical Physics</i> , 2005, 122, 224310.	3.0	51
303	Theoretical Reduction Potentials for Nitrogen Oxides from CBS-QB3 Energetics and (C)PCM Solvation Calculations. <i>Inorganic Chemistry</i> , 2005, 44, 4024-4028.	4.0	82
304	Intramolecular Dynamics of 1,2,3-Trifluorobenzene Radical Anions As Studied by OD ESR and Quantum-Chemical Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4404-4409.	2.5	26
305	On the Electrophilicity of Hydroxyl Radical: A Laser Flash Photolysis and Computational Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 7094-7109.	13.7	89
306	Accurate Calculation of the Heats of Formation for Large Main Group Compounds with Spin-Component Scaled MP2 Methods. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3067-3077.	2.5	241
307	Intrinsic Conformational Preferences of Substituted Cyclohexanes and Tetrahydropyrans Evaluated at the CCSD(T) Complete Basis Set Limit: Implications for the Anomeric Effect. <i>Journal of Physical Chemistry A</i> , 2005, 109, 11073-11079.	2.5	58
308	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.	2.5	56

#	ARTICLE	IF	CITATIONS
309	Global Search for Minimum Energy (H ₂ O) _n Clusters, n = 3~5. Journal of Physical Chemistry A, 2005, 109, 6773-6778.	2.5	89
310	Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. Journal of Chemical Physics, 2005, 122, 024302.	3.0	57
311	Reactivity of Alkanes on Zeolites: A Computational Study of Propane Conversion Reactions. Journal of Physical Chemistry A, 2005, 109, 10734-10741.	2.5	45
312	The Chiral Molecule CHClFI: First Determination of Its Molecular Parameters by Fourier Transform Microwave and Millimeter-Wave Spectroscopies Supplemented by ab Initio Calculations. Journal of Physical Chemistry A, 2005, 109, 5708-5716.	2.5	14
313	Thermochemistry Is Not a Lower Bound to the Activation Energy of Endothermic Reactions: A Kinetic Study of the Gas-Phase Reaction of Atomic Chlorine with Ammonia. Journal of Physical Chemistry A, 2006, 110, 6844-6850.	2.5	34
314	Energetics of Xylose Decomposition as Determined Using Quantum Mechanics Modeling. Journal of Physical Chemistry A, 2006, 110, 11824-11838.	2.5	140
315	Consistent Theoretical Description of 1,3-Dipolar Cycloaddition Reactions. Journal of Physical Chemistry A, 2006, 110, 2583-2586.	2.5	95
316	Conformational and Orientational Guidance of the Analgesic Dipeptide Kyotorphin Induced by Lipidic Membranes: Putative Correlation toward Receptor Docking. Journal of Physical Chemistry B, 2006, 110, 3385-3394.	2.6	17
317	Quantum Chemical Investigation of Low-Temperature Intramolecular Hydrogen Transfer Reactions of Hydrocarbons. Journal of Physical Chemistry A, 2006, 110, 10863-10871.	2.5	60
318	Theoretical Study of the Reduction Mechanism of Sulfoxides by Thiols. Journal of Physical Chemistry A, 2006, 110, 7628-7636.	2.5	33
319	The Special Five-Membered Ring of Proline: An Experimental and Theoretical Investigation of Alkali Metal Cation Interactions with Proline and Its Four- and Six-Membered Ring Analogues. Journal of Physical Chemistry A, 2006, 110, 3933-3946.	2.5	82
320	Chlorofluoroiodomethane as a potential candidate for parity violation measurements. Physical Chemistry Chemical Physics, 2006, 8, 79-92.	2.8	46
321	Matrix isolation and computational study of the photochemistry of p-azidoaniline. Physical Chemistry Chemical Physics, 2006, 8, 719-727.	2.8	42
322	Mechanism for Catechol Ring Cleavage by Non-Heme Iron Intradiol Dioxygenases: A Hybrid DFT Study. Journal of the American Chemical Society, 2006, 128, 12941-12953.	13.7	82
323	Mechanisms of Glycerol Dehydration. Journal of Physical Chemistry A, 2006, 110, 6145-6156.	2.5	239
324	A computational exploration of some transnitrosation and thiolation reactions involving CH ₃ SNO, CH ₃ ONO and CH ₃ NHNO. Organic and Biomolecular Chemistry, 2006, 4, 1352.	2.8	11
325	Gas-Phase Deprotonation of Uracil~Cu ²⁺ and Thiouracil~Cu ²⁺ Complexes. Journal of Physical Chemistry A, 2006, 110, 1943-1950.	2.5	69
326	Ab Initio Procedure for Aqueous-Phase pK _a Calculation: The Acidity of Nitrous Acid. Journal of Physical Chemistry A, 2006, 110, 11371-11376.	2.5	97

#	ARTICLE	IF	CITATIONS
327	Active Thermochemical Tables: Accurate Enthalpy of Formation of Hydroperoxyl Radical, HO ₂ . Journal of Physical Chemistry A, 2006, 110, 6592-6601.	2.5	255
328	Radical radical reaction dynamics: A combined crossed-beam and theoretical study. International Reviews in Physical Chemistry, 2006, 25, 613-653.	2.3	27
329	Generation of Oxynitrenes and Confirmation of Their Triplet Ground States. Journal of the American Chemical Society, 2006, 128, 13142-13150.	13.7	29
330	Gas-Phase Generation and Electronic Structure Investigation of Chlorosulfanyl Thiocyanate, ClSSCN. Inorganic Chemistry, 2006, 45, 5971-5975.	4.0	23
331	Macroscopic pK _a Calculations for Fluorescein and Its Derivatives. Journal of Chemical Theory and Computation, 2006, 2, 1520-1529.	5.3	49
332	Quantum Chemical and Statistical Rate Study of the Reaction of O(3P) with Allene: O-Addition and H-Abstraction Channels. Journal of Physical Chemistry A, 2006, 110, 12166-12176.	2.5	24
333	Detailed Kinetic Study of the Ring Opening of Cycloalkanes by CBS-QB3 Calculations. Journal of Physical Chemistry A, 2006, 110, 12693-12704.	2.5	97
334	A Single Transition State Serves Two Mechanisms. The Branching Ratio for CH ₂ O + CH ₃ Cl on Improved Potential Energy Surfaces. Journal of Physical Chemistry A, 2006, 110, 2801-2806.	2.5	20
335	Normal Modes of Redox-Active Tyrosine: Conformation Dependence and Comparison to Experiment. Journal of Physical Chemistry B, 2006, 110, 10970-10981.	2.6	31
336	Quantum Chemical and Theoretical Kinetics Study of the O(3P) + C ₂ H ₂ Reaction: A Multistate Process. Journal of Physical Chemistry A, 2006, 110, 6696-6706.	2.5	48
337	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	2.5	52
338	Effect of Side Chains on Competing Pathways for β -Scission Reactions of Peptide-Backbone Alkoxy Radicals. Journal of Physical Chemistry A, 2006, 110, 10316-10323.	2.5	19
339	High-Temperature Reactions of OH Radicals with Benzene and Toluene. Journal of Physical Chemistry A, 2006, 110, 5081-5090.	2.5	118
340	Kinetic Modeling of the Propyl Radical β -Scission Reaction: An Application of Composite Energy Methods. Industrial & Engineering Chemistry Research, 2006, 45, 530-535.	3.7	10
341	First-Principle Kinetic Modeling of the 1-Chloroethyl Unimolecular Decomposition Reaction. Industrial & Engineering Chemistry Research, 2006, 45, 2981-2985.	3.7	2
342	Multilevel and Density Functional Electronic Structure Calculations of Proton Affinities and Gas-Phase Basicities Involved in Biological Phosphoryl Transfer. Journal of Physical Chemistry A, 2006, 110, 791-797.	2.5	17
343	Conformational Flexibility of Alanine Zwitterion Determines Shapes of Raman and Raman Optical Activity Spectral Bands. Journal of Physical Chemistry A, 2006, 110, 4689-4696.	2.5	90
344	Enthalpy of Formation of the Cyclopentadienyl Radical: Photoacoustic Calorimetry and ab Initio Studies. Journal of Physical Chemistry A, 2006, 110, 5130-5134.	2.5	22

#	ARTICLE	IF	CITATIONS
345	Accurate Heats of Formation of the σ -Arduengo-Type Carbene and Various Adducts Including H ₂ from ab Initio Molecular Orbital Theory. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1968-1974.	2.5	48
346	Thionitroxides, RSNHO: The Structure of the SNO Moiety in σ -S-Nitrosohemoglobin, A Possible NO Reservoir and Transporter. <i>Journal of the American Chemical Society</i> , 2006, 128, 1422-1423.	13.7	31
347	Primary Mechanism of the Thermal Decomposition of Tricyclodecane. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11298-11314.	2.5	82
348	Collision-Induced Dissociation of HS-(HCN): An Unsymmetrical Hydrogen Bonding in a Proton-Bound Dimer Anion. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1342-1349.	2.5	13
349	H ₂ CO ₃ and Its Oligomers: Structures, Stabilities, Vibrational and NMR Spectra, and Acidities. <i>Inorganic Chemistry</i> , 2006, 45, 5961-5970.	4.0	46
350	Reactivity of Isobutane on Zeolites: A First Principles Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2455-2460.	2.5	45
351	Reactions of F+(3P) and F+(1D) with Silicon Oxide. Possibility of Spin-Forbidden Processes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7130-7137.	2.5	0
352	Boric acid adsorption on humic acids: Ab initio calculation of structures, stabilities, ¹¹ B NMR and ¹¹ B, ¹⁰ B isotopic fractionations of surface complexes. <i>Geochimica Et Cosmochimica Acta</i> , 2006, 70, 5089-5103.	3.9	43
353	Intramolecular Hydrogen Bonds. Methodologies and Strategies for Their Strength Evaluation. , 2006, , 51-107.		16
354	Assessment of Model Chemistries for Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1009-1018.	5.3	214
355	Effect of Metal Ions (Li ⁺ , Na ⁺ , K ⁺ , Mg ²⁺ , Ca ²⁺ , Ni ²⁺ , Cu ²⁺ , and Zn ²⁺) and Water Coordination on the Structure of Glycine and Zwitterionic Glycine. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1960-1967.	2.5	140
356	The correlation consistent composite approach (ccCA): An alternative to the Gaussian-n methods. <i>Journal of Chemical Physics</i> , 2006, 124, 114104.	3.0	269
357	Stabilization Energies of Extensively Conjugated Propargylic Radicals. <i>Journal of Organic Chemistry</i> , 2006, 71, 2214-2219.	3.2	15
358	Theoretical Comparison of the Linear and Bent Structures for the Weakly Bound CO ₂ -HF Complex. <i>Journal of the Chinese Chemical Society</i> , 2006, 53, 519-530.	1.4	1
359	Protonation thermochemistry of aminoacetonitrile. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 1187-1191.	1.5	5
360	Theoretical influence of third molecule on reaction channels of weakly bound complex CO ₂ -HF systems. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1640-1652.	2.0	2
361	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3122-3128.	2.0	29
362	On the stability of non-conventional π -complexes between Ni ⁺ and toluene, phenyl-silane and phenyl-germane. <i>Journal of Physical Organic Chemistry</i> , 2006, 19, 495-502.	1.9	3

#	ARTICLE	IF	CITATIONS
381	A theoretical examination of the isomerization of BrONO ₂ to BrOONO. Chemical Physics, 2006, 323, 369-375.	1.9	5
382	Computational study of keto↔enol equilibria of tropolone in gas and aqueous solution phase. Chemical Physics, 2006, 331, 61-66.	1.9	15
383	Gas-Phase Protonation and Deprotonation of Acrylonitrile Derivatives Ni _{1/2} Ci _{1/2} CHi _{3/4} CHi _{1/2} X (X=CH ₃ , NH ₂ ,) Tj ETQo 0 0 0 rgBT /Overlo	3.3	17
384	Formation of Phosphaethyne Dimers: A Mechanistic Study. Chemistry - A European Journal, 2006, 12, 8044-8055.	3.3	15
385	First Experimental Observation of Gas-Phase Nitrosyl Thiocyanate. European Journal of Inorganic Chemistry, 2006, 2006, 2469-2475.	2.0	21
386	Theoretical study on structures and stabilities of [H,Ge,C,N]. Journal of Computational Chemistry, 2006, 27, 505-514.	3.3	4
387	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. ChemPhysChem, 2006, 7, 1119-1126.	2.1	53
388	The Origin of Systematic Error in the Standard Enthalpies of Formation of Hydrocarbons Computed via Atomization Schemes. ChemPhysChem, 2006, 7, 1664-1667.	2.1	45
389	A Theoretical Investigation of the Gas-Phase Oxidation Reaction of the Saturated tert-Butyl Radical. ChemPhysChem, 2006, 7, 2526-2532.	2.1	10
390	Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer. Helvetica Chimica Acta, 2006, 89, 2254-2272.	1.6	39
391	Conceptual, Qualitative, and Quantitative Theories of 1,3-Dipolar and Diels-Alder Cycloadditions Used in Synthesis. Advanced Synthesis and Catalysis, 2006, 348, 2337-2361.	4.3	273
392	Kinetic modeling of tert-butyl radical decomposition reaction. AIChE Journal, 2006, 52, 3216-3221.	3.6	3
393	Adsorption of Oleic Acid on Silica Gel Derived from Rice Ash Hulls: Experimental and Theoretical Studies. Adsorption Science and Technology, 2006, 24, 797-814.	3.2	10
394	The evaluation of bond dissociation energies for NO ₂ scission in nitro compounds using density functional and complete basis set methods. Chinese Physics B, 2006, 15, 329-333.	1.3	7
395	Accurate ab initio predictions of ionization energies and heats of formation for the 2-propyl, phenyl, and benzyl radicals. Journal of Chemical Physics, 2006, 124, 044323.	3.0	26
396	The correlation-consistent composite approach: Application to the G3/99 test set. Journal of Chemical Physics, 2006, 125, 104111.	3.0	134
398	A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106.	3.0	208
399	Accurate ab initio Predictions of Ionization Energies and Heats of Formation for Cyclopropenylidene, Propargylene and Propadienylidene. Chinese Journal of Chemical Physics, 2006, 19, 29-38.	1.3	30

#	ARTICLE	IF	CITATIONS
400	THEORETICAL CALCULATION OF BOND DISSOCIATION ENERGIES AND HEATS OF FORMATION FOR ALKYL NITRATE AND NITRITE COMPOUNDS WITH DENSITY FUNCTIONAL THEORY AND COMPLETE BASIS SET METHOD. Journal of Theoretical and Computational Chemistry, 2007, 06, 449-458.	1.8	5
401	THE ORIGIN OF THE ROTATIONAL BARRIER IN DIMETHYL ETHER AND DIMETHYL SULFIDE: A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2007, 06, 421-434.	1.8	2
402	ASSOCIATION OF URACIL WITH Zn ²⁺ AND THE HYDRATED Zn ²⁺ : A DFT INVESTIGATION. Journal of Theoretical and Computational Chemistry, 2007, 06, 197-212.	1.8	1
403	Experimental and theoretical studies of the electronic structure and the ionization and dissociation processes of trifluoromethyl peroxyxynitrate. Journal of Chemical Physics, 2007, 126, 184301.	3.0	4
404	Theoretical prediction of the ionization energies of the C ₄ H ₇ radicals: 1-Methylallyl, 2-methylallyl, cyclopropylmethyl, and cyclobutyl radicals. Journal of Chemical Physics, 2007, 127, 154302.	3.0	12
405	Performance of the correlation consistent composite approach for transition states: A comparison to G3B theory. Journal of Chemical Physics, 2007, 127, 154117.	3.0	34
406	Potential Energy Surfaces of Nitrogen Dioxide for the Ground State. Chinese Physics Letters, 2007, 24, 1879-1882.	3.3	0
407	Raman spectra, ab initio calculations, phase transitions and conformations of 1,3-disilabutane. Phase Transitions, 2007, 80, 529-538.	1.3	2
408	Potential energy surfaces of ozone in the ground state. Chinese Physics B, 2007, 16, 2650-2655.	1.3	4
409	Halogenated Methyl Nitrates, CX ₃ ONO ₂ (X = F, Cl). A Computational Study of their Properties and Capacity to Act as Sink Compounds in the Troposphere. AIP Conference Proceedings, 2007, , .	0.4	0
410	Quantum Mechanics for Organic Chemistry. , 0, , 1-41.		1
411	Gas-phase reaction thermodynamics in preparation of pyrolytic carbon by propylene pyrolysis. Computational Materials Science, 2007, 40, 504-524.	3.0	11
412	Mass spectrometric and quantum chemical determination of proton water clustering equilibria. Geochimica Et Cosmochimica Acta, 2007, 71, 2436-2447.	3.9	21
413	Gas phase protonation of \hat{I}^{\pm} , \hat{I}^2 and \hat{I}^3 -dicarbonyls: Thermochemistry and structures. International Journal of Mass Spectrometry, 2007, 267, 63-80.	1.5	10
414	A theoretical study of hydration effects on the prototropic tautomerism of selenouracils. Organic and Biomolecular Chemistry, 2007, 5, 3092.	2.8	22
415	Energetics of Cresols and of Methylphenoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 8741-8748.	2.5	25
416	Amide Resonance Correlates with a Breadth of C ¹⁵ N Rotation Barriers. Journal of the American Chemical Society, 2007, 129, 2521-2528.	13.7	246
417	Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	2.5	101

#	ARTICLE	IF	CITATIONS
418	QM/MM Metadynamics Study of the Direct Decarboxylation Mechanism for Orotidine-5'-monophosphate Decarboxylase Using Two Different QM Regions: Acceleration Too Small To Explain Rate of Enzyme Catalysis. Journal of Physical Chemistry B, 2007, 111, 12573-12581.	2.6	53
419	Mechanism of Formation of Silver N -Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. Organometallics, 2007, 26, 6170-6183.	2.3	58
420	Theoretical Study of the Thermodynamics and Kinetics of Hydrogen Abstractions from Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 11771-11786.	2.5	134
421	Theoretical and spectroscopic study of the reaction of diethylhydroxylamine on silicon(100)-2Å-1. Physical Chemistry Chemical Physics, 2007, 9, 1629-1634.	2.8	10
422	Conformational Properties of 1-Fluoro-1-silacyclohexane, $\text{C}_5\text{H}_{10}\text{SiHF}$: Gas Electron Diffraction, Low-Temperature NMR, Temperature-Dependent Raman Spectroscopy, and Quantum Chemical Calculations. Organometallics, 2007, 26, 6544-6550.	2.3	54
423	Rate coefficients of H-atom abstraction from ethers and isomerization of alkoxyalkylperoxy radicals. Physical Chemistry Chemical Physics, 2007, 9, 5133.	2.8	76
424	Infrared Multiphoton Dissociation Spectra as a Probe of Ion Molecule Reaction Mechanism: The Formation of the Protonated Water Dimer via Sequential Bimolecular Reactions with 1,1,3,3-Tetrafluorodimethyl Ether. Journal of Physical Chemistry A, 2007, 111, 8792-8802.	2.5	8
425	Theoretical Study of the Benzyl + O_2 Reaction: Kinetics, Mechanism, and Product Branching Ratios. Journal of Physical Chemistry A, 2007, 111, 13200-13208.	2.5	87
426	Photoionization of 1-Alkenylperoxy and Alkylperoxy Radicals and a General Rule for the Stability of Their Cations. Journal of the American Chemical Society, 2007, 129, 14019-14025.	13.7	38
427	Ab Initio Thermochemistry and Kinetics for Carbon-Centered Radical Addition and β -Scission Reactions. Journal of Physical Chemistry A, 2007, 111, 8416-8428.	2.5	67
428	Ab Initio Energies and Product Branching Ratios for the $\text{O} + \text{C}_3\text{H}_6$ Reaction. Journal of Physical Chemistry A, 2007, 111, 12977-12984.	2.5	12
429	On the Chaperon Mechanism: Application to $\text{ClO} + \text{ClO} (\text{N}_2) \rightarrow \text{ClOCl} (\text{N}_2)$. Journal of Physical Chemistry A, 2007, 111, 8689-8698.	2.5	10
430	Computational Methods in Organic Thermochemistry. 1. Hydrocarbon Enthalpies and Free Energies of Formation. Journal of Organic Chemistry, 2007, 72, 5555-5566.	3.2	48
431	Computational Studies of Intramolecular Hydrogen Atom Transfers in the β -Hydroxyethylperoxy and β -Hydroxyethoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 5032-5042.	2.5	37
432	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2007, 3, 569-582.	5.3	207
433	Systematically Convergent Correlation Consistent Basis Sets for Molecular Core Valence Correlation Effects: The Third-Row Atoms Gallium through Krypton. Journal of Physical Chemistry A, 2007, 111, 11383-11393.	2.5	138
434	Quantitative Computational Thermochemistry of Transition Metal Species. Journal of Physical Chemistry A, 2007, 111, 11269-11277.	2.5	153
435	Application of the Computationally Efficient Self-Consistent-Charge Density-Functional Tight-Binding Method to Magnesium-Containing Molecules. Journal of Physical Chemistry A, 2007, 111, 5743-5750.	2.5	15

#	ARTICLE	IF	CITATIONS
436	Thermochemical and Kinetic Analysis of the Thermal Decomposition of Monomethylhydrazine: An Elementary Reaction Mechanism. Journal of Physical Chemistry A, 2007, 111, 3748-3760.	2.5	31
437	Computational Study of the Curtius-like Rearrangements of Phosphoryl, Phosphinyl, and Phosphinoyl Azides and Their Corresponding Nitrenes. Journal of Organic Chemistry, 2007, 72, 9426-9438.	3.2	28
438	Energetics of C-F, C-Cl, C-Br, and C-I Bonds in 2-Haloethanols. Enthalpies of Formation of XCH ₂ CH ₂ OH (X = F, Cl, Br, I) Compounds and of the 2-Hydroxyethyl Radical. Journal of Physical Chemistry A, 2007, 111, 1713-1720.	2.5	29
439	Hydrogen Migration and Vinylidene Pathway for Formation of Methane in the 193 nm Photodissociation of Propene: CH ₃ CHCH ₂ and CD ₃ CD ₂ CD ₂ . Journal of Physical Chemistry A, 2007, 111, 8330-8335.	2.5	6
440	Insights on Co-Catalyst-Promoted Enamine Formation between Dimethylamine and Propanal through Ab Initio and Density Functional Theory Study. Journal of Organic Chemistry, 2007, 72, 8202-8215.	3.2	75
441	Energetics of the Allyl Group. Journal of Organic Chemistry, 2007, 72, 8770-8779.	3.2	23
442	A New Look at the Ylidic Bond in Phosphorus Ylides and Related Compounds: Energy Decomposition Analysis Combined with a Domain-Averaged Fermi Hole Analysis. Journal of Physical Chemistry A, 2007, 111, 2859-2869.	2.5	27
443	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels: Ethyl Propanoate and Methyl Butanoate. Journal of Physical Chemistry A, 2007, 111, 3727-3739.	2.5	145
444	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions: H, O, and P Atoms. Journal of Chemical Theory and Computation, 2007, 3, 486-504.	5.3	138
445	Reactions of SO ₃ with the O/H Radical Pool under Combustion Conditions. Journal of Physical Chemistry A, 2007, 111, 3984-3991.	2.5	64
446	Comparison of Density Functionals for Reactions of Sulfur Ylides with Aldehydes and Olefins. Journal of Physical Chemistry A, 2007, 111, 12019-12025.	2.5	9
447	Computation of Accurate Activation Barriers for Methyl-Transfer Reactions of Sulfonium and Ammonium Salts in Aqueous Solution. Journal of Chemical Theory and Computation, 2007, 3, 1028-1035.	5.3	33
448	Theoretical Reinvestigation of the O(3P) + C ₆ H ₆ Reaction: A Quantum Chemical and Statistical Rate Calculations. Journal of Physical Chemistry A, 2007, 111, 3836-3849.	2.5	34
449	Ab Initio Study of Bonding between Nucleophilic Species and the Nitroso Group. Journal of Physical Chemistry A, 2007, 111, 1300-1306.	2.5	5
450	Reactions of Hydrogen Atom with Hydrogen Peroxide. Journal of Physical Chemistry A, 2007, 111, 13554-13566.	2.5	44
451	Gaussian-4 theory using reduced order perturbation theory. Journal of Chemical Physics, 2007, 127, 124105.	3.0	598
452	N-Nitrosation of Amines by NO ₂ and NO: A Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 2200-2205.	2.5	33
453	Theoretical Methods for Computing Enthalpies of Formation of Gaseous Compounds. Reviews in Computational Chemistry, 2007, , 147-211.	1.5	31

#	ARTICLE	IF	CITATIONS
455	Unexpected Conformational Properties of 1-Trifluoromethyl-1-Silacyclohexane, C ₅ H ₁₀ SiHCF ₃ : Gas Electron Diffraction, Low-Temperature NMR Spectropic Studies, and Quantum Chemical Calculations. Chemistry - A European Journal, 2007, 13, 1776-1783.	3.3	51
456	Hydrogen Peroxide Decomposition by a Non-Heme Iron(III) Catalase Mimic: A DFT Study. Chemistry - A European Journal, 2007, 13, 4230-4245.	3.3	36
457	Contra-thermodynamic Behavior in Intermolecular Hydrogen Transfer of Alkylperoxy Radicals. ChemPhysChem, 2007, 8, 1969-1978.	2.1	4
458	Thermochemistry, bonding, and reactivity of Ni + and Ni 2+ in the gas phase. Mass Spectrometry Reviews, 2007, 26, 474-516.	5.4	36
459	Thermochemistry for enthalpies and reaction paths of nitrous acid isomers. International Journal of Chemical Kinetics, 2007, 39, 378-398.	1.6	35
460	Infrared and Raman Spectra, conformations, ab initio calculations and spectral assignments of 1,3-disilabutane (SiH ₃ CH ₂ SiH ₂ CH ₃). Journal of Raman Spectroscopy, 2007, 38, 1159-1173.	2.5	8
461	Tribological degradation of two vegetable-based lubricants at elevated temperatures. Journal of Synthetic Lubrication: Research, Development and Application of Synthetic Lubricants and Functional Fluids, 2007, 24, 167-179.	0.7	8
462	Theoretical study on the reaction mechanism of CH ₂ ClO ₂ with HO ₂ . Computational and Theoretical Chemistry, 2007, 812, 1-11.	1.5	9
463	A computational study of the keto-enol equilibria of sulphur substituted analogues of hydroxycyclopropanone. Computational and Theoretical Chemistry, 2007, 814, 105-112.	1.5	2
464	Extension of the composite CBS-QB3 method to singlet diradical calculations. Chemical Physics Letters, 2007, 435, 152-156.	2.6	31
465	Theoretical study of reaction mechanism for NCO+HCNO. Chemical Physics Letters, 2007, 442, 1-6.	2.6	17
466	Theoretical characterization of halogenated methylperoxy nitrites CX ₃ OOONO (X, Y = H, F, Cl). Chemical Physics Letters, 2007, 446, 268-275.	2.6	6
467	Isomers on the [S ₂ , F ₂] potential energy surface: Straightening out experimental and theoretical findings using a high-level theoretical approach. Chemical Physics Letters, 2007, 448, 24-30.	2.6	26
468	Chemical methods for the hydrogen termination of silicon dangling bonds. Chemical Physics Letters, 2007, 448, 237-242.	2.6	12
469	Cyano substituent effects on enol and enethiol acidity and basicity: The protonation and deprotonation of 3-hydroxy-2-propenenitrile and its thio analogue. International Journal of Mass Spectrometry, 2007, 267, 125-133.	1.5	18
470	Quantum chemical calculations on the structure and stability of Mg ²⁺ +XH ₃ OH complexes in the gas phase (X=C, Si, and Ge). International Journal of Mass Spectrometry, 2007, 263, 267-275.	1.5	10
471	CASSCF calculations for photoinduced processes in large molecules: Choosing when to use the RASSCF, ONIOM and MMVB approximations. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 207-227.	3.9	55
472	Rate constants for the H abstraction from alkanes (R-H) by R [•] O ₂ radicals: A systematic study on the impact of R and R [•] . Proceedings of the Combustion Institute, 2007, 31, 149-157.	3.9	89

#	ARTICLE	IF	CITATIONS
473	Protonation of phenylboronic acid: Comparison of G3B3 and G2MP2 methods. International Journal of Quantum Chemistry, 2007, 107, 182-188.	2.0	0
474	Gaussian-4 theory. Journal of Chemical Physics, 2007, 126, 084108.	3.0	1,741
475	The Application of Composite Energy Methods to n-butyl Radical β -scission Reaction Kinetic Estimations. Theoretical Chemistry Accounts, 2007, 117, 207-212.	1.4	7
476	Calculation of acidic dissociation constants in water: solvation free energy terms. Their accuracy and impact. Theoretical Chemistry Accounts, 2007, 118, 281-293.	1.4	69
477	The 1-D hindered rotor approximation. Theoretical Chemistry Accounts, 2007, 118, 881-898.	1.4	168
478	Multilevel quantum chemical calculation of the enthalpy of formation of [1,2,5]oxadiazolo[3,4-e][1,2,3,4]-tetrazine-4,6-di-N-dioxide. Combustion, Explosion and Shock Waves, 2007, 43, 562-566.	0.8	31
479	CHH-DFT determination of the molecular structure infrared spectra, UV spectra and chemical reactivity of three antitubercular compounds: Rifampicin, Isoniazid and Pyrazinamide. Journal of Molecular Modeling, 2007, 13, 505-518.	1.8	48
480	Elucidation of structure-reactivity relationships in hindered phenols via quantum chemistry and transition state theory. Chemical Engineering Science, 2007, 62, 5232-5239.	3.8	22
481	Kinetics and thermochemistry of the addition of atomic chlorine to acetylene. Proceedings of the Combustion Institute, 2007, 31, 193-200.	3.9	4
482	G3 calculations of the proton affinity and ionization energy of dimethyl methylphosphonate. Journal of Chemical Thermodynamics, 2008, 40, 1116-1119.	2.0	19
483	Computational study of the molecular structure and reactive sites of the R and S isomers of persin diene. Computational and Theoretical Chemistry, 2008, 869, 67-74.	1.5	5
484	Hydrogenation of conjugated CC and CO bonds: Quantum chemical preview before metal catalysis. Computational and Theoretical Chemistry, 2008, 870, 61-64.	1.5	4
485	Core-valence correlation consistent basis sets for second-row atoms (Al-Ar) revisited. Theoretical Chemistry Accounts, 2008, 120, 119-131.	1.4	26
486	Accurate thermochemistry from quantum chemical calculations?. Monatshefte für Chemie, 2008, 139, 309-318.	1.8	29
487	On the heat of formation of nitromethane. Journal of Physical Organic Chemistry, 2008, 21, 747-757.	1.9	3
488	Application of CCSD(T)/(ECP + GCM) for studying gas-phase electron and proton affinities. International Journal of Quantum Chemistry, 2008, 108, 2454-2458.	2.0	2
489	Experimental measurements and kinetic modeling of $\text{CO}/\text{H}_2/\text{O}_2/\text{NO}_x$ conversion at high pressure. International Journal of Chemical Kinetics, 2008, 40, 454-480.	1.6	164
490	Carbon-Centered Radical Addition and β -Scission Reactions: Modeling of Activation Energies and Pre-exponential Factors. ChemPhysChem, 2008, 9, 124-140.	2.1	87

#	ARTICLE	IF	CITATIONS
491	Theoretical Investigation of the OH [•] -Initiated Oxidation of Benzaldehyde in the Troposphere. ChemPhysChem, 2008, 9, 1453-1459.	2.1	19
492	Why Are Selenouracils as Basic as but Stronger Acids than Uracil in the Gas Phase?. ChemPhysChem, 2008, 9, 1715-1720.	2.1	5
493	Calculation of the enthalpies of formation and proton affinities of some isoquinoline derivatives. Journal of Chemical Thermodynamics, 2008, 40, 1627-1631.	2.0	13
494	Investigation of thermodynamic properties of gaseous SiC(X ^Å and a ^Å) with accurate model chemistry calculations. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 5440-5456.	2.6	14
495	Accurate calculation of the pKa of trifluoroacetic acid using high-level ab initio calculations. Chemical Physics Letters, 2008, 451, 163-168.	2.6	80
496	Antioxidant and cytotoxic activities of canadine: Biological effects and structural aspects. Bioorganic and Medicinal Chemistry, 2008, 16, 3641-3651.	3.0	32
497	On the interaction of peptides with calcium ions as studied by matrix-assisted laser desorption/ionization Fourier transform mass spectrometry: Towards peptide fishing using metal ion baits. Analytica Chimica Acta, 2008, 627, 136-147.	5.4	7
498	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. Chemical Physics, 2008, 344, 273-280.	1.9	12
499	Dinitraminic acid (HDN) isomerization and self-decomposition revisited. Chemical Physics, 2008, 348, 53-60.	1.9	17
500	CBS-QB3 computational examination of substituent effects on the interconversion of 1,3,5-cyclooctatriene and bicyclo[4.2.0]-2,4-octadiene. Tetrahedron, 2008, 64, 2101-2103.	1.9	14
501	Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study. Computational and Theoretical Chemistry, 2008, 851, 54-62.	1.5	9
502	Sugars in the gas phase: The conformational properties of erythrose, threose, and erythrulose characterized by quantum chemistry calculations. Computational and Theoretical Chemistry, 2008, 858, 113-119.	1.5	9
503	CHIH-DFT computational molecular characterization of phenanthro [9,10-c]-1,2,5-thiadiazole 1,1-dioxide. Computational and Theoretical Chemistry, 2008, 862, 60-65.	1.5	6
504	Vibrational spectra, conformations, ab initio calculations and vibrational assignments of 3-pentyn-2-ol. Journal of Molecular Structure, 2008, 879, 102-112.	3.6	4
505	Vibrational spectra, ab initio calculations and vibrational assignments of 3-butyne-1-ol. Journal of Molecular Structure, 2008, 886, 90-102.	3.6	7
506	Thermodynamic properties of the most stable gaseous small silicon-carbon clusters in their ground states. European Physical Journal D, 2008, 49, 21-35.	1.3	22
507	Predictions of Substituent Effects in Thermal Azide 1,3-Dipolar Cycloadditions: Implications for Dynamic Combinatorial (Reversible) and Click (Irreversible) Chemistry. Journal of Organic Chemistry, 2008, 73, 1333-1342.	3.2	80
508	The Unusual Reaction of Semiquinone Radicals with Molecular Oxygen. Journal of Organic Chemistry, 2008, 73, 1830-1841.	3.2	117

#	ARTICLE	IF	CITATIONS
527	Thermodynamic model for arsenic speciation in sulfidic waters: A novel use of ab initio computations. <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 4457-4468.	3.9	112
528	Calculation of the structures, stabilities, and vibrational spectra of arsenites, thioarsenites and thioarsenates in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 5232-5242.	3.9	27
529	Enthalpies of Formation and Bond Dissociation Energies of Lower Alkyl Hydroperoxides and Related Hydroperoxy and Alkoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5010-5016.	2.5	98
530	Experimental and Theoretical Studies of Sodium Cation Complexes of the Deamidation and Dehydration Products of Asparagine, Glutamine, Aspartic Acid, and Glutamic Acid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3328-3338.	2.5	30
531	Experimental and Theoretical Studies of Potassium Cation Interactions with the Acidic Amino Acids and Their Amide Derivatives. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12056-12065.	2.6	50
532	Assessment of Multicoefficient Correlation Methods, Second-Order Møller-Plesset Perturbation Theory, and Density Functional Theory for $\text{H}_3\text{O}^+(\text{H}_2\text{O})_n$ ($n=1\text{--}5$) and $\text{OH}^-(\text{H}_2\text{O})_n$ ($n=1\text{--}4$). <i>Journal of Physical Chemistry B</i> , 2008, 112, 2372-2381.	2.6	29
533	Theoretical Prediction of pK_a Values for Methacrylic Acid Oligomers Using Combined Quantum Mechanical and Continuum Solvation Methods. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12687-12694.	2.5	59
534	Thermochemistry and kinetics of acetylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7139.	2.8	19
535	Structures, vibrational spectra, and relative energetics of $\text{FC}(\text{O})\text{ONO}$ and $\text{FC}(\text{O})\text{NO}_2$ isomers at DFT and ab initio levels. <i>Molecular Physics</i> , 2008, 106, 2301-2308.	1.7	0
536	Threshold Collision-Induced Dissociation of Hydrogen-Bonded Dimers of Carboxylic Acids. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1773-1782.	2.5	26
537	Ab Initio Study on Mechanisms and Kinetics for Reaction of NCS with NO. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5495-5501.	2.5	9
538	Theoretical Study on the Gas-Phase Acidity of Multiple Sites of Cu^{+} -Adenine and Cu^{2+} -Adenine Complexes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7418-7425.	2.5	22
539	Theoretical Study of the Nitroalkane Thermolysis. 1. Computation of the Formation Enthalpy of the Nitroalkanes, Their Isomers and Radical Products. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4458-4464.	2.5	38
540	Computational Methods in Organic Chemistry. 3. Correction of Computed Enthalpies for Multiple Conformations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1656-1660.	2.5	17
541	Nature of Glycine and Its $\dot{\text{C}}\alpha$ -Carbon Radical in Aqueous Solution: A Theoretical Investigation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1788-1794.	5.3	24
542	Origins of Stereoselectivity in the Diels-Alder Addition of Chiral Hydroxyalkyl Vinyl Ketones to Cyclopentadiene: A Quantitative Computational Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13006-13016.	2.5	8
543	$\text{C}\alpha\text{--H}$ Bond Dissociation Enthalpies in Norbornane. An Experimental and Computational Study. <i>Organic Letters</i> , 2008, 10, 1613-1616.	4.6	16
544	Polyfunctional Methodology for Improved DFT Thermochemical Predictions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10624-10634.	2.5	1

#	ARTICLE	IF	CITATIONS
545	Energetic Differences between the Five- and Six-Membered Ring Hydrocarbons: Strain Energies in the Parent and Radical Molecules. <i>Journal of Organic Chemistry</i> , 2008, 73, 6213-6223.	3.2	26
546	Thermodynamics and Mechanism of the Deamidation of Sodium-Bound Asparagine. <i>Journal of the American Chemical Society</i> , 2008, 130, 10227-10232.	13.7	40
547	Experimental and Theoretical Studies of Sodium Cation Interactions with α -D-Arabinose, Xylose, Glucose, and Galactose. <i>Journal of Physical Chemistry A</i> , 2008, 112, 10156-10167.	2.5	39
548	Theoretical Thermodynamics for Large Molecules: Walking the Thin Line between Accuracy and Computational Cost. <i>Accounts of Chemical Research</i> , 2008, 41, 569-579.	15.6	329
549	Theoretical Kinetic Study of Thermal Unimolecular Decomposition of Cyclic Alkyl Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 11598-11610.	2.5	73
550	Theoretical Investigation of Nitration and Nitrosation of Dimethylamine by N_2O_4 . <i>Journal of Physical Chemistry A</i> , 2008, 112, 7098-7105.	2.5	24
551	Theoretical Explanation of Nonexponential OH Decay in Reactions with Benzene and Toluene under Pseudo-First-Order Conditions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7608-7615.	2.5	57
552	Enol Formation and Ring-Opening in OH-Initiated Oxidation of Cycloalkenes. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13444-13451.	2.5	18
553	first principles Study of the Reaction of Formic and Acetic Acids with Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6918-6928.	2.5	20
554	Hartree-Fock complete basis set limit properties for transition metal diatomics. <i>Journal of Chemical Physics</i> , 2008, 128, 044101.	3.0	34
555	Computational study of the perhalogenated methyl nitrates CX_3ONO_2 , $CX_3\dot{X}ONO_2$ ($X, Y \in F, Cl$). <i>Molecular Physics</i> , 2008, 106, 1025-1032.		4
556	Theoretical Study on Mechanism of Reaction of OH with HO_2NO_2 . <i>Chinese Journal of Chemical Physics</i> , 2008, 21, 32-38.	1.3	3
557	Density Functional Theory Study of Infrared and Ultraviolet Spectra of Urea L-Malic Acid. <i>Chinese Journal of Chemical Physics</i> , 2008, 21, 535-540.	1.3	2
558	Performance of the correlation-consistent composite approach for sulfur species. <i>Journal of Sulfur Chemistry</i> , 2008, 29, 353-365.	2.0	19
559	Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Sc–Zn. <i>Journal of Chemical Physics</i> , 2008, 128, 144122.	3.0	20
560	Non-Covalent Complexes. , 2008, , 323-337.		0
561	A theoretical investigation into the formation of sesquiterpene episulfides. <i>Journal of Sulfur Chemistry</i> , 2009, 30, 119-127.	2.0	1
562	The resolution of the identity approximation applied to the correlation consistent composite approach. <i>Journal of Chemical Physics</i> , 2009, 131, 044130.	3.0	21

#	ARTICLE	IF	CITATIONS
563	THEORETICAL STUDIES ON HEATS OF FORMATION OF PYRIDINE N-OXIDES USING DENSITY FUNCTIONAL THEORY AND COMPLETE BASIS METHOD. Journal of Theoretical and Computational Chemistry, 2009, 08, 541-549.	1.8	5
564	Ab initio thermochemistry using optimal-balance models with isodesmic corrections: The ATOMIC protocol. Journal of Chemical Physics, 2009, 130, 144113.	3.0	29
565	Infrared spectra of protonated polycyclic aromatic hydrocarbon molecules: Azulene. Journal of Chemical Physics, 2009, 131, 184307.	3.0	30
566	Understanding the substituent effect on the acidity of alcohols and <i>p</i> -substituted phenols. Molecular Simulation, 2009, 35, 1269-1278.	2.0	13
567	Penning ionization and ion fragmentation of formamide HCONH ₂ by He ⁺ , Ne ⁺ , and Ar ⁺ in molecular beams. Journal of Chemical Physics, 2009, 131, 134309.	3.0	6
568	The Effect of a Complexed Lithium Cation on a Norcaradiene-Based Radical Clock. Chemistry - A European Journal, 2009, 15, 2425-2433.	3.3	7
569	The Variable Strength of the Sulfur-Sulfur Bond: 78 to 41 kcal mol ⁻¹ G3, CBS-Q, and DFT Bond Energies of Sulfur (S ₈) and Disulfanes XSSX (X = H, F, Cl, CH ₃ , CN, NH ₂ , OH, Tj ETQq020 rgBT / Overlock 1	3.3	10
570	Theoretical studies of the reactions of CF ₃ CHClOCHF ₂ /CF ₃ CHFOCHF ₂ with OH radical and Cl atom and their product radicals with OH. Journal of Computational Chemistry, 2009, 30, 565-580.	3.3	20
571	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with least-square calibration. Journal of Computational Chemistry, 2009, 30, 1007-1015.	3.3	6
572	Extensive theoretical studies of a new energetic material: Tetrazino-tetrazine-tetraoxide (TTTO). Journal of Computational Chemistry, 2009, 30, 1816-1820.	3.3	55
573	Barrier heights for H-atom abstraction by H ₂ from <i>n</i> -butanol: A simple yet exacting test for model chemistries?. Journal of Computational Chemistry, 2010, 31, 1236-1248.	3.3	80
574	Vibrational spectroscopic studies, conformations and <i>ab initio</i> calculations of 1,2-bis(trifluorosilyl)ethane (SiF ₃ CH ₂ CH ₂ SiF ₃). Journal of Raman Spectroscopy, 2009, 40, 2111-2122.	2.5	6
575	Theoretical investigation of tautomerism in N-hydroxy amidines. Journal of Molecular Modeling, 2009, 15, 807-816.	1.8	31
576	Kinetic studies of chlorobenzene reactions with hydrogen atoms and phenyl radicals and the thermochemistry of 1-chlorocyclohexadienyl radicals. Proceedings of the Combustion Institute, 2009, 32, 351-357.	3.9	4
577	Gas-phase acidity, bond dissociation energy and enthalpy of formation of fluorine-substituted benzenes: A theoretical study. Journal of Fluorine Chemistry, 2009, 130, 621-628.	1.7	20
578	Structural studies of cyclic ureas: 3. Enthalpy of formation of barbital. Journal of Chemical Thermodynamics, 2009, 41, 1400-1407.	2.0	19
579	Activation enthalpies of pericyclic reactions: the performances of some recently proposed functionals. Theoretical Chemistry Accounts, 2009, 122, 257-264.	1.4	16
580	A theoretical study of the thermodynamics and kinetics of small organosulfur compounds. Theoretical Chemistry Accounts, 2009, 123, 391-412.	1.4	32

#	ARTICLE	IF	CITATIONS
581	Density functional methods in the study of oxygen transfer reactions. Theoretical Chemistry Accounts, 2009, 123, 59-66.	1.4	3
582	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215.	1.4	4
583	Structure-activity relationship of nitrosating agents in the nitrosation reactions of ammonia: a theoretical study. Theoretical Chemistry Accounts, 2009, 124, 261-268.	1.4	9
584	PCM study of the solvent and substituent effects on bond dissociation energies of the C-NO bond. International Journal of Quantum Chemistry, 2009, 109, 1403-1409.	2.0	5
585	Isomer-specific product detection of CN radical reactions with ethene and propene by tunable VUV photoionization mass spectrometry. International Journal of Mass Spectrometry, 2009, 280, 113-118.	1.5	34
586	How reliable are gas-phase proton affinity values of small carbanions? A comparison of experimental data with values calculated using Gaussian-3 and CBS compound methods. International Journal of Mass Spectrometry, 2009, 285, 86-94.	1.5	12
587	The elimination of water from a conformationally complex alcohol: A computational study of the gas phase dehydration of n-butanol. Journal of Molecular Structure, 2009, 928, 149-157.	3.6	53
588	Assessment of mixed basis set and ONIOM methods on the activation energy of ring opening reactions of substituted cyclobutenes. Computational and Theoretical Chemistry, 2009, 893, 98-105.	1.5	3
589	Characterization of the semiquinones and quinones of (â)-epicatechin by means of computational chemistry. Computational and Theoretical Chemistry, 2009, 897, 6-11.	1.5	8
590	Absolute and relative pKa calculations of mono and diprotic pyridines by quantum methods. Computational and Theoretical Chemistry, 2009, 912, 5-12.	1.5	61
591	Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study. Computational and Theoretical Chemistry, 2009, 907, 66-73.	1.5	15
592	Theoretical studies on bond dissociation energies for some pyridine N-oxide biological compounds by density functional theory and CBS-4M method. Computational and Theoretical Chemistry, 2009, 907, 126-130.	1.5	12
593	Theoretical and experimental interpretations of phenol oxidation by the hydroxyl radical. Computational and Theoretical Chemistry, 2009, 910, 74-79.	1.5	36
594	Thermodynamics and mechanism of protonated asparagine decomposition. Journal of the American Society for Mass Spectrometry, 2009, 20, 852-866.	2.8	42
595	The reaction of hydroxyethyl radicals with O ₂ : A theoretical analysis and experimental product study. Proceedings of the Combustion Institute, 2009, 32, 271-277.	3.9	90
596	Atomization energies from coupled-cluster calculations augmented with explicitly-correlated perturbation theory. Chemical Physics, 2009, 356, 14-24.	1.9	92
597	Accurate multi-coefficient electronic structure methods MLSE(Cn)-DFT for thermochemical kinetics. Chemical Physics Letters, 2009, 475, 141-145.	2.6	3
598	Current technologies for analysis of biomass thermochemical processing: A review. Analytica Chimica Acta, 2009, 651, 117-138.	5.4	252

#	ARTICLE	IF	CITATIONS
599	Accurate Methods for Large Molecular Systems. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9646-9663.	2.6	188
600	On the Effect of Tether Composition on <i>cis</i> / <i>trans</i> Selectivity in Intramolecular Diels-Alder Reactions. <i>Chemistry - an Asian Journal</i> , 2009, 4, 126-134.	3.3	12
601	Steric and Solvation Effects in Ionic S_N2 Reactions. <i>Journal of the American Chemical Society</i> , 2009, 131, 16162-16170.	13.7	72
602	Accurate Reaction Enthalpies and Sources of Error in DFT Thermochemistry for Aldol, Mannich, and α -Aminoxylation Reactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10376-10384.	2.5	124
603	Catching CO_2 in a Bowl. <i>Inorganic Chemistry</i> , 2009, 48, 7105-7110.	4.0	12
604	Kinetic Barriers of H-Atom Transfer Reactions in Alkyl, Allylic, and Oxoallylic Radicals as Calculated by Composite Ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2473-2482.	2.5	43
605	Energetics of <i>tert</i> -Butoxyl Addition Reaction to Norbornadiene: A Method for Estimating the π -Bond Strength of a Carbon-Carbon Double Bond. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6524-6530.	2.5	4
606	Mechanism of S_H2 Reactions of Disulfides: Frontside vs Backside, Stepwise vs Concerted. <i>Journal of Organic Chemistry</i> , 2009, 74, 5356-5360.	3.2	31
607	Energetics and Dynamics of the Reactions of O(3P) with Dimethyl Methylphosphonate and Sarin. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13752-13761.	2.5	7
608	Mechanisms of Peroxynitrite-Mediated Nitration of Tyrosine. <i>Chemical Research in Toxicology</i> , 2009, 22, 894-898.	3.3	82
609	Hydrogen Bonding Described Using Dispersion-Corrected Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2009, 113, 4726-4732.	2.6	60
610	Energetics and Structure of Hydroxynicotinic Acids. Crystal Structures of 2-, 4-, 6-Hydroxynicotinic and 5-Chloro-6-hydroxynicotinic Acids. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14291-14309.	2.6	21
611	Mechanism and Kinetic Isotope Effect of the Reaction of $C_2(X1^+g)$ Radicals with H_2 and D_2 . <i>Journal of Physical Chemistry A</i> , 2009, 113, 8963-8970.	2.5	8
612	Structures and Thermochemistry of the Alkali Metal Monoxide Anions, Monoxide Radicals, and Hydroxides. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9501-9510.	2.5	17
613	Gas-Phase Infrared Spectra of Vinyl Selenol and Vinyl Tellurol. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12857-12863.	2.5	7
614	Carbon-Centered Radicals in Cigarette Smoke: Acyl and Alkylaminocarbonyl Radicals. <i>Analytical Chemistry</i> , 2009, 81, 631-641.	6.5	33
615	Supersilylated Tetraphosphene Derivatives $M_2[t-Bu_3SiPPPPSi-t-Bu_3]$ ($M = Li, Na, Rb, Cs$) and $Ba[t-Bu_3SiPPPPSi-t-Bu_3]$: Reactivity and <i>Cis</i> - <i>Trans</i> Isomerization. <i>Inorganic Chemistry</i> , 2009, 48, 1005-1017.	4.0	29
616	Effect of Halogenation on the Mechanism of the Atmospheric Reactions between Methylperoxy Radicals and NO. A computational Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3545-3554.	2.5	9

#	ARTICLE	IF	CITATIONS
617	Vacuum-Ultraviolet Photoionization Measurement and ab Initio Calculation of the Ionization Energy of Gas-Phase SiO ₂ . Journal of Physical Chemistry A, 2009, 113, 1225-1230.	2.5	21
618	Kinetics of the Gas-Phase Reaction of OH with Chlorobenzene. Journal of Physical Chemistry A, 2009, 113, 10452-10459.	2.5	13
619	Ab Initio Reaction Path Analysis for the Initial Hydrogen Abstraction from Organic Acids by Hydroxyl Radicals. Journal of Physical Chemistry A, 2009, 113, 7852-7860.	2.5	15
620	O(³ P) + C ₂ H ₄ Potential Energy Surface: Study at the Multireference Level. Journal of Physical Chemistry A, 2009, 113, 12663-12674.	2.5	21
621	H ₂ CO ₃ (s): A New Candidate for CO ₂ Capture and Sequestration. Environmental Science & Technology, 2009, 43, 2575-2580.	10.0	22
622	Quantum-Mechanical Study of 10-R-9-borabicyclo[3.3.2]decane Alkene Hydroboration. Journal of Organic Chemistry, 2009, 74, 8626-8637.	3.2	11
623	Accurate Benchmark Calculations on the Gas-Phase Basicities of Small Molecules. Journal of Physical Chemistry A, 2009, 113, 10096-10103.	2.5	18
624	A DFT Study on the Mechanism of the Annulation Reaction of Trichloronitroethylene with Aniline in the Synthesis of Quinoxalinone-N-oxides. Journal of Organic Chemistry, 2009, 74, 4727-4739.	3.2	10
625	Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone. Journal of Physical Chemistry A, 2009, 113, 5786-5799.	2.5	114
626	H/Br Exchange in BBr ₃ by HSiR ₃ (R = H, CH ₃), Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 387 Barrier. Journal of Physical Chemistry A, 2009, 113, 12035-12043.	2.5	12
627	Density Functional Study of the High-Temperature Oxidation of <i>o</i> -, <i>m</i> - and <i>p</i> -Xylyl Radicals. Journal of Physical Chemistry A, 2009, 113, 10652-10666.	2.5	19
628	Basicity of organic bases and superbases in acetonitrile by the polarized continuum model and DFT calculations. New Journal of Chemistry, 2009, 33, 588-597.	2.8	72
629	Computational Study of the Acid Dissociation of Esters and Lactones. A Case Study of Diketene. Journal of Organic Chemistry, 2009, 74, 4943-4948.	3.2	24
630	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	1.7	96
631	Experimental and Theoretical Studies of Redox Reactions of <i>o</i> -Chloranil in Aqueous Solution. Journal of Physical Chemistry B, 2009, 113, 8080-8085.	2.6	35
632	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. Journal of Chemical Theory and Computation, 2009, 5, 808-821.	5.3	462
633	The Effects of Chemical Substitution and Polymerization on the <i>p</i> K _a Values of Sulfonic Acids. Journal of Physical Chemistry B, 2009, 113, 14094-14101.	2.6	41
634	Acidities of Arsenic (III) and Arsenic (V) Thio- and Oxyacids in Aqueous Solution using the CBS-QB3/CPCM Method. Journal of Physical Chemistry A, 2009, 113, 5105-5111.	2.5	17

#	ARTICLE	IF	CITATIONS
635	Ab Initio Thermochemistry with High-Level Isodesmic Corrections: Validation of the ATOMIC Protocol for a Large Set of Compounds with First-Row Atoms (H, C, N, O, F). Journal of Physical Chemistry A, 2009, 113, 11517-11534.	2.5	30
636	Ionic Hydrogen-Bond Networks and Ion Solvation. 1. An Efficient Monte Carlo/Quantum Mechanical Method for Structural Search and Energy Computations: Ammonium/Water. Journal of Physical Chemistry A, 2009, 113, 2967-2974.	2.5	24
637	RRKM and Ab Initio Investigation of the NH (X) Oxidation by Dioxygen. Journal of Physical Chemistry A, 2009, 113, 6468-6476.	2.5	30
638	Computational Calculation of Equilibrium Constants: Addition to Carbonyl Compounds. Journal of Physical Chemistry A, 2009, 113, 11423-11428.	2.5	35
639	C<sup>i>-Nitroso Donors of Nitric Oxide. Journal of Organic Chemistry, 2009, 74, 1450-1453.	3.2	23
640	Theoretical Investigation of Mechanisms for the Gas-Phase Unimolecular Decomposition of DMMP. Journal of Physical Chemistry A, 2009, 113, 13762-13771.	2.5	33
641	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.	5.3	12
642	Steric Effects and Solvent Effects on S_N2 Reactions. Journal of Physical Chemistry A, 2009, 113, 9109-9114.	2.5	42
643	Unrestricted Coupled Cluster and Brueckner Doubles Variations of W1 Theory. Journal of Chemical Theory and Computation, 2009, 5, 2687-2693.	5.3	232
644	Optimization and Basis-Set Dependence of a Restricted-Open-Shell Form of B2-PLYP Double-Hybrid Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 9861-9873.	2.5	77
645	Benchmark Thermochemistry of the C_nH_{2n}+2 Alkane Isomers (C_n = 2âˆ’8) and Performance of DFT and Composite Ab Initio Methods for Dispersion-Driven Isomeric Equilibria. Journal of Physical Chemistry A, 2009, 113, 8434-8447.	2.5	128
646	Density Functional Theory in Prediction of Four Stepwise Protonation Constants for Nitrilotripropanoic Acid (NTPA). Journal of Physical Chemistry A, 2009, 113, 3639-3647.	2.5	23
647	Phosphine Polymerization by Nitric Oxide: Experimental Characterization and Theoretical Predictions of Mechanism. Inorganic Chemistry, 2009, 48, 1223-1231.	4.0	12
648	Uracil and Thymine Reactivity in the Gas Phase: The S_N2 Reaction and Implications for Electron Delocalization in Leaving Groups. Journal of the American Chemical Society, 2009, 131, 18376-18385.	13.7	19
649	Theoretical Kinetic Study of the Reactions of Cycloalkylperoxy Radicals. Journal of Physical Chemistry A, 2009, 113, 6924-6935.	2.5	51
650	Atomization energies of the carbon clusters C_n (C_n = 2âˆ’10) revisited by means of W4 theory as well as density functional, G₃, and CBS methods. Molecular Physics, 2009, 107, 977-990.	1.7	41
651	Theoretical study of the gas-phase ozonolysis of Î²-pinene (C10H16). Physical Chemistry Chemical Physics, 2009, 11, 5643.	2.8	83
652	Absolute rate coefficients over extended temperature ranges and mechanisms of the CF(X2Î) reactions with F2, Cl2 and O2. Physical Chemistry Chemical Physics, 2009, 11, 4319.	2.8	4

#	ARTICLE	IF	CITATIONS
653	The gas-phase ozonolysis of β -caryophyllene (C ₁₅ H ₂₄). Part II: A theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4173.	2.8	66
654	Hydroxyl Radical Initiated Oxidation of s-Triazine: Hydrogen Abstraction Is Faster than Hydroxyl Addition. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8596-8606.	2.5	28
655	A Hierarchy of Homodesmotic Reactions for Thermochemistry. <i>Journal of the American Chemical Society</i> , 2009, 131, 2547-2560.	13.7	508
656	Calculation of Some Biologically Important Carbon Acids - An Assessment of Contemporary Theoretical Procedures. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 295-306.	5.3	131
657	DFT Studies of the Ring-Opening Mechanism of SB-3CT, a Potent Inhibitor of Matrix Metalloproteinase 2. <i>Organic Letters</i> , 2009, 11, 2559-2562.	4.6	23
658	Accurate DFT Descriptions for Weak Interactions of Molecules Containing Sulfur. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 23-28.	5.3	38
659	The Unimolecular Decomposition and H Abstraction Reactions by HO and HO[₂] from n-Butanol. , 2009, , .		11
661	Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry. <i>Current Organic Chemistry</i> , 2010, 14, 1600-1611.	1.6	6
662	Performance of the major semiempirical, ab initio, and density functional theory methods in evaluating isomerization enthalpies for linear to branched heptanes. <i>Nature Precedings</i> , 2010, , .	0.1	6
663	An Experimental and Theoretical Study of the Reaction Between NH(X ⁺) + SO(X ⁺). <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 1009-1024.	2.8	1
664	Composition and temporal behavior of ambient ions in the boreal forest. <i>Atmospheric Chemistry and Physics</i> , 2010, 10, 8513-8530.	4.9	170
665	The mechanism of formation of the hydroperoxyl radical in the CF ₃ COOH + 3O ₂ system: a quantum-chemical study. <i>Russian Journal of Physical Chemistry B</i> , 2010, 4, 705-708.	1.3	6
666	Structure and Thermochemical Properties of 2-Methoxyfuran, 3-Methoxyfuran, and Their Carbon-Centered Radicals Using Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7984-7995.	2.5	16
667	Development of Detailed Kinetic Models for the Thermal Conversion of Biomass via First Principle Methods and Rate Estimation Rules. <i>ACS Symposium Series</i> , 2010, , 201-243.	0.5	23
668	Quantum Mechanical Modeling of Sugar Thermochemistry. <i>ACS Symposium Series</i> , 2010, , 179-199.	0.5	1
669	A universal approach for continuum solvent pK _a calculations: are we there yet?. <i>Theoretical Chemistry Accounts</i> , 2010, 125, 3-21.	1.4	408
670	Theoretical study of the competitive decomposition and isomerization of 1-hexyl radical. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 87-98.	1.4	16
671	Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. <i>Theoretical Chemistry Accounts</i> , 2010, 126, 289-304.	1.4	64

673	Gas-phase enthalpies of formation, acidities, and strain energies of the [m, n]polyprismanes (m,n-polyprismanes) Tj ETQq1 1 0.784314 rgBT 1.4 26 127, 697-709.		
674	Acid/base and hydrogen bonding effects on the proton-coupled electron transfer of quinones and hydroquinones in acetonitrile: Mechanistic investigation by voltammetry, 1H NMR and computation. Electrochimica Acta, 2010, 55, 6507-6516.	5.2	45
675	Structural and heat of formation studies of halogenated methyl hydro-peroxides. Chemical Physics, 2010, 371, 36-42.	1.9	8
676	Low temperature n-butane oxidation skeletal mechanism, based on multilevel approach. Combustion and Flame, 2010, 157, 641-652.	5.2	15
677	A study of factors affecting the accurac of combined calculation methods. Journal of Structural Chemistry, 2010, 51, 211-216.	1.0	1
678	Thermochemistry of paracetamol. Journal of Thermal Analysis and Calorimetry, 2010, 100, 391-401.	3.6	33
679	GeCl2 cycloaddition reactions to unsaturated organic compounds taking ethylene, buta-1,3-diene, and hexa-1,3,5-triene as examples: a quantum chemical study. Russian Chemical Bulletin, 2010, 59, 1099-1109.	1.5	0
680	Hydrogen Radical Additions to Unsaturated Hydrocarbons and the Reverse β -Scission Reactions: Modeling of Activation Energies and Pre-exponential Factors. ChemPhysChem, 2010, 11, 195-210.	2.1	50
681	From a Network of Computed Reaction Enthalpies to Atom-Based Thermochemistry (NEAT). Chemistry - A European Journal, 2010, 16, 4826-4835.	3.3	23
682	Kinetic Stability and Propellant Performance of Green Energetic Materials. Chemistry - A European Journal, 2010, 16, 6590-6600.	3.3	69
683	Bonding in Cationic MCH_2^+ ($M=La, Hf, Rn$): A Theoretical Study on Periodic Trends. Chemistry - A European Journal, 2010, 16, 5882-5888.	3.3	51
685	Experimental Confirmation of the Low-Temperature Oxidation Scheme of Alkanes. Angewandte Chemie - International Edition, 2010, 49, 3169-3172.	13.8	180
686	Computational studies on the reactions of α -butenyl and α -butenylperoxy radicals. International Journal of Chemical Kinetics, 2010, 42, 273-288.	1.6	49
687	Atmospheric chemistry of isopropyl formate and <i>tert</i> -butyl formate. International Journal of Chemical Kinetics, 2010, 42, 479-498.	1.6	18
688	Vibrational spectroscopy of intermediates in benzene-to-pheno conversion by FeO^+ . Journal of the American Society for Mass Spectrometry, 2010, 21, 750-757.	2.8	21
689	A phenomenological relationship between molecular geometry change and conformational energy change. Journal of Molecular Structure, 2010, 978, 14-19.	3.6	24
690	Synthesis and characterization of the first phosphonic diamide containing thiazolyl groups: Structural properties and tautomeric equilibrium. Journal of Molecular Structure, 2010, 978, 67-73.	3.6	20

692	Infrared and Raman spectra, conformations, ab initio calculations and spectral assignments of ethylmethyldichlorogermane. Journal of Molecular Structure, 2010, 976, 105-114.	3.6	2
693	Density functional based reactivity parameters: Thermodynamic or kinetic concepts?. Computational and Theoretical Chemistry, 2010, 943, 127-137.	1.5	25
694	Theoretical investigation on the structures and thermodynamic properties of mixed boron-, nitrogen- and oxygen-containing three- and four-membered rings B N OH (n= 3, m= 3, p= 3). Computational and Theoretical Chemistry, 2010, 942, 121-130.	1.5	1
695	Gas phase isomerization enthalpies of organic compounds: A semiempirical, density functional theory, and ab initio post-Hartree-Fock theoretical study. Computational and Theoretical Chemistry, 2010, 948, 102-107.	1.5	50
696	Theoretical studies on the pKa values of perfluoroalkyl carboxylic acids. Computational and Theoretical Chemistry, 2010, 949, 60-69.	1.5	94
697	A comparison of high-level theoretical methods to predict the heats of formation of azo compounds. Computational and Theoretical Chemistry, 2010, 956, 55-60.	1.5	35
698	Formation enthalpies and bond dissociation enthalpies for C1-C4 mononitroalkanes by composite and DFT/B3LYP methods. Computational and Theoretical Chemistry, 2010, 958, 1-6.	1.5	17
699	Theoretical investigation of the isomerization and dissociation reactions of all the HOONO2 isomers. Computational and Theoretical Chemistry, 2010, 959, 42-48.	1.5	1
700	Vibrational spectra, conformational equilibrium, ab initio calculations and spectral assignments of ethylmethylgermane. Vibrational Spectroscopy, 2010, 54, 56-64.	2.2	0
701	Bio-butanol: Combustion properties and detailed chemical kinetic model. Combustion and Flame, 2010, 157, 363-373.	5.2	267
702	Modeling of 1,3-hexadiene, 2,4-hexadiene and 1,4-hexadiene-doped methane flames: Flame modeling, benzene and styrene formation. Combustion and Flame, 2010, 157, 1331-1345.	5.2	43
703	A lean methane premixed laminar flame doped with components of diesel fuel part III: Indane and comparison between n-butylbenzene, n-propylcyclohexane and indane. Combustion and Flame, 2010, 157, 1236-1260.	5.2	30
704	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.	2.6	26
705	A theoretical analysis of the acid-base equilibria of hydroxylamine in aqueous solution. Chemical Physics Letters, 2010, 490, 159-164.	2.6	17
706	Conformational energies of C_4H_8 isomers. Chemical Physics Letters, 2010, 495, 182-186.	2.6	74
707	Heats of formation and protonation thermochemistry of gaseous benzaldehyde, tropone and quinone methides. Chemical Physics Letters, 2010, 495, 192-197.	2.6	8
708	Assessment of Gaussian-4 theory for energy barriers. Chemical Physics Letters, 2010, 499, 168-172.	2.6	74

#	ARTICLE	IF	CITATIONS
709	Theoretical study on the formation of tetraoxygen conformational isomerism in the CO ₂ with O ₃ reaction. Chemical Physics Letters, 2010, 499, 51-55.	2.6	5
710	The ability of triplet nitrenes to abstract hydrogen atoms. Journal of Physical Organic Chemistry, 2010, 23, 370-375.	1.9	22
711	Simplification of the CBS-QB3 method for predicting gas-phase deprotonation free energies. International Journal of Quantum Chemistry, 2010, 110, 323-330.	2.0	31
712	Gas phase constant pressure heat capacities (C _{p,gas}) for the C ₁ through C ₁₀ straight chain alkanes, isobutane, hydrogen atom, hydroxyl and methyl radicals, and water between 298.15 and 1500 K: A comparison of theoretical values against experimental data. Nature Precedings, 2010, , .	0.1	2
713	Theoretical studies on the all-anti zigzag geometries of perfluoro-n-alkyl chains. Nature Precedings, 0, , .	0.1	5
714	THEORETICAL STUDY ON OXYGEN-OXYGEN HOMOLYTIC BOND DISSOCIATION ENTHALPIES OF PEROXIDES. Journal of Theoretical and Computational Chemistry, 2010, 09, 625-635.	1.8	2
715	Imaging the dynamics of chlorine atom reactions with alkenes. Journal of Chemical Physics, 2010, 133, 074306.	3.0	24
716	Theoretical Study of the HOCH ₂ OO [•] + HO ₂ [•] Reaction: Detailed Molecular Mechanisms of the Three Reaction Channels. Zeitschrift Fur Physikalische Chemie, 2010, 224, 1081-1093.	2.8	8
717	Method and basis set dependence of anharmonic ground state nuclear wave functions and zero-point energies: Application to SSSH. Journal of Chemical Physics, 2010, 132, 054105.	3.0	8
718	Theoretical Investigation of <i>N</i> -Nitrosodimethylamine Formation from Nitrosation of Trimethylamine. Journal of Physical Chemistry A, 2010, 114, 455-465.	2.5	13
719	Probing Substituent Effects in Aryl-Aryl Interactions Using Stereoselective Diels-Alder Cycloadditions. Journal of the American Chemical Society, 2010, 132, 3304-3311.	13.7	176
720	Thermochemical Properties of <i>exo</i> -Tricyclo[5.2.1.0 ^{2,6}]decane (JP-10 Jet Fuel) and Derived Tricyclodecyl Radicals. Journal of Physical Chemistry A, 2010, 114, 9545-9553.	2.5	42
721	Radicals from the Gas-Phase Pyrolysis of Catechol: 1. <i>o</i> -Semiquinone and <i>ipso</i> -Catechol Radicals. Journal of Physical Chemistry A, 2010, 114, 2306-2312.	2.5	31
722	Computational Study of Main Mechanisms for Gas-Phase Decomposition of 1,1- and 1,2-Dinitroethane. Journal of Energetic Materials, 2010, 28, 318-337.	2.0	4
723	On the Anomalous Decomposition and Reactivity of Ammonium and Potassium Dinitramide. Journal of Physical Chemistry A, 2010, 114, 2845-2854.	2.5	36
724	Homoselenocysteine - An oxygen or selenium acid in the gas phase?. Canadian Journal of Chemistry, 2010, 88, 744-753.	1.1	2
725	Accuracy of computational solvation free energies for neutral and ionic compounds: Dependence on level of theory and solvent model. Nature Precedings, 0, , .	0.1	12
726	Matrix Metalloproteinase 2 (MMP2) Inhibition: DFT and QM/MM Studies of the Deprotonation-Initialized Ring-Opening Reaction of the Sulfoxide Analogue of SB-3CT. Journal of Physical Chemistry B, 2010, 114, 1030-1037.	2.6	20

#	ARTICLE	IF	CITATIONS
727	Radicals from the Gas-Phase Pyrolysis of Catechol. 2. Comparison of the Pyrolysis of Catechol and Hydroquinone. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10110-10116.	2.5	30
728	Study of a Benzoylperoxy Radical in the Gas Phase: Ultraviolet Spectrum and $C_6H_5C(O)O_2 + HO_2$ Reaction between 295 and 357 K. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10367-10379.	2.5	8
729	Reaction of the C_2H Radical with 1-Butyne (C_4H_6): Low-Temperature Kinetics and Isomer-Specific Product Detection. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3340-3354.	2.5	57
730	Unimolecular \dot{I}^2 -Hydroxyperoxy Radical Decomposition with OH Recycling in the Photochemical Oxidation of Isoprene. <i>Environmental Science & Technology</i> , 2010, 44, 250-256.	10.0	122
731	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6235-6249.	2.5	33
732	Infrared Spectrum of the Propargyl Peroxyl Radical, $HC\equiv CH_2OO\dot{X}$. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1498-1507.	2.5	12
733	Vinyl Cations Substituted with \dot{I}^2 σ -Donors Have Triplet Ground States. <i>Journal of the American Chemical Society</i> , 2010, 132, 215-222.	13.7	35
734	Dissociative Photoionization of Sulfur Chlorides and Oxochlorides: Thermochemistry and Bond Energies Based on Accurate Appearance Energies. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9115-9123.	2.5	16
735	Type II Isopentenyl Diphosphate Isomerase: Probing the Mechanism with Alkyne/Allene Diphosphate Substrate Analogues. <i>Biochemistry</i> , 2010, 49, 6228-6233.	2.5	21
736	Heats of Formation of C_6H_5 , $C_6H_5^+$, and C_6H_5NO by Threshold Photoelectron Photoion Coincidence and Active Thermochemical Tables Analysis. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13134-13145.	2.5	87
737	Photoelectron Circular Dichroism Spectroscopy in an Orbital Congested System: The Terpene Endoborneol. <i>Journal of Physical Chemistry A</i> , 2010, 114, 847-853.	2.5	32
738	Conformational and Thermodynamic Properties of Gaseous Levulinic Acid. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12323-12329.	2.5	19
739	Isomer-Selective Study of the OH Initiated Oxidation of Isoprene in the Presence of O_2 and NO. I. The Minor Inner OH-Addition Channel. <i>Journal of Physical Chemistry A</i> , 2010, 114, 904-912.	2.5	22
740	Si^{IV} -Ge-based Oxynitrides: From Molecules to Solids. <i>Chemistry of Materials</i> , 2010, 22, 3884-3899.	6.7	9
741	Vibrational Spectra, Crystal Structures, Constitutional and Rotational Isomerism of $FC(O)SCN$ and $FC(O)NCS$. <i>Inorganic Chemistry</i> , 2010, 49, 11142-11157.	4.0	14
742	Energetics and Structure of Nicotinic Acid (Niacin). <i>Journal of Physical Chemistry B</i> , 2010, 114, 5475-5485.	2.6	39
743	G4-SP, G4(MP2)-SP, G4-sc, and G4(MP2)-sc: Modifications to G4 and G4(MP2) for the Treatment of Medium-Sized Radicals. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2647-2653.	5.3	42
744	Detailed Modeling of Low-Temperature Propane Oxidation: 1. The Role of the $Propyl + O_2$ Reaction. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6594-6607.	2.5	70

#	ARTICLE	IF	CITATIONS
745	Isomerization and Decomposition of a Model Nerve Agent: A Computational Analysis of the Reaction Energetics and Kinetics of Dimethyl Ethylphosphonate. Journal of Physical Chemistry A, 2010, 114, 10717-10725.	2.5	17
746	Bond Dissociation Energies of Organophosphorus Compounds: an Assessment of Contemporary Ab Initio Procedures. Journal of Physical Chemistry A, 2010, 114, 2864-2873.	2.5	35
747	Stability and Structure of Protonated Clusters of Ammonia and Water, $H^+ \cdot (NH_3)_m \cdot (H_2O)_n$. Journal of Physical Chemistry A, 2010, 114, 7301-7310.	2.5	24
748	Crossed-Beam Imaging of the H Abstraction Channel in the Reaction of CN with 1-Pentene. Journal of Physical Chemistry Letters, 2010, 1, 2417-2421.	4.6	17
749	Vibrational Spectroscopy of Intermediates in Methane-to-Methanol Conversion by FeO^+ . Journal of Physical Chemistry A, 2010, 114, 5104-5112.	2.5	49
750	Focal point analysis of torsional isomers of acrylic acid. Molecular Physics, 2010, 108, 2601-2609.	1.7	4
751	First-Principles Prediction of the pK_a s of Anti-inflammatory Oxicams. Journal of Physical Chemistry A, 2010, 114, 11992-12003.	2.5	44
752	Accurate Proton Affinity and Gas-Phase Basicity Values for Molecules Important in Biocatalysis. Journal of Physical Chemistry B, 2010, 114, 13911-13921.	2.6	127
753	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. Industrial & Engineering Chemistry Research, 2010, 49, 10399-10420.	3.7	71
754	Accurate Predictions of Water Cluster Formation, $(H_2O)_n = 2 \times 10^n$. Journal of Physical Chemistry A, 2010, 114, 11725-11737.	2.5	213
755	Comment on "Important role of reaction field in photodegradation of deca-bromodiphenyl ether: Theoretical and experimental investigations of solvent effects" by Q. Xie, J. Chen, J. Shao, C. Chen, H. Zhao, C. Hao [Chemosphere 76(11) (2009) 1486-1490]. Chemosphere, 2010, 80, 676-678.	8.2	1
756	Theoretical Study of the Thermal Decomposition of Dimethyl Disulfide. Journal of Physical Chemistry A, 2010, 114, 10531-10549.	2.5	57
757	Intramolecular Hydrogen Migration in Alkylperoxy and Hydroperoxyalkylperoxy Radicals: Accurate Treatment of Hindered Rotors. Journal of Physical Chemistry A, 2010, 114, 5689-5701.	2.5	225
758	Quantum Chemical Study of the Acrolein $(CH_2=CHCHO) + OH + O_2$ Reactions. Journal of Physical Chemistry A, 2010, 114, 8302-8311.	2.5	63
759	The mechanism of the Stevens and Sommelet-Hauser Rearrangements. A Theoretical Study. Journal of Organic Chemistry, 2010, 75, 3608-3617.	3.2	73
760	Theoretical Calculation of Jet Fuel Thermochemistry. 1. Tetrahydrodicyclopentadiene (JP10) Thermochemistry Using the CBS-QB3 and G3(MP2)//B3LYP Methods. Journal of Organic Chemistry, 2010, 75, 4387-4391.	3.2	17
761	A Theoretical Approach for Accurate Predictions of the Enthalpies of Formation of Carotenes. Journal of Physical Chemistry A, 2010, 114, 12334-12344.	2.5	4
762	What happens at the microscopic level when CO ₂ reacts with ammonia or amines in solution or on cryogenic surfaces?. Energy and Environmental Science, 2010, 3, 1079.	30.8	10

#	ARTICLE	IF	CITATIONS
763	Computational Tests of Quantum Chemical Models for Structures, Vibrational Frequencies, and Heats of Formation of Molecules with Phosphorus and Sulfur Atoms. Journal of Physical Chemistry A, 2010, 114, 8142-8155.	2.5	12
764	Reaction free energies in organic solvents: comparing different quantum mechanical methods. Molecular Simulation, 2010, 36, 1197-1207.	2.0	4
765	Origins of Stereoselectivity in the <i>trans</i> Diels-Alder Paradigm. Journal of the American Chemical Society, 2010, 132, 9335-9340.	13.7	101
766	Theoretical Calculations of Acid Dissociation Constants: A Review Article. Annual Reports in Computational Chemistry, 2010, , 113-138.	1.7	160
767	Theoretical Study on the Mechanism of the Reaction of CF ₃ S with NO ₂ . Journal of Physical Chemistry A, 2010, 114, 1147-1152.	2.5	6
768	Probing the Influence of Anomeric Effects on the Lithium Ion Affinity in 1,3-Diaza Systems: A Computational Study. Journal of Physical Chemistry A, 2010, 114, 10684-10693.	2.5	8
769	The effect of tetramethylammonium ion on the voltammetric behavior of polycyclic aromatic hydrocarbons: computations explain a long-standing anomaly. Physical Chemistry Chemical Physics, 2010, 12, 14775.	2.8	16
770	Are cyclopentadienylberyllium, magnesium and calcium hydrides carbon or metal acids in the gas phase?. Dalton Transactions, 2010, 39, 4593.	3.3	11
771	Computational Investigation of the Reaction Mechanisms of Nitroxyl and Thiols. Journal of Organic Chemistry, 2010, 75, 4014-4024.	3.2	31
772	Arsine and its fluoro, chloro derivatives: a computational thermochemical study. Molecular Physics, 2010, 108, 1-11.	1.7	11
773	Modeling the influence of resonance stabilization on the kinetics of hydrogen abstractions. Physical Chemistry Chemical Physics, 2010, 12, 1278-1298.	2.8	51
774	Guided ion beam and theoretical studies of sequential bond energies of water to sodium cysteine cation. Physical Chemistry Chemical Physics, 2010, 12, 13419.	2.8	10
775	Probing the influence of electronic effects of organic additives on the morphology of sodium chloride crystals: a combined experimental and computational study. CrystEngComm, 2010, 12, 4168.	2.6	1
776	Towards cleaner combustion engines through groundbreaking detailed chemical kinetic models. Chemical Society Reviews, 2011, 40, 4762.	38.1	111
777	The enthalpies of formation of AsX _n molecules, where X = H, F or Cl, and n = 1, 2 or 3, by RCCSD(T) and UCCSD(T)-F12x calculations. Physical Chemistry Chemical Physics, 2011, 13, 9540.	2.8	15
778	Acid-base thermochemistry of gaseous oxygen and sulfur substituted amino acids (Ser, Thr, Cys, Met). Physical Chemistry Chemical Physics, 2011, 13, 18561.	2.8	34
779	Dynamics of H and D abstraction in the reaction of Cl atom with butane-1,1,1,4,4,4-d6. Physical Chemistry Chemical Physics, 2011, 13, 8433.	2.8	9
780	Dissociative photoionization mechanism of methanol isotopologues (CH ₃ OH, CD ₃ OH, CH ₃ OD and) Tj ETQq1 1 0.784314 rgBT /Overbo Chemistry Chemical Physics, 2011, 13, 13009.	2.8	48

#	ARTICLE	IF	CITATIONS
781	The association reaction between C ₂ H and 1-butyne: a computational chemical kinetics study. Physical Chemistry Chemical Physics, 2011, 13, 4583.	2.8	7
782	Detailed product analysis during the low temperature oxidation of n-butane. Physical Chemistry Chemical Physics, 2011, 13, 296-308.	2.8	108
783	Multiscale Modelling in Computational Heterogeneous Catalysis. Topics in Current Chemistry, 2011, 307, 69-107.	4.0	48
784	Unraveling the Mechanism of Cascade Reactions of Zincke Aldehydes. Journal of the American Chemical Society, 2011, 133, 3895-3905.	13.7	88
785	Understanding the Complex Dissociation Dynamics of Energy Selected Dichloroethylene Ions: Neutral Isomerization Energies and Heats of Formation by Imaging Photoelectron-Photoion Coincidence. Journal of Physical Chemistry A, 2011, 115, 726-734.	2.5	20
786	Atmospheric Reaction of the HOSO Radical with NO ₂ : A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 11008-11015.	2.5	12
787	Theoretical Study of Isomerization and Dissociation Transition States of C ₃ H ₅ O Radical Isomers: Ab Initio Characterization of the Critical Points and Statistical Transition-State Theory Modeling of the Dynamics. Journal of Physical Chemistry A, 2011, 115, 1701-1712.	2.5	15
788	Access to Oxetane-Containing <i>psico</i> -Nucleosides from 2-Methyleneoxetanes: A Role for Neighboring Group Participation?. Journal of Organic Chemistry, 2011, 76, 9962-9974.	3.2	26
789	Direct Detection of Products from the Pyrolysis of 2-Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2011, 115, 428-438.	2.5	160
790	Novel Products from C ₆ H ₅ + C ₆ H ₆ /C ₆ H ₅ Reactions. Journal of Physical Chemistry A, 2011, 115, 5284-5293.	2.5	45
791	Kinetic Modeling of the Free-Radical Process during the Initiated Thermal Cracking of Normal Alkanes with 1-Nitropropane as an Initiator. Industrial & Engineering Chemistry Research, 2011, 50, 9054-9062.	3.7	18
792	Thermodynamics and Mechanisms for Decomposition of Protonated Glycine and Its Protonated Dimer. Journal of Physical Chemistry A, 2011, 115, 11144-11155.	2.5	39
793	The Development of Continuous Process for Alkene Ozonolysis Based on Combined in Situ FTIR, Calorimetry, and Computational Chemistry. Organic Process Research and Development, 2011, 15, 91-97.	2.7	30
794	Theoretical Investigation into Competing Unimolecular Reactions Encountered in the Pyrolysis of Acetamide. Journal of Physical Chemistry A, 2011, 115, 14092-14099.	2.5	10
795	Conformational behaviours of 2-substituted cyclohexanones: a complete basis set, hybrid-DFT study and NBO interpretation. Molecular Simulation, 2011, 37, 1207-1220.	2.0	4
796	Thermal Decomposition Mechanisms of the Methoxyphenols: Formation of Phenol, Cyclopentadienone, Vinylacetylene, and Acetylene. Journal of Physical Chemistry A, 2011, 115, 13381-13389.	2.5	80
797	Kinetics and Mechanisms of the Allyl + Allyl and Allyl + Propargyl Recombination Reactions. Journal of Physical Chemistry A, 2011, 115, 7610-7624.	2.5	39
798	Pyrolysis Mechanisms of Thiophene and Methylthiophene in Asphaltenes. Journal of Physical Chemistry A, 2011, 115, 2882-2891.	2.5	27

#	ARTICLE	IF	CITATIONS
799	A Computational Study of <i>tert</i> -Butylbenzenium Ions. Journal of Physical Chemistry A, 2011, 115, 3106-3115.	2.5	15
800	Group Additivity Values for Estimating the Enthalpy of Formation of Organic Compounds: An Update and Reappraisal. 1. C, H, and O. Journal of Physical Chemistry A, 2011, 115, 10576-10586.	2.5	31
801	Thermal Decomposition of 2-Butanol as a Potential Nonfossil Fuel: A Computational Study. Journal of Physical Chemistry A, 2011, 115, 2837-2846.	2.5	36
802	G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2). Journal of Chemical Theory and Computation, 2011, 7, 112-120.	5.3	145
803	High-Level ab Initio Predictions for the Ionization Energies and Heats of Formation of Five-Membered-Ring Molecules: Thiophene, Furan, Pyrrole, 1,3-Cyclopentadiene, and Borole, $C_4H_4XC_4H_4X$ ($X = S, O, NH$). J. Phys. Chem. A, 2011, 115, 2210-2219.	2.5	22
804	Effects of Olefin Group and Its Position on the Kinetics for Intramolecular H-Shift and HO_2 Elimination of Alkenyl Peroxy Radicals. Journal of Physical Chemistry A, 2011, 115, 655-663.	2.5	46
805	Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. Journal of Physical Chemistry A, 2011, 115, 13628-13641.	2.5	25
806	Computational Study of Bond Dissociation Enthalpies for a Large Range of Native and Modified Lignins. Journal of Physical Chemistry Letters, 2011, 2, 2846-2852.	4.6	318
807	Projected Coupled Cluster Amplitudes from a Different Basis Set As Initial Guess. Journal of Chemical Theory and Computation, 2011, 7, 909-914.	5.3	2
808	Computational Study of the Reactions of Methanol with the Hydroperoxyl and Methyl Radicals. 1. Accurate Thermochemistry and Barrier Heights. Journal of Physical Chemistry A, 2011, 115, 2811-2829.	2.5	95
809	Ab Initio Analysis and Harmonic Force Fields of Gallium Nitride Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 6467-6477.	3.1	16
810	Mechanism and Kinetics of the Reaction $NO_3 + C_2H_4$. Journal of Physical Chemistry A, 2011, 115, 4894-4901.	2.5	15
811	Transition States and Energetics of Nucleophilic Additions of Thiols to Substituted α,β -Unsaturated Ketones: Substituent Effects Involve Enone Stabilization, Product Branching, and Solvation. Journal of Organic Chemistry, 2011, 76, 5074-5081.	3.2	84
812	Thermochemical Properties of Formamide Revisited: New Experiment and Quantum Mechanical Calculations. Journal of Chemical & Engineering Data, 2011, 56, 4183-4187.	1.9	27
813	Searching for Computational Strategies to Accurately Predict pK_a s of Large Phenolic Derivatives. Journal of Chemical Theory and Computation, 2011, 7, 2528-2538.	5.3	62
814	The Pyrolysis of Isoxazole Revisited: A New Primary Product and the Pivotal Role of the Vinylnitrene. A Low-Temperature Matrix Isolation and Computational Study. Journal of the American Chemical Society, 2011, 133, 18911-18923.	13.7	59
815	Solvent effect on keto-enol tautomerism in a new β -diketone: a comparison between experimental data and different theoretical approaches. New Journal of Chemistry, 2011, 35, 2840.	2.8	38
816	Extraordinary Difference in Reactivity of Ozone (OOO) and Sulfur Dioxide (OSO): A Theoretical Study. Journal of Chemical Theory and Computation, 2011, 7, 2104-2111.	5.3	63

#	ARTICLE	IF	CITATIONS
817	Systematic Computational Study on the Unimolecular Reactions of Alkylperoxy (RO_2), Hydroperoxyalkyl (QOOH), and Hydroperoxyalkylperoxy (O_2QOOH) Radicals. Journal of Physical Chemistry A, 2011, 115, 3301-3325.	2.5	196
818	Simulant Molecules with Trivalent or Pentavalent Phosphorus Atoms: Bond Dissociation Energies and Other Thermodynamic and Structural Properties from Quantum Chemical Models. Journal of Physical Chemistry A, 2011, 115, 8532-8539.	2.5	5
819	Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 3420-3437.	5.3	45
820	Kinetics and Mechanism of S-Nitrosothiol Acid-Catalyzed Hydrolysis: Sulfur Activation Promotes Facile NO Release. Journal of Physical Chemistry B, 2011, 115, 3112-3126.	2.6	27
821	Reply to Comments by O. V. Dorofeeva on <i>J. Chem. Eng. Data</i> 2010, 55, 5359-5364. Journal of Chemical & Engineering Data, 2011, 56, 684-685.	1.9	9
822	Theoretical calculation of heats of formation, bond dissociation energies, and gas-phase acidities of fluoromethanes, chloromethanes, and eight other monoderivatives of methane. Computational and Theoretical Chemistry, 2011, 968, 64-70.	2.5	6
823	Calculation of the properties of molecules in the pyridine catalyst system for the photochemical conversion of CO_2 to methanol. Computational and Theoretical Chemistry, 2011, 977, 123-127.	2.5	37
824	Chlorodifluoroacetyl Cyanide, $\text{ClF}_2\text{CC}(\text{O})\text{CN}$: Synthesis, Structure, and Spectroscopic Characterization. Inorganic Chemistry, 2011, 50, 9650-9659.	4.0	6
825	Kinetics of $\text{Al} + \text{H}_2\text{O}$ Reaction: Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 4476-4481.	2.5	40
826	A Mechanistic Study of the 2-Thienylmethyl + HO_2 Radical Recombination Reaction. Journal of Physical Chemistry A, 2011, 115, 14546-14557.	2.5	6
827	Inductive Effect: A Quantum Theory of Atoms in Molecules Perspective. Journal of Physical Chemistry A, 2011, 115, 12544-12554.	2.5	11
828	Theoretical studies in the molecular Platonic solids: Pure and mixed carbon, nitrogen, phosphorus, and silicon tetrahedranes. Nature Precedings, 2011, , .	0.1	1
830	Proton-donating power of 100% perchloric acid: An MP2 study. Kinetics and Catalysis, 2011, 52, 805-808.	1.0	1
831	The pure rotational spectra of the two lowest energy conformers of the asymmetric ether $\text{C}_4\text{H}_9\text{OC}_2\text{H}_5$. Journal of Molecular Spectroscopy, 2011, 269, 113-118.	1.2	4
832	Combustion chemistry and fuel-nitrogen conversion in a laminar premixed flame of morpholine as a model biofuel. Combustion and Flame, 2011, 158, 1647-1666.	5.2	64
833	Ab-initio assessment of conventional standard-state thermodynamic properties of geochemically relevant gaseous and aqueous species. Computers and Geosciences, 2011, 37, 646-661.	4.2	5
834	Theoretical Study of the Reaction of Carbon Monoxide with Oxygen Molecules in the Ground Triplet and Singlet Delta States. Journal of Physical Chemistry A, 2011, 115, 1795-1803.	2.5	15
835	High-Pressure Rate Rules for Alkyl + O_2 Reactions. 1. The Dissociation, Concerted Elimination, and Isomerization Channels of the Alkyl Peroxy Radical. Journal of Physical Chemistry A, 2011, 115, 13425-13442.	2.5	223

#	ARTICLE	IF	CITATIONS
836	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 269-279.	0.4	22
837	Computational Methods To Calculate Accurate Activation and Reaction Energies of 1,3-Dipolar Cycloadditions of 24 1,3-Dipoles. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13906-13920.	2.5	122
838	Ab initio Calculations. , 2011, , 175-390.		1
839	Density Functional Calculations. , 2011, , 445-519.		3
840	First-principles prediction of acidities in the gas and solution phase. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 649-660.	14.6	94
841	Gaussian theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 810-825.	14.6	189
842	Complete basis set, hybrid-DFT study, and NBO interpretations of the conformational behavior of 1,2-dihaloethanes. <i>Structural Chemistry</i> , 2011, 22, 253-262.	2.0	13
843	Theoretical studies on tautomerism of tetrazole 5-thion. <i>Structural Chemistry</i> , 2011, 22, 175-181.	2.0	22
844	Theoretical study of substituent and solvent effects on the thermodynamics for cis/trans isomerization and intramolecular rearrangements of 2,2-diphenyl-1,3-dioxane-4,5-dione. <i>Structural Chemistry</i> , 2011, 22, 615-625.	2.0	5
845	Theoretical investigation of reactivities of amines in the N-nitrosation reactions by N ₂ O ₃ . <i>Journal of Molecular Modeling</i> , 2011, 17, 669-680.	1.8	9
846	Cyclic dimers of tetrafluorobutatriene. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 507-515.	1.4	4
847	A computational study of the radical-radical reaction of O(3P) + C ₂ H ₅ with comparisons to gas-phase kinetics and crossed-beam experiments. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 105-118.	1.4	4
848	Computational study on the reaction of CH ₃ SCH ₂ CH ₃ with OH radical: mechanism and enthalpy of formation. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 771-780.	1.4	17
849	An examination of density functionals on aldol, Mannich and 1,2-aminooxylation reaction enthalpy calculations. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 153-160.	1.4	8
850	Avoiding gas-phase calculations in theoretical pK _a predictions. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 1-13.	1.4	65
851	Synthesis, structural and vibrational properties of 1-(4-Fluorobenzoyl)-3-(isomeric) 1,2,4-triazole. <i>Journal of Molecular Modeling</i> , 2011, 17, 105-118.	3.6	142
852	Interference-corrected explicitly-correlated second-order perturbation theory. <i>Chemical Physics Letters</i> , 2011, 503, 157-161.	2.6	25
853	Experimental study of the gas phase chemistry of C ₃ H ₃ ⁺ with several cyclic molecules. <i>International Journal of Mass Spectrometry</i> , 2011, 299, 139-144.	1.5	3

#	ARTICLE	IF	CITATIONS
854	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. Combustion and Flame, 2011, 158, 16-41.	5.2	240
855	Theoretical rate coefficients for allyl+HO ₂ and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	3.9	75
856	High pressure oxidation of C ₂ H ₄ /NO mixtures. Proceedings of the Combustion Institute, 2011, 33, 449-457.	3.9	38
857	Complete basis set, hybrid DFT study and NBO interpretations of conformational behaviors of trans-2,3- and trans-2,5-dihalo-1,4-dithianes. Journal of Physical Organic Chemistry, 2011, 24, 212-221.	1.9	12
858	Thermochemistry, bond energies and internal rotor barriers of methyl sulfinic acid, methyl sulfinic acid ester and their radicals. Journal of Physical Organic Chemistry, 2011, 24, 366-377.	1.9	10
859	Thermodynamic Characterization of Three Polymorphic Forms of Piracetam. Journal of Pharmaceutical Sciences, 2011, 100, 594-603.	3.3	20
860	First principle-based simulation of ethane steam cracking. AIChE Journal, 2011, 57, 482-496.	3.6	69
861	Construction of an ab initio kinetic model for industrial ethane pyrolysis. AIChE Journal, 2011, 57, 2458-2471.	3.6	19
862	Accurate Bond Energies of Hydrocarbons from Complete Basis Set Extrapolated Multi-Reference Singles and Doubles Configuration Interaction. ChemPhysChem, 2011, 12, 3354-3364.	2.1	13
863	Oxidative Addition of the C ₁ -C ₂ Bond in the C ₁ -O ₄ Linkage of Lignin to Transition Metals Using a Relativistic Pseudopotential-Based ccCA-ONION Method. ChemPhysChem, 2011, 12, 3320-3330.	2.1	26
864	The shape of gaseous n-butylbenzene: Assessment of computational methods and comparison with experiments. Journal of Computational Chemistry, 2011, 32, 1550-1560.	3.3	6
865	Probing the structural and electronic effects to stabilize nonplanar forms of thioamide derivatives: A computational study. Journal of Computational Chemistry, 2011, 32, 2170-2176.	3.3	10
866	Accurate prediction of the enthalpies of formation for xanthophylls. Journal of Computational Chemistry, 2011, 32, 3175-3187.	3.3	2
869	Experimental Detection of Trinitramide, N(NO ₂) ₃ . Angewandte Chemie - International Edition, 2011, 50, 1145-1148.	13.8	38
870	Diatomic [CuO] ⁺ and Its Role in the Spin-Selective Hydrogen- and Oxygen-Atom Transfers in the Thermal Activation of Methane. Angewandte Chemie - International Edition, 2011, 50, 4966-4969.	13.8	156
871	Conformational preferences and pK _a value of selenocysteine residue. Biopolymers, 2011, 95, 345-353.	2.4	34
872	Modeling the Gas-Phase Thermochemistry of Organosulfur Compounds. Chemistry - A European Journal, 2011, 17, 7656-7673.	3.3	44
873	Kinetic study on gas phase zinc reduction of silicon tetrachloride. Chemical Engineering Journal, 2011, 168, 889-895.	12.7	14

#	ARTICLE	IF	CITATIONS
874	Structure-reactivity trends of C1–C4 alkanolic acid methyl esters. <i>Combustion and Flame</i> , 2011, 158, 1037-1048.	5.2	61
875	Experimental and modeling study of the thermal decomposition of methyl decanoate. <i>Combustion and Flame</i> , 2011, 158, 1288-1300.	5.2	50
876	An experimental and kinetic investigation of premixed furan/oxygen/argon flames. <i>Combustion and Flame</i> , 2011, 158, 756-773.	5.2	113
877	Role of peroxy chemistry in the high-pressure ignition of n-butanol – Experiments and detailed kinetic modelling. <i>Combustion and Flame</i> , 2011, 158, 1444-1455.	5.2	121
878	Quantum chemical and RRKM/master equation studies of cyclopropene ozonolysis. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 305-312.	2.5	13
879	Rate coefficients of the reactions of isopentane with H and CH ₃ radicals: Quantum mechanical approach. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 357-364.	2.5	7
880	Deprotonation studies of Cu+–guanine and Cu ₂ +–guanine complexes by theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 490-496.	2.5	5
881	DFT study on the one-electron reduction of CF ₃ X (X=Cl, Br, I) molecules. <i>Computational and Theoretical Chemistry</i> , 2011, 966, 340-351.	2.5	5
882	A theoretical study of the NCN (3̂) biradical thermochemical properties: Implications for combustion chemistry. <i>Computational and Theoretical Chemistry</i> , 2011, 967, 67-74.	2.5	8
883	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <i>Chemical Physics Letters</i> , 2011, 510, 165-178.	2.6	353
884	Modeling reaction pathways of low energy particle deposition on thiophene via ab initio calculations. <i>Chemical Physics Letters</i> , 2011, 510, 197-201.	2.6	2
885	Kinetics of elementary reactions in low-temperature autoignition chemistry. <i>Progress in Energy and Combustion Science</i> , 2011, 37, 371-421.	31.2	586
886	Theoretical study of the thermochemistry and the kinetics of the SF _x Cl (x= 0–5) series. <i>Journal of Fluorine Chemistry</i> , 2011, 132, 474-481.	1.7	10
887	Ab initio energetics of nonsubstituted monocyclic pyrones. <i>Journal of Chemical Thermodynamics</i> , 2011, 43, 9-16.	2.0	6
888	New experimental evidences about the formation and consumption of ketohydroperoxides. <i>Proceedings of the Combustion Institute</i> , 2011, 33, 325-331.	3.9	64
889	The infrared and Raman spectra, ab initio calculations and spectral assignments of cyclopropylmethyl dichlorosilane (c-C ₃ H ₅)SiCl ₂ CH ₃ . <i>Vibrational Spectroscopy</i> , 2011, 56, 136-145.	2.2	8
890	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.	2.8	16
891	Electronic and vibrational spectroscopy of intermediates in methane-to-methanol conversion by CoO+. <i>Journal of Chemical Physics</i> , 2011, 135, 084311.	3.0	17

#	ARTICLE	IF	CITATIONS
892	Theoretical study on the gas and solution phase enthalpies, free energies and equilibrium constants for the isomerisation of [1.1]paracyclophane derivatives as potential molecular switches. Molecular Simulation, 2011, 37, 369-378.	2.0	0
894	Photoionization of epichlorohydrin enantiomers and clusters studied with circularly polarized vacuum ultraviolet radiation. Journal of Chemical Physics, 2011, 134, 064306.	3.0	38
895	Potential energy surface for dissociation including spin-orbit effects. Molecular Physics, 2012, 110, 2599-2609.	1.7	6
896	Ab initio calculation of ionization potential and electron affinity of six common explosive compounds. Reports in Theoretical Chemistry, 0, , 11.	0.0	31
897	Prediction of Thermodynamic and Kinetic Parameters for Interfacial Reactions of the SiO ₂ System by Quantum Chemistry Methods. Soft Materials, 2012, 10, 285-312.	1.7	3
898	From quantum chemical formation free energies to evaporation rates. Atmospheric Chemistry and Physics, 2012, 12, 225-235.	4.9	247
899	Amine substitution into sulfuric acid-ammonia clusters. Atmospheric Chemistry and Physics, 2012, 12, 3591-3599.	4.9	82
900	Carbonic acid revisited: Vibrational spectra, energetics and the possibility of detecting an elusive molecule. AIP Advances, 2012, 2, .	1.3	17
901	Mechanisms and Kinetics for the Thermal Decomposition of 2-Azido- <i>N,N</i> -Dimethylethanamine (DMAZ). Journal of Physical Chemistry A, 2012, 116, 3561-3576.	2.5	16
902	Liquid-phase dehydration of propylene glycol using solid-acid catalysts. Applied Catalysis A: General, 2012, 449, 59-68.	4.3	26
903	High-Level ab Initio Enthalpies of Formation of 2,5-Dimethylfuran, 2-Methylfuran, and Furan. Journal of Physical Chemistry A, 2012, 116, 11768-11775.	2.5	38
904	Hybrid Quantum and Classical Simulations of the Formate Dehydrogenase Catalyzed Hydride Transfer Reaction on an Accurate Semiempirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2012, 8, 4786-4796.	5.3	25
905	Hydride Dissociation Energies of Six-Membered Heterocyclic Organic Hydrides Predicted by ONIOM-G4Method. Journal of Chemical Information and Modeling, 2012, 52, 63-75.	5.4	16
906	Thermochemical Data and Additivity Group Values for Ten Species of <i>o</i> -Xylene Low-Temperature Oxidation Mechanism. Journal of Physical Chemistry A, 2012, 116, 592-610.	2.5	7
907	Quantum chemical study of the mechanism for OH-initiated atmospheric oxidation reaction of (Z)-CF ₃ CFCHF. Computational and Theoretical Chemistry, 2012, 991, 22-31.	2.5	9
908	High-Pressure Rate Rules for Alkyl + O ₂ Reactions. 2. The Isomerization, Cyclic Ether Formation, and β^2 -Scission Reactions of Hydroperoxy Alkyl Radicals. Journal of Physical Chemistry A, 2012, 116, 5068-5089.	2.5	172
909	Density functional theory for N ₂ O bond dissociation energies of N-nitroacylamide compounds in acetonitrile—Theoretical method assessment and prediction. Canadian Journal of Chemistry, 2012, 90, 526-533.	1.1	0
910	Complete basis set, hybrid-DFT study and NBO interpretation of conformational analysis of 2-methoxytetrahydropyran and its thiopyran and selenopyran analogues in relation to the anomeric effect. Molecular Simulation, 2012, 38, 1022-1031.	2.0	6

#	ARTICLE	IF	CITATIONS
911	Kinetics of $\dot{\text{I}}$ hydrogen abstractions from thiols, sulfides and thiocarbonyl compounds. Physical Chemistry Chemical Physics, 2012, 14, 12773.	2.8	29
912	Hydrogen abstraction from n-butanol by the methyl radical: high level ab initio study of abstraction pathways and the importance of low energy rotational conformers. Physical Chemistry Chemical Physics, 2012, 14, 9615.	2.8	15
913	Probing the O \cdots Br halogen bonding in X-ray crystal structures with ab initio calculations. CrystEngComm, 2012, 14, 1833.	2.6	13
914	Unusually Fast 1,6-H Shifts of Enolic Hydrogens in Peroxy Radicals: Formation of the First-Generation C ₂ and C ₃ Carbonyls in the Oxidation of Isoprene. Journal of Physical Chemistry A, 2012, 116, 6134-6141.	2.5	34
915	Bimolecular Rate Constant and Product Branching Ratio Measurements for the Reaction of C ₂ H with Ethene and Propene at 79 K. Journal of Physical Chemistry A, 2012, 116, 3907-3917.	2.5	32
916	Examining the heavy <i>p</i> -block with a pseudopotential-based composite method: Atomic and molecular applications of rp-ccCA. Journal of Chemical Physics, 2012, 137, 214111.	3.0	14
917	CO ₂ capture in aqueous ammonia solutions: a computational chemistry perspective. Physical Chemistry Chemical Physics, 2012, 14, 16301.	2.8	15
918	New mechanistic insights to the O(3P) + propene reaction from multiplexed photoionization mass spectrometry. Physical Chemistry Chemical Physics, 2012, 14, 10410.	2.8	51
919	Dissociation energies of X-H bonds in amino acids. Physical Chemistry Chemical Physics, 2012, 14, 3148.	2.8	38
920	Low-temperature combustion chemistry of biofuels: pathways in the initial low-temperature (550) Tj ETQq1 1 0.784314 rgBT/Overlook	2.8	88
921	Thermal Decomposition of 1-Pentanol and Its Isomers: A Theoretical Study. Journal of Physical Chemistry A, 2012, 116, 9238-9244.	2.5	44
922	Assessment of Density Functional Theory in Predicting Structures and Free Energies of Reaction of Atmospheric Prenucleation Clusters. Journal of Chemical Theory and Computation, 2012, 8, 2071-2077.	5.3	168
923	Computational Study of Isopropylbenzenium Ions. Journal of Physical Chemistry A, 2012, 116, 3710-3716.	2.5	10
924	Thermochemical Parameters and <i>p</i> K _a Values for Chlorinated Congeners of Thiophenol. Journal of Chemical & Engineering Data, 2012, 57, 1834-1842.	1.9	14
925	Synchrotron Photoionization Measurements of OH-Initiated Cyclohexene Oxidation: Ring-Preserving Products in OH + Cyclohexene and Hydroxycyclohexyl + O ₂ Reactions. Journal of Physical Chemistry A, 2012, 116, 6720-6730.	2.5	17
926	Improvement of the Modeling of the Low-Temperature Oxidation of <i>n</i> -Butane: Study of the Primary Reactions. Journal of Physical Chemistry A, 2012, 116, 6142-6158.	2.5	72
927	Study of the Low Temperature Oxidation of Propane. Journal of Physical Chemistry A, 2012, 116, 12214-12228.	2.5	57
928	Role of O ₂ + QOOH in Low-Temperature Ignition of Propane. 1. Temperature and Pressure Dependent Rate Coefficients. Journal of Physical Chemistry A, 2012, 116, 3325-3346.	2.5	223

#	ARTICLE	IF	CITATIONS
929	What is Wrong with Quantitative Structure–Property Relations Models Based on Three-Dimensional Descriptors?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1984-1993.	5.4	38
930	BDE261: A Comprehensive Set of High-Level Theoretical Bond Dissociation Enthalpies. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4975-4986.	2.5	62
931	The Reactivity of Air-Stable Pyridine- and Pyrimidine-Containing Diarylamine Antioxidants. <i>Journal of Organic Chemistry</i> , 2012, 77, 6895-6907.	3.2	40
932	Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3187-3206.	5.3	81
933	A Density Functional with Spherical Atom Dispersion Terms. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4989-5007.	5.3	463
934	Isomerization energies of tetrahedranes to 1,3-cyclobutadienes: A challenge for theoretical methods. <i>Computational and Theoretical Chemistry</i> , 2012, 979, 1-9.	2.5	8
935	Singlet–triplet excitation energies of naphthyl cations: High level composite method calculations suggest a singlet ground state. <i>Computational and Theoretical Chemistry</i> , 2012, 983, 69-75.	2.5	9
936	Effect of halogen substituents on C–N bond strength in nitromethane. <i>Computational and Theoretical Chemistry</i> , 2012, 985, 80-89.	2.5	3
937	Theoretical investigation on two-dimensional molecule-based second-order nonlinear optical materials of the disubstituted o-carborane derivatives. <i>Computational and Theoretical Chemistry</i> , 2012, 992, 142-149.	2.5	9
938	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.	2.5	20
939	Kinetic modeling for hydrogen-abstraction reaction of methylcyclohexane with the CH ₃ radical. <i>Chemical Engineering Science</i> , 2012, 79, 200-209.	3.8	5
940	A comprehensive study of methyl decanoate pyrolysis. <i>Energy</i> , 2012, 43, 146-160.	8.8	37
941	Calculation of the properties of the S ₃ ^{•−} radical anion and its complexes with Cu ⁺ in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 95, 79-92.	3.9	28
942	Comparison of some dispersion-corrected and traditional functionals with CCSD(T) and MP2 ab initio methods: Dispersion, induction, and basis set superposition error. <i>Journal of Chemical Physics</i> , 2012, 137, 134109.	3.0	49
943	Proton affinities of deoxyribonucleosides via the ONIOM–cCA methodology. <i>Journal of Computational Chemistry</i> , 2012, 33, 2590-2601.	3.3	6
944	Solvent Effect on the Potential Energy Surfaces for the One-Electron Reduction of CF ₃ X (X = Cl, Br, I) Molecules: A DFT PCM Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11694-11701.	2.5	4
945	Ab Initio Composite Approaches. <i>Annual Reports in Computational Chemistry</i> , 2012, 8, 29-51.	1.7	3
946	Detection of Mercury–TpT Dinucleotide Binding by Raman Spectra: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8313-8320.	2.5	19

#	ARTICLE	IF	CITATIONS
947	Theoretical Studies on the Unimolecular Decomposition of Ethylene Glycol. <i>Journal of Physical Chemistry A</i> , 2012, 116, 55-63.	2.5	30
948	Complete basis set, hybrid-density functional theory study, and natural bond orbital interpretations of the conformational behavior of halocarbonyl, thiocarbonyl, and selenocarbonyl isocyanates. <i>Canadian Journal of Chemistry</i> , 2012, 90, 333-343.	1.1	1
949	A pass too far: dissociation of internal energy selected paracyclophane cations, theory and experiment. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11920.	2.8	17
950	Experimental and modeling investigation of the low-temperature oxidation of n-heptane. <i>Combustion and Flame</i> , 2012, 159, 3455-3471.	5.2	165
951	The importance of deformation on the strength of beryllium bonds. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 74-79.	2.5	33
952	Accurate pKa calculations for trimethylaminium ion with a variety of basis sets and methods combined with CPCM continuum solvation methods. <i>Computational and Theoretical Chemistry</i> , 2012, 999, 1-6.	2.5	11
953	Complexes of prodigiosin (a naturally occurring pyrrolylpyrromethene) with H ⁺ , Cl ⁻ , and CO ₂ : A computational study. <i>Computational and Theoretical Chemistry</i> , 2012, 997, 103-109.	2.5	2
954	A computational study on the structures and energetics of isobutanol pyrolysis. <i>Computational and Theoretical Chemistry</i> , 2012, 997, 94-102.	2.5	9
955	Progress toward the Syntheses of (+)-GB 13, (+)-Himgaline, and Himandridine. New Insights into Intramolecular Imine/Enamine Aldol Cyclizations. <i>Journal of the American Chemical Society</i> , 2012, 134, 8162-8170.	13.7	29
956	Theoretical Determination of One-Electron Oxidation Potentials for Nucleic Acid Bases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 5107-5123.	5.3	72
957	On the possible catalysis by single water molecules of gas-phase hydrogen abstraction reactions by OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12992.	2.8	32
958	Explicitly correlated W ⁿ -F ⁿ theory: W1-F12 and W2-F12. <i>Journal of Chemical Physics</i> , 2012, 136, 124114.	3.0	229
959	Gas-Phase Studies of Purine 3-Methyladenine DNA Glycosylase II (AlkA) Substrates. <i>Journal of the American Chemical Society</i> , 2012, 134, 9622-9633.	13.7	28
960	Insufficient Hartree-Fock Exchange in Hybrid DFT Functionals Produces Bent Alkynyl Radical Structures. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 289-293.	4.6	19
961	Database of Small Molecule Thermochemistry for Combustion. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9033-9057.	2.5	178
962	Thermochemistry and Bond Dissociation Energies of Ketones. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5707-5722.	2.5	45
963	Thermochemical Properties for Hydrogenated and Oxy-Hydrogenated Aluminum Species. <i>Soft Materials</i> , 2012, 10, 313-343.	1.7	4
964	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 527-541.	5.3	661

#	ARTICLE	IF	CITATIONS
965	Tunneling in Hydrogen-Transfer Isomerization of <i>n</i> -Alkyl Radicals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 319-332.	2.5	70
966	C-H Bond Amination by Photochemically Generated Transient Borylnitrenes at Room Temperature: A Combined Experimental and Theoretical Investigation of the Insertion Mechanism and Influence of Substituents. <i>Organometallics</i> , 2012, 31, 3894-3903.	2.3	30
967	Explicitly correlated benchmark calculations on C ₈ H ₈ isomer energy separations: how accurate are DFT, double-hybrid, and composite <i>ab initio</i> procedures?. <i>Molecular Physics</i> , 2012, 110, 2477-2491.	1.7	63
968	Is Quantum Tunneling Relevant in Free-Radical Polymerization?. <i>Macromolecular Reaction Engineering</i> , 2012, 6, 496-506.	1.5	15
969	Product channels in the reaction of the CH ₃ SO radical with NO ₂ : DFT and <i>ab initio</i> studies. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1904-1912.	2.0	3
970	Theoretical thermochemistry: Enthalpies of formation of a set of nitrogen-containing compounds. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1688-1700.	2.0	14
971	Thermodynamic and kinetic analysis on the reaction of dimethyl sulfide radical with oxygen. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1945-1958.	2.0	11
972	Density functional study of the phenylethyl + O ₂ reaction: Kinetic analysis for the low-temperature autoignition of ethylbenzenes. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1968-1983.	2.0	8
973	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.	13.7	67
974	Evaluation of the reaction rate constants for the gas-phase Al-CH ₄ "air combustion chemistry. <i>Combustion Theory and Modelling</i> , 2012, 16, 842-868.	1.9	23
975	Direct measurement of Criegee intermediate (CH ₂ OO) reactions with acetone, acetaldehyde, and hexafluoroacetone. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10391.	2.8	143
976	Chlorodifluoroacetyl Azide, ClF ₂ CC(O)N ₃ : Preparation, Properties, and Decomposition. <i>Journal of Organic Chemistry</i> , 2012, 77, 6456-6462.	3.2	18
977	Kinetics for the hydrogen-abstraction of CH ₄ with NO ₂ . <i>Journal of Computational Chemistry</i> , 2012, 33, 1870-1879.	3.3	2
978	Gas phase basicities of polyfunctional molecules. Part 3: Amino acids. <i>Mass Spectrometry Reviews</i> , 2012, 31, 391-435.	5.4	59
979	The Kinetics and Thermodynamics of CO ₂ Capture by Aqueous Ammonia Derived Using Meta-GGA Density Functional Theory and Wavefunction-Based Model Chemistry Methods. <i>ACS Symposium Series</i> , 2012, , 99-131.	0.5	1
980	Mechanisms of ethylene glycol carbonylation with carbon dioxide. <i>Computational and Theoretical Chemistry</i> , 2012, 992, 103-109.	2.5	10
981	Theoretical Study of the Thermal Decomposition of the 5-Methyl-2-furanylmethyl Radical. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6675-6684.	2.5	61
982	Polarized continuum model study of bond dissociation energies of the "NO ₂ bond" A density functional theory study and natural bond order analysis. <i>Canadian Journal of Chemistry</i> , 2012, 90, 433-440.	1.1	0

#	ARTICLE	IF	CITATIONS
983	Thermochemical Properties and Bond Dissociation Energies of C3â€“C5 Cycloalkyl Hydroperoxides and Peroxy Radicals: Cycloalkyl Radical + 3O2 Reaction Thermochemistry. Journal of Physical Chemistry A, 2012, 116, 7550-7563.	2.5	13
984	Thermodynamics and Mechanisms of Protonated Diglycine Decomposition: A Computational Study. Journal of the American Society for Mass Spectrometry, 2012, 23, 621-631.	2.8	37
985	Molecular dynamics investigations of chlorine peroxide dissociation on a neural network ab initio potential energy surface. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	6
986	A theoretical study on the reaction mechanism of O2 with C4H9â€• radical. Journal of Molecular Modeling, 2012, 18, 2219-2226.	1.8	3
987	Kinetic mechanism of COâ€“H2 system oxidation promoted by excited singlet oxygen molecules. Combustion and Flame, 2012, 159, 16-29.	5.2	23
988	Experimental and modeling study of the oxidation of n-butylbenzene. Combustion and Flame, 2012, 159, 1399-1416.	5.2	59
989	A shock tube and chemical kinetic modeling study of the pyrolysis and oxidation of butanols. Combustion and Flame, 2012, 159, 2009-2027.	5.2	87
990	Fuel-nitrogen conversion in the combustion of small amines using dimethylamine and ethylamine as biomass-related model fuels. Combustion and Flame, 2012, 159, 2254-2279.	5.2	74
991	Gas-phase basicity and acidity of tryptophan. International Journal of Mass Spectrometry, 2012, 316-318, 47-56.	1.5	13
992	Mechanistic and kinetic study of the gas-phase reaction of vinyl acetate with ozone. Atmospheric Environment, 2012, 49, 197-205.	4.1	10
993	The interplay of hydrogen bonds in the solid state structure of NH-pyrazoles bearing cyano and amino substituents. Journal of Molecular Structure, 2012, 1014, 63-69.	3.6	5
994	Experimental and computational thermodynamic study of ortho-, meta-, and para-methylbenzamide. Journal of Chemical Thermodynamics, 2012, 47, 81-89.	2.0	17
995	The quinones of bicyclo[3.1.0]hexatriene: A computational study of their chemistry and thermochemistry. Journal of Chemical Thermodynamics, 2012, 52, 43-56.	2.0	3
996	Pressure dependence of phenylperoxy radical formation in the reaction of phenyl radical with molecular oxygen. International Journal of Chemical Kinetics, 2012, 44, 41-50.	1.6	20
997	Molecular size dependent falloff rate constants for the recombination reactions of alkyl radicals with O₂ and implications for simplified kinetics of alkylperoxy radicals. International Journal of Chemical Kinetics, 2012, 44, 59-74.	1.6	78
998	Computational study on the recombination reaction between benzyl and propargyl radicals. International Journal of Chemical Kinetics, 2012, 44, 206-218.	1.6	63
999	Detailed chemical kinetic modeling of JPâ€‘10 (<i>exo</i>-tetrahydrodicyclopentadiene) highâ€‘temperature oxidation: Exploring the role of biradical species in initial decomposition steps. International Journal of Chemical Kinetics, 2012, 44, 179-193.	1.6	43
1000	Converting ab initio energies to enthalpies of formation of free radicals. I. New atom equivalents for alkyl radicals. AIChE Journal, 2012, 58, 600-609.	3.6	2

#	ARTICLE	IF	CITATIONS
1001	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	381
1002	Computational thermochemistry of glycolaldehyde. International Journal of Quantum Chemistry, 2013, 113, 1147-1154.	2.0	4
1003	Structure and energetics of cyclopropane carboxaldehyde. International Journal of Quantum Chemistry, 2013, 113, 1155-1161.	2.0	4
1004	Theoretical study of gas phase reactions of important SOA intermediates: (<i>cis</i> - and <i>trans</i> -) BEPOX and β -EPOX with OH radical. International Journal of Quantum Chemistry, 2013, 113, 1162-1170.	2.0	0
1005	Computational study of tautomerism and aromaticity in mono- and dithio-substituted tropolone. International Journal of Quantum Chemistry, 2013, 113, 1245-1252.	2.0	9
1006	MP2 study of the proton-donating power of 100% fluorosulfonic and chlorosulfonic acids. Kinetics and Catalysis, 2013, 54, 284-289.	1.0	2
1007	Theoretical study of the complex reaction of O(3P) with trans-2-butene. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	4
1008	Density functional and chemical model study of the competition between methyl and hydrogen scission of propane and β -scission of the propyl radical. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	8
1009	In Silico Studies toward Understanding the Interactions of DNA Base Pairs with Protonated Linear/Cyclic Diamines. Journal of Physical Chemistry B, 2013, 117, 9840-9850.	2.6	4
1010	Reaction of Dimethyl Ether with Hydroxyl Radicals: Kinetic Isotope Effect and Prereactive Complex Formation. Journal of Physical Chemistry A, 2013, 117, 8343-8351.	2.5	47
1011	Anthrone and Related Hydroxyarenes: Tautomerization and Hydrogen Bonding. Journal of Organic Chemistry, 2013, 78, 7674-7682.	3.2	23
1012	Dissociation or Cyclization: Options for a Triad of Radicals Released from Oxime Carbamates. Journal of the American Chemical Society, 2013, 135, 7349-7354.	13.7	68
1013	Terahertz Spectra of Biotin Based on First Principle, Molecular Mechanical, and Hybrid Simulations. IEEE Transactions on Terahertz Science and Technology, 2013, 3, 357-362.	3.1	0
1014	Quantum Chemical Investigation on Indole: Vibrational Force Field and Theoretical Determination of Its Aqueous pK_a Value. Journal of Physical Chemistry A, 2013, 117, 6846-6858.	2.5	10
1015	Association reaction between SiH ₃ and H ₂ O ₂ : a computational study of the reaction mechanism and kinetics. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	7
1016	Styrene and ethylbenzene absorption in ionic liquids: comparing DFT affinity calculations with experimental data. Molecular Simulation, 2013, 39, 94-108.	2.0	0
1017	[BH ₃ C(NO ₂) ₃] ⁺ : The First Room-Temperature Stable (Trinitromethyl)borate. Angewandte Chemie - International Edition, 2013, 52, 11002-11006.	13.8	23
1018	Thermal decomposition of 2-phenylethanol: A computational study on mechanism. Chemical Physics Letters, 2013, 556, 29-34.	2.6	12

#	ARTICLE	IF	CITATIONS
1019	The Iminyl Radical O_2 SN. Angewandte Chemie - International Edition, 2013, 52, 7981-7984.	13.8	35
1020	Theoretical studies on the structures, heats of formation, energetic properties and pyrolysis mechanisms of nitrogen-rich difurazano[3,4-b:3',4'-e]piperazine derivatives and their analogues. Structural Chemistry, 2013, 24, 1071-1087.	2.0	34
1021	Structure of genipin in solution: a combined experimental and theoretical study. RSC Advances, 2013, 3, 13764.	3.6	15
1022	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, 1-57.		1
1023	Spin-component-scaled double hybrids: An extensive search for the best fifth-generation functionals blending DFT and perturbation theory. Journal of Computational Chemistry, 2013, 34, 2327-2344.	3.3	292
1024	Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. Journal of Chemical Theory and Computation, 2013, 9, 3947-3958.	5.3	38
1025	Theoretical study on the kinetics and the mechanism for the gas-phase reaction of 1-naphthylmethyl radical with molecular oxygen. Chemical Physics Letters, 2013, 585, 27-32.	2.6	3
1026	Ultraviolet Photodissociation of the <i>N</i> -Methylpyridinium Ion: Action Spectroscopy and Product Characterization. Journal of Physical Chemistry A, 2013, 117, 10839-10846.	2.5	6
1027	Experimental and Kinetic Modeling Study of Methanol Ignition and Oxidation at High Pressure. International Journal of Chemical Kinetics, 2013, 45, 283-294.	1.6	55
1028	Ionization of ammonium dinitramide: decomposition pathways and ionization products. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	9
1029	Halogenation effects in intramolecular furan Diels-Alder reactions: broad scope synthetic and computational studies. Organic and Biomolecular Chemistry, 2013, 11, 7946.	2.8	15
1030	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	4.6	38
1031	Low-Temperature Combustion Chemistry of <i>n</i> -Butanol: Principal Oxidation Pathways of Hydroxybutyl Radicals. Journal of Physical Chemistry A, 2013, 117, 11983-12001.	2.5	40
1032	Theoretical study of structure and physical properties of $(Al_2O_3)_n$ clusters. Physica Scripta, 2013, 88, 058307.	2.5	20
1033	On the kinetics of the $C_5H_5 + C_5H_5$ reaction. Proceedings of the Combustion Institute, 2013, 34, 557-564.	3.9	72
1034	Rate Rules, Branching Ratios, and Pressure Dependence of the $HO_2 + Olefin$ Addition Channels. Journal of Physical Chemistry A, 2013, 117, 6458-6473.	2.5	57
1035	Facile Rearrangement of 3-Oxoalkyl Radicals is Evident in Low-Temperature Gas-Phase Oxidation of Ketones. Journal of the American Chemical Society, 2013, 135, 14256-14265.	13.7	18
1036	The Pivotal Role of Oxyallyl Diradicals in Photo-Favorskii Rearrangements: Transient Spectroscopic and Computational Studies. Journal of the American Chemical Society, 2013, 135, 15209-15215.	13.7	22

#	ARTICLE	IF	CITATIONS
1037	Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate CH ₃ CHOO. Science, 2013, 340, 177-180.	12.6	379
1038	Theoretical studies on the kinetics and mechanism of the reaction of atomic hydrogen with carbon dioxide. Kinetics and Catalysis, 2013, 54, 671-676.	1.0	1
1039	Terahertz Spectra of Biotin Based on First Principle, Molecular Mechanical, and Hybrid Simulations. IEEE Journal of Biomedical and Health Informatics, 2013, 17, 768-773.	6.3	3
1040	Directly measuring reaction kinetics of $\dot{\text{E}}^{\text{TM}}\text{QOOH}$ – a crucial but elusive intermediate in hydrocarbon autoignition. Physical Chemistry Chemical Physics, 2013, 15, 10753.	2.8	58
1041	Thermochemical Properties for Isooctane and Carbon Radicals: Computational Study. Journal of Physical Chemistry A, 2013, 117, 421-429.	2.5	20
1042	Annuloselectivity in Cycloadditions of Ketenes with Imines: A DFT Study. Journal of Organic Chemistry, 2013, 78, 347-355.	3.2	32
1043	Functional group dependence of the acid catalyzed ring opening of biomass derived furan rings: an experimental and theoretical study. Catalysis Science and Technology, 2013, 3, 106-115.	4.1	51
1044	Thermodynamics of the Carbon Dioxide–Epoxide Copolymerization and Kinetics of the Metal-Free Degradation: A Computational Study. Macromolecules, 2013, 46, 83-95.	4.8	73
1045	Unimolecular decomposition of 2,5-dimethylfuran: a theoretical chemical kinetic study. Physical Chemistry Chemical Physics, 2013, 15, 596-611.	2.8	50
1046	Rate constants of hydrogen abstraction by methyl radical from n-butanol and a comparison of CanTherm, MultiWell and Variflex. Proceedings of the Combustion Institute, 2013, 34, 483-491.	3.9	16
1047	G3X-K theory: A composite theoretical method for thermochemical kinetics. Chemical Physics Letters, 2013, 558, 109-113.	2.6	46
1048	Theoretical kinetic investigation of thermal decomposition of methylcyclohexane. Computational and Theoretical Chemistry, 2013, 1026, 38-45.	2.5	11
1049	How acidic are monomeric structural units of heparin?. Chemical Physics Letters, 2013, 590, 187-191.	2.6	17
1050	Fragmentation reactions of Si ₂ Cl ₆ ⁺ in the gas phase – A quantum-chemical and mass-spectrometric assessment. International Journal of Mass Spectrometry, 2013, 354-355, 378-390.	1.5	5
1051	Conformation-specific dissociative photoionization of oxalyl chloride in the gas phase. Chemical Physics, 2013, 416, 26-32.	1.9	6
1052	Design and implementation of a next-generation software interface for on-the-fly quantum and force field calculations in automated reaction mechanism generation. Computers and Chemical Engineering, 2013, 52, 35-45.	3.8	48
1053	Thermochemistry and kinetics of isobutanol oxidation by the OH radical. Fuel, 2013, 106, 431-436.	6.4	10
1054	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.	2.5	11

#	ARTICLE	IF	CITATIONS
1055	Mechanistic study on the reaction of the CH ₂ ClO ₂ radical with NO. Chemical Physics Letters, 2013, 579, 28-34.	2.6	1
1056	NNO ₂ bond dissociation energies in acetonitrile: An assessment of contemporary computational methods. Journal of Molecular Graphics and Modelling, 2013, 43, 66-71.	2.4	2
1057	Critical Evaluation of Implicit Solvent Models for Predicting Aqueous Oxidation Potentials of Neutral Organic Compounds. Journal of Chemical Theory and Computation, 2013, 9, 5046-5058.	5.3	105
1058	An experimental and kinetic modeling investigation on a rich premixed n-propylbenzene flame at low pressure. Proceedings of the Combustion Institute, 2013, 34, 1785-1793.	3.9	41
1059	New experimental evidence and modeling study of the ethylbenzene oxidation. Proceedings of the Combustion Institute, 2013, 34, 325-333.	3.9	48
1060	Energetics of H-atom addition to naphthalene: A thermochemical cycle from tetralin to naphthalene. Journal of Chemical Thermodynamics, 2013, 61, 83-89.	2.0	3
1061	The reaction of 2,5-dimethylfuran with hydrogen atoms " An experimental and theoretical study. Proceedings of the Combustion Institute, 2013, 34, 233-239.	3.9	40
1062	Theoretical investigation into the low-temperature oxidation of ethylbenzene. Proceedings of the Combustion Institute, 2013, 34, 315-323.	3.9	16
1063	Theoretical study of the reaction 2,5-dimethylfuran + H " products. Proceedings of the Combustion Institute, 2013, 34, 241-249.	3.9	44
1064	VUV photoionization and dissociation of o-nitrotoluene: Experimental and theoretical insights. Journal of Electron Spectroscopy and Related Phenomena, 2013, 191, 41-47.	1.7	6
1065	Experimental and Modeling Study of Premixed Laminar Flames of Ethanol and Methane. Energy & Fuels, 2013, 27, 2226-2245.	5.1	44
1066	Low temperature oxidation of benzene and toluene in mixture with n-decane. Proceedings of the Combustion Institute, 2013, 34, 297-305.	3.9	42
1067	Effects of Protonation and C5 Methylation on the Electrophilic Addition Reaction of Cytosine: A Computational Study. Journal of Physical Chemistry B, 2013, 117, 3-12.	2.6	16
1068	Hierarchy of Relative Bond Dissociation Enthalpies and Their Use to Efficiently Compute Accurate Absolute Bond Dissociation Enthalpies for C-H, C-C, and C-F Bonds. Journal of Physical Chemistry A, 2013, 117, 3666-3675.	2.5	32
1069	An improved B3LYP method in the calculation of organic thermochemistry and reactivity. Computational and Theoretical Chemistry, 2013, 1015, 64-71.	2.5	56
1070	Unimolecular Reaction Mechanism of an Imidazolin-2-ylidene: An iPEPICO Study on the Complex Dissociation of an Arduengo-Type Carbene. Chemistry - A European Journal, 2013, 19, 7090-7099.	3.3	33
1071	The ammonium nitrate and its mechanism of decomposition in the gas phase: a theoretical study and a DFT benchmark. Physical Chemistry Chemical Physics, 2013, 15, 10849.	2.8	43
1072	Absolute photoionization cross-sections of selected furanic and lactonic potential biofuels. International Journal of Mass Spectrometry, 2013, 348, 39-46.	1.5	20

#	ARTICLE	IF	CITATIONS
1073	Reaction Rate and Isomer-Specific Product Branching Ratios of $C_2H + C_4H_8$: 1-Butene, <i>cis</i> -2-Butene, <i>trans</i> -2-Butene, and Isobutene at 79 K. Journal of Physical Chemistry A, 2013, 117, 5093-5105.	2.5	14
1074	Threshold Photoionization of Fluorenyl, Benzhydryl, Diphenylmethylene, and Their Dimers. Journal of Physical Chemistry A, 2013, 117, 5260-5268.	2.5	14
1075	Novel inhibitors of a Grb2 SH3C domain interaction identified by a virtual screen. Bioorganic and Medicinal Chemistry, 2013, 21, 4027-4033.	3.0	6
1076	Mechanisms of Lactone Hydrolysis in Acidic Conditions. Journal of Organic Chemistry, 2013, 78, 6880-6889.	3.2	29
1077	Revealing the chemistry of biomass pyrolysis by means of tunable synchrotron photoionisation-mass spectrometry. RSC Advances, 2013, 3, 4786.	3.6	54
1078	Thermodynamically sick molecules: searching for defective experimental enthalpies of formation values using empirical and quantum chemistry methods. Structural Chemistry, 2013, 24, 2017-2026.	2.0	1
1079	First principles modelling of free-radical polymerisation kinetics. International Reviews in Physical Chemistry, 2013, 32, 467-513.	2.3	63
1080	Mechanisms of Prebiotic Adenine Synthesis from HCN by Oligomerization in the Gas Phase. Astrobiology, 2013, 13, 465-475.	3.0	32
1081	Computational Nanochemistry Report on the Oxicams Conceptual DFT Indices and Chemical Reactivity. Journal of Physical Chemistry B, 2013, 117, 6339-6351.	2.6	35
1082	Enthalpies of formation of mono substituted nitrobenzenes: A quantum chemistry study. Computational and Theoretical Chemistry, 2013, 1011, 37-43.	2.5	13
1083	Theoretical study of substituents effect on C–NO ₂ bond strength in mono substituted nitrobenzenes. Computational and Theoretical Chemistry, 2013, 1017, 7-13.	2.5	13
1084	Dissociation of the Fluorine Molecule. Journal of Physical Chemistry A, 2013, 117, 5518-5528.	2.5	22
1085	The conversion of protonated cytosine-SO ₃ ⁺ to uracil-SO ₃ ⁺ : Insights into the novel induced hydrolytic deamination through bisulfite catalysis. Physical Chemistry Chemical Physics, 2013, 15, 9034.	2.8	9
1086	Shock tube measurements and model development for morpholine pyrolysis and oxidation at high pressures. Combustion and Flame, 2013, 160, 1559-1571.	5.2	12
1087	Theoretical study on the molecular tautomerism of the 3-hydroxy-pyridin-4-one system. Molecular Physics, 2013, 111, 958-967.	1.7	8
1088	Spectroscopic Characterization and Constitutional and Rotational Isomerism of ClC(O)SCN and ClC(O)NCS. Journal of Physical Chemistry A, 2013, 117, 2383-2399.	2.5	6
1089	Thermochemical Properties of Methyl-Substituted Cyclic Alkyl Ethers and Radicals for Oxiranes, Oxetanes, and Oxolanes: C–H Bond Dissociation Enthalpy Trends with Ring Size and Ether Site. Journal of Physical Chemistry A, 2013, 117, 378-392.	2.5	19
1090	Base initiated depolymerization of polycarbonates to epoxide and carbon dioxide co-monomers: a computational study. Green Chemistry, 2013, 15, 1578.	9.0	53

#	ARTICLE	IF	CITATIONS
1091	Computational Quantification of the Physicochemical Effects of Heme Distortion: Redox Control in the Reaction Center Cytochrome Subunit of <i>Blastochloris viridis</i> . <i>Inorganic Chemistry</i> , 2013, 52, 1228-1237.	4.0	20
1092	Reaction Kinetics of Hydrogen Abstraction Reactions by Hydroperoxyl Radical from 2-Methyltetrahydrofuran and 2,5-Dimethyltetrahydrofuran. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5028-5041.	2.5	31
1093	Determination of Proton Affinities and Acidity Constants of Sugars. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5211-5219.	2.5	81
1094	Mechanism of Homogeneous Reduction of CO ₂ by Pyridine: Proton Relay in Aqueous Solvent and Aromatic Stabilization. <i>Journal of the American Chemical Society</i> , 2013, 135, 142-154.	13.7	151
1095	Theoretical study on the structures, stabilities and electronic properties of S ₂ O ₅ ²⁻ isomers in the gas and solution phases. <i>Molecular Physics</i> , 2013, 111, 581-588.	1.7	1
1096	A Classical Trajectory Study of the Dissociation and Isomerization of C ₂ H ₅ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 11624-11639.	2.5	9
1097	Theoretical calculations of stability constants and pK _a values of metal complexes in solution: application to pyridoxamine-copper(II) complexes and their biological implications in AGE inhibition. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 16303.	2.8	34
1098	Quantum Chemical and Kinetics Study of the Thermal Gas Phase Decomposition of 2-Chloropropene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10218-10227.	2.5	9
1099	Product Branching Fractions of the CH + Propene Reaction from Synchrotron Photoionization Mass Spectrometry. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6450-6457.	2.5	22
1100	Kinetics and Mechanism of the Tropospheric Oxidation of Vinyl Acetate Initiated by OH Radical: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3739-3750.	2.5	44
1101	Isomer Specific Product Detection in the Reaction of CH with Acrolein. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11013-11026.	2.5	13
1102	Explicitly Correlated Methods within the ccCA Methodology. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1402-1407.	5.3	26
1103	Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of N-Cl and N-Br Bonds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 460-472.	2.5	22
1104	Energetics of Atmospherically Implicated Clusters Made of Sulfuric Acid, Ammonia, and Dimethyl Amine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3819-3825.	2.5	102
1105	Reactive Bond-Order Potential for Si-, C-, and H-Containing Materials. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1323-1334.	3.1	10
1106	CIMS Sulfuric Acid Detection Efficiency Enhanced by Amines Due to Higher Dipole Moments: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14109-14119.	2.5	33
1107	Theoretical study on thermochemical parameters and IR spectra of chlorinated isomers of nitrobenzene. <i>Canadian Journal of Chemistry</i> , 2013, 91, 999-1008.	1.1	4
1108	Theoretical study of the complex reaction of O(3P) with cis-2-butene. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	4

#	ARTICLE	IF	CITATIONS
1109	Human farnesyl pyrophosphate synthase inhibition by nitrogen bisphosphonates: a 3D-QSAR study. Journal of Computer-Aided Molecular Design, 2013, 27, 739-754.	2.9	12
1110	Theoretical Support for the Involvement of a Radical Pathway in the Formation of Allenylzincs from Propargyl Iodides and Dialkylzincs: Influence of Zinc Coordination. Journal of Organic Chemistry, 2013, 78, 1589-1603.	3.2	11
1111	Computational Prediction of One-Electron Reduction Potentials and Acid Dissociation Constants for Guanine Oxidation Intermediates and Products. Journal of Physical Chemistry B, 2013, 117, 9518-9531.	2.6	43
1112	Kinetics of Decomposition and Isomerization of Methylcyclohexane: Starting Point for Studying Monoalkylated Cyclohexanes Combustion. Energy & Fuels, 2013, 27, 1679-1687.	5.1	44
1113	G3 Assisted Rational Design of Chemical Sensor Array Using Carbonitrile Neutral Receptors. Sensors, 2013, 13, 13835-13860.	3.8	4
1114	Understanding the Initial Decomposition Pathways of the <i>n</i> -Alkane/Nitroalkane Binary Mixture. Chinese Journal of Chemistry, 2013, 31, 1087-1094.	4.9	12
1115	Photochemistry of aqueous pyruvic acid. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 11714-11719.	7.1	118
1116	Free energy barrier in the growth of sulfuric acid-ammonia and sulfuric acid-dimethylamine clusters. Journal of Chemical Physics, 2013, 139, 084312.	3.0	164
1117	DENSITY FUNCTIONAL STUDY OF THE EFFECTS OF THE SUBSTITUENTS ON THE CHEMICAL REACTIVITY OF THE INDIGO MOLECULE. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350013.	1.8	8
1118	Biomass pyrolysis: Thermal decomposition mechanisms of furfural and benzaldehyde. Journal of Chemical Physics, 2013, 139, 104310.	3.0	63
1119	Proton affinities of candidates for positively charged ambient ions in boreal forests. Atmospheric Chemistry and Physics, 2013, 13, 10397-10404.	4.9	11
1121	Kinetics of Homolytic Substitutions by Hydrogen Atoms at Thiols and Sulfides. ChemPhysChem, 2013, 14, 1703-1722.	2.1	12
1122	Kinetic Modeling of Hydrogen Abstractions Involving Sulfur Radicals. ChemPhysChem, 2013, 14, 3751-3771.	2.1	19
1124	Development of Gasoline Combustion Reaction Model. , 0, , .		9
1125	Unusual Structure-Energy Correlations in Intramolecular Diels-Alder Reaction Transition States. Molecules, 2014, 19, 15535-15545.	3.8	3
1128	A New Paradigm in Oxidative Cleavage Reaction: The Use of Continuous Reactors To Enable Safe Scale Up of Ozonolysis. ACS Symposium Series, 2014, , 353-382.	0.5	5
1129	Quantum chemical prediction of structure and stability of the benzodihydropyrimidine tautomers. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450056.	1.8	2
1130	Reaction mechanism and kinetic study of the OH initiated tropospheric oxidation of 3-methyl-2-buten-1-ol: A quantum chemical investigation. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450052.	1.8	1

#	ARTICLE	IF	CITATIONS
1131	Assessment of theoretical procedures for a diverse set of isomerization reactions involving double-bond migration in conjugated dienes. Chemical Physics, 2014, 441, 166-177.	1.9	49
1132	Intramolecular stabilization of the silylene center due to the donor-acceptor interaction with a valence-unbonded nitrogen atom. A theoretical consideration. Russian Chemical Bulletin, 2014, 63, 2599-2604.	1.5	0
1133	Determination of acidic dissociation constants of glutamine and isoleucine in water using ab initio methods. Turkish Journal of Biochemistry, 0, , .	0.5	1
1134	Photoionization and Pyrolysis of a 1,4-Azaborinine: Retro-Hydroboration in the Cation and Identification of Novel Organoboron Ring Systems. Chemistry - A European Journal, 2014, 20, 9683-9692.	3.3	22
1135	Decomposition of Diazomeldrum™s Acid: A Threshold Photoelectron Spectroscopy Study. Journal of Physical Chemistry A, 2014, 118, 11235-11243.	2.5	9
1136	Further Insight into the Reaction $\text{FeO}^{+} + \text{H}_2 \rightarrow \text{Fe}^{+} + \text{H}_2\text{O}$: Temperature Dependent Kinetics, Isotope Effects, and Statistical Modeling. Journal of Physical Chemistry A, 2014, 118, 6789-6797.	2.5	38
1137	Systematic testing of Gaussian and complete basis set methods with dispersion corrections for environmentally relevant clusters. Chemical Physics Letters, 2014, 615, 50-55.	2.6	1
1138	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.	1.8	3
1139	An efficient extrapolation to the (T)/CBS limit. Journal of Chemical Physics, 2014, 140, 184116.	3.0	1
1140	Hypervalence in monoxides and dioxides of superalkali clusters. Journal of Chemical Physics, 2014, 140, 204319.	3.0	12
1141	A computational study on the mechanism and kinetics of the reaction between $\text{CH}_3\text{CH}_2\text{S}$ and OH. RSC Advances, 2014, 4, 62835-62843.	3.6	2
1142	A polarizable dipole-dipole interaction model for evaluation of the interaction energies for $\text{Ni}(\text{H}_2\text{O})_4$ and $\text{Cu}(\text{H}_2\text{O})_4$ hydrogen-bonded complexes. Journal of Computational Chemistry, 2014, 35, 415-426.	3.3	21
1143	Yield of Formyl Radical from the Vinyl + O_2 Reaction. International Journal of Chemical Kinetics, 2014, 46, 260-274.	1.6	10
1144	The p <i>K_a</i> theoretical estimation of $\text{C}_6\text{H}_5\text{N}$, N_2H_5 , O_2H and S_2H acids in dimethylsulfoxide solution. Journal of Physical Organic Chemistry, 2014, 27, 926-934.	1.9	10
1145	Theoretical study on $\text{S}(\text{H})_2$ reaction of methyl radical with three-membered ring. International Journal of Quantum Chemistry, 2014, 114, 1594-1601.	2.0	1
1146	Detection of nitrobenzene compounds in surface water by ion mobility spectrometry coupled with molecularly imprinted polymers. Journal of Hazardous Materials, 2014, 280, 588-594.	12.4	37
1147	Practical hyperdynamics method for systems with large changes in potential energy. Journal of Chemical Physics, 2014, 141, 234109.	3.0	12
1148	Unraveling polar Diels-Alder reactions with conceptual DFT analysis and the distortion/interaction model. Organic and Biomolecular Chemistry, 2014, 12, 187-199.	2.8	31

#	ARTICLE	IF	CITATIONS
1149	Burning velocities and kinetics of H ₂ /NF ₃ /N ₂ , CH ₄ /NF ₃ /N ₂ , and C ₃ H ₈ /NF ₃ /N ₂ flames. Combustion and Flame, 2014, 161, 1425-1431.	5.2	9
1150	A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi. Combustion and Flame, 2014, 161, 711-724.	5.2	54
1151	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. Combustion and Flame, 2014, 161, 2270-2287.	5.2	29
1152	Theoretic studies on the kinetics and mechanism of multi-channel gas-phase unimolecular reactions of 1-chloropropane and 2-chloropropane. Structural Chemistry, 2014, 25, 21-28.	2.0	4
1153	Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons. Journal of Chemical Physics, 2014, 140, 044317.	3.0	85
1154	Molecular properties of the PCO radical: heat of formation and the isomerization pathways. Journal of Molecular Modeling, 2014, 20, 2074.	1.8	14
1155	Thermodynamics and Mechanism of Protonated Cysteine Decomposition: A Guided Ion Beam and Computational Study. Journal of the American Society for Mass Spectrometry, 2014, 25, 512-523.	2.8	8
1156	Carbonic acid: molecule, crystal and aqueous solution. Chemical Communications, 2014, 50, 503-514.	4.1	29
1157	Theoretical study on the acidity behavior of some N-methylpyrazole derivatives: CBS-Q method and United Atom (UA) molecular cavity effect. Computational and Theoretical Chemistry, 2014, 1032, 65-72.	2.5	3
1158	A Computational Study of RXH _n Xâ€“H Bond Dissociation Enthalpies. Journal of Physical Chemistry A, 2014, 118, 2353-2359.	2.5	11
1160	Experimental and ab Initio Investigations of H ₂ S-Assisted Propane Oxidative Dehydrogenation Reactions. Journal of Physical Chemistry A, 2014, 118, 1541-1556.	2.5	11
1161	Computational estimates of thermochemistry and <i>p</i> K _a values of cyclopropenyl imine superbases. International Journal of Quantum Chemistry, 2014, 114, 392-399.	2.0	17
1162	Assessment of CCSD(T), MP2, DFT-D, CBS-QB3, and G4(MP2) methods for conformational study of alanine and proline dipeptides. Chemical Physics Letters, 2014, 600, 112-117.	2.6	38
1163	Oxidation Products of Biogenic Emissions Contribute to Nucleation of Atmospheric Particles. Science, 2014, 344, 717-721.	12.6	456
1164	Isomer-Specific Product Detection of Gas-Phase Xylyl Radical Rearrangement and Decomposition Using VUV Synchrotron Photoionization. Journal of Physical Chemistry A, 2014, 118, 3593-3604.	2.5	57
1166	Nitryl Cyanide, NCNO ₂ . Angewandte Chemie - International Edition, 2014, 53, 6893-6897.	13.8	45
1167	Determination of thermodynamic parameters of C2â€“C3 nitroalkanes using anharmonic oscillator approximation and explicit treatment of internal rotation. Computational and Theoretical Chemistry, 2014, 1039, 55-61.	2.5	1
1168	Kinetic Modeling of H-Atom Hydrogen Abstractions from Unsaturated and Saturated Oxygenate Compounds by Carbon-Centered Radicals. ChemPhysChem, 2014, 15, 1849-1866.	2.1	20

#	ARTICLE	IF	CITATIONS
1169	Conformational behaviors of trans-2,3- and trans-2,5-dihalo-1,4-diselenanes. A complete basis set, hybrid-density functional theory study and natural bond orbital interpretations. Journal of Molecular Modeling, 2014, 20, 2249.	1.8	9
1170	(E)-2-(Benzo[d]thiazol-2-yl)-3-heteroarylacrylonitriles as efficient Michael acceptors for cysteine: Real application in biological imaging. Sensors and Actuators B: Chemical, 2014, 193, 391-399.	7.8	8
1171	Ab initio chemical kinetics for the HCCO + OH reaction. Chemical Physics Letters, 2014, 592, 175-181.	2.6	8
1172	Thermochemistry, Reaction Paths, and Kinetics on the Secondary Isooctane Radical Reaction with 3 O ₂ . International Journal of Chemical Kinetics, 2014, 46, 71-103.	1.6	8
1173	Personal Adventures in the Synthesis of Copolymers from Carbon Dioxide and Cyclic Ethers. Advances in Inorganic Chemistry, 2014, , 1-23.	1.0	7
1174	Ab Initio Analysis of Silicon Nano-Clusters. Journal of Physical Chemistry C, 2014, 118, 1397-1406.	3.1	12
1175	A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , .	0.1	20
1176	Roaming dynamics in radical addition–elimination reactions. Nature Communications, 2014, 5, 4064.	12.8	47
1177	Partial Ionic Character beyond the Pauling Paradigm: Metal Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 28069-28074.	3.1	6
1178	The MC-DFT approach including the SCS-MP2 energies to the new minnesota-type functionals. Journal of Computational Chemistry, 2014, 35, 1560-1567.	3.3	4
1179	Photoionization Mass Spectrometric Measurements of Initial Reaction Pathways in Low-Temperature Oxidation of 2,5-Dimethylhexane. Journal of Physical Chemistry A, 2014, 118, 10188-10200.	2.5	19
1180	Theoretical Kinetics Studies on the Reaction of CF ₃ •CF ₂ with Hydroxyl Radical. Journal of Physical Chemistry A, 2014, 118, 9941-9950.	2.5	12
1181	Molecular Dynamics of Methylamine, Methanol, and Methyl Fluoride Cations in Intense 7 Micron Laser Fields. Journal of Physical Chemistry A, 2014, 118, 10067-10072.	2.5	4
1182	A Dissociative Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation and Infrared Experiments Reveal Characteristics of the Strongly Hydrolytic Arsenic(III). Inorganic Chemistry, 2014, 53, 11861-11870.	4.0	10
1183	Theoretical study of the mechanisms and kinetics of the reactions of hydroperoxy (HO ₂) radicals with hydroxymethylperoxy (HOCH ₂ O ₂) and methoxymethylperoxy (CH ₃ OCH ₂ O ₂) radicals. Physical Chemistry Chemical Physics, 2014, 16, 22805-22814.	2.8	12
1184	The Catalytic Mechanism of Diarylamine Radical-Trapping Antioxidants. Journal of the American Chemical Society, 2014, 136, 16643-16650.	13.7	42
1185	Dynamics of Cl + propane, butanes revisited: a crossed beam slice imaging study. Physical Chemistry Chemical Physics, 2014, 16, 414-420.	2.8	6
1186	Thermochemistry of C ₇ H ₁₆ to C ₁₀ H ₂₂ Alkane Isomers: Primary, Secondary, and Tertiary C–H Bond Dissociation Energies and Effects of Branching. Journal of Physical Chemistry A, 2014, 118, 9364-9379.	2.5	44

#	ARTICLE	IF	CITATIONS
1187	Photoelectron ⁺ Photofragment Coincidence Studies of the <i>tert</i> -Butoxide Anion (CH ₃) ₃ CO ⁺ , the Carbanion Isomer (CH ₃) ₂ CH ₂ COH ⁺ , and Corresponding Radicals. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10223-10232.	2.5	4
1188	Computational electrochemistry: prediction of liquid-phase reduction potentials. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15068-15106.	2.8	407
1189	Low-temperature combustion chemistry of novel biofuels: resonance-stabilized QOOH in the oxidation of diethyl ketone. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13027-13040.	2.8	25
1190	Group Additivity Determination for Enthalpies of Formation of Carbenium Ions. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 19446-19452.	3.7	11
1191	The Successful Merger of Theoretical Thermochemistry with Fragment-Based Methods in Quantum Chemistry. <i>Accounts of Chemical Research</i> , 2014, 47, 3596-3604.	15.6	34
1192	Solar driven uphill conversion of dicyclopentadiene to cyclopentadiene: an important synthon for energy systems and fine chemicals. <i>RSC Advances</i> , 2014, 4, 54558-54564.	3.6	7
1193	A new insight into the 5-carboxycytosine and 5-formylcytosine under typical bisulfite conditions: a deamination mechanism study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3573.	2.8	9
1194	Thermal Dehydroboration: Experimental and Theoretical Studies of Olefin Elimination from Trialkylboranes and Its Relationship to Alkylborane Isomerization and Transalkylation. <i>Organometallics</i> , 2014, 33, 4251-4259.	2.3	14
1195	Azidonation derivatives of 1,1 TM ,4,4 TM -tetramethyl-2-tetrazene as nitrogen-rich compounds for NTO/MMH replacement - Synthesis, characterization and properties. , 2014, , .		0
1197	Assessment of the Density Functional Tight Binding Method for Protic Ionic Liquids. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4633-4643.	5.3	44
1198	Structure, Stability, and Spectroscopic Properties of H-Bonded Complexes of HOSO and CH ₃ SO with H ₂ O. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7855-7862.	2.5	12
1199	Accurate Bond Energies of Biodiesel Methyl Esters from Multireference Averaged Coupled-Pair Functional Calculations. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7392-7403.	2.5	44
1200	PAH Growth Initiated by Propargyl Addition: Mechanism Development and Computational Kinetics. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2865-2885.	2.5	69
1201	Trends in Bond Dissociation Energies of Alcohols and Aldehydes Computed with Multireference Averaged Coupled-Pair Functional Theory. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3039-3050.	2.5	36
1202	Oxidation of Reduced Sulfur Species: Carbon Disulfide. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6798-6809.	2.5	37
1203	Thermochemistry and Kinetics of Angelica and Cognate Lactones. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4172-4183.	2.5	11
1204	Molecular Dynamics of Methanol Monocation (CH ₃ OH ⁺) in Strong Laser Fields. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1769-1776.	2.5	11
1205	Comparison of Unimolecular Decomposition Pathways for Carboxylic Acids of Relevance to Biofuels. <i>Journal of Physical Chemistry A</i> , 2014, 118, 260-274.	2.5	34

#	ARTICLE	IF	CITATIONS
1206	CH ₂ NH ₂ + O ₂ and CH ₃ CHNH ₂ + O ₂ Reaction Kinetics: Photoionization Mass Spectrometry Experiments and Master Equation Calculations. Journal of Physical Chemistry A, 2014, 118, 2176-2186.	2.5	52
1207	Dynamics of Chlorine Atom Reactions with Hydrocarbons: Insights from Imaging the Radical Product in Crossed Beams. Journal of Physical Chemistry A, 2014, 118, 9281-9295.	2.5	27
1208	Catalyst activation and the dimerization energy of alkylaluminium compounds. Journal of Organometallic Chemistry, 2014, 772-773, 161-171.	1.8	59
1209	Experimental Study of the Mesospheric Removal of NF ₃ by Neutral Meteoric Metals and Lyman- α Radiation. Journal of Physical Chemistry A, 2014, 118, 4120-4129.	2.5	6
1210	Dehydrohalogenation of ethyl halides. Tetrahedron Letters, 2014, 55, 4860-4868.	1.4	36
1211	Hydrogen abstraction reactions of hydroxyl radicals with 1,1,2,2-tetrachloroethane, 1,1,1,2-tetrachloroethane and pentachloroethane studied by using semi-classical transition state theory. Molecular Physics, 2014, 112, 2979-2986.	1.7	0
1212	Proton Affinity Calculations with High Level Methods. Journal of Chemical Theory and Computation, 2014, 10, 3123-3128.	5.3	30
1213	Reactivity for the Diels-Alder Reaction of Cumulenes: A Distortion-Interaction Analysis along the Reaction Pathway. Journal of Physical Chemistry A, 2014, 118, 2638-2645.	2.5	79
1214	Theoretical Study of the Oxidation Mechanisms of Naphthalene Initiated by Hydroxyl Radicals: The OH-Addition Pathway. Journal of Physical Chemistry A, 2014, 118, 4593-4610.	2.5	65
1215	Theoretical ρ -K _a calculations with continuum model solvents, alternative protocols to thermodynamic cycles. International Journal of Quantum Chemistry, 2014, 114, 1350-1363.	2.0	88
1216	Solv-ccCA: Implicit Solvation and the Correlation Consistent Composite Approach for the Determination of ρ -K _a . Journal of Chemical Theory and Computation, 2014, 10, 1500-1510.	5.3	21
1217	Hydration of Atmospherically Relevant Molecular Clusters: Computational Chemistry and Classical Thermodynamics. Journal of Physical Chemistry A, 2014, 118, 2599-2611.	2.5	98
1218	Absolute Rate Constants for Hydrogen Atom Transfer from Tertiary Amides to the Cumyloxyl Radical: Evaluating the Role of Stereoelectronic Effects. Journal of Organic Chemistry, 2014, 79, 7179-7184.	3.2	29
1219	Products from the Oxidation of Linear Isomers of Hexene. Journal of Physical Chemistry A, 2014, 118, 673-683.	2.5	50
1220	Kinetic Modeling of $\dot{\text{H}}$ -Hydrogen Abstractions from Unsaturated and Saturated Oxygenate Compounds by Hydrogen Atoms. Journal of Physical Chemistry A, 2014, 118, 9296-9309.	2.5	20
1221	Thermal decomposition and isomerization of 1-heptyl radical: a computational investigation. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
1222	Theoretical Study of Chain Transfer to Agent Kinetics in Butyl Acrylate Polymerization. Industrial & Engineering Chemistry Research, 2014, 53, 9058-9066.	3.7	15
1223	Kinetics of Homoallylic/Homobenzylic Rearrangement Reactions under Combustion Conditions. Journal of Physical Chemistry A, 2014, 118, 6741-6748.	2.5	16

#	ARTICLE	IF	CITATIONS
1224	A study of the rotational barriers for some organic compounds using the G3 and G3CEP theories. Journal of Molecular Modeling, 2014, 20, 2199.	1.8	17
1225	Shock Wave Study of the Thermal Dissociations of C ₃ F ₆ and c-C ₃ F ₆ . I. Dissociation of Hexafluoropropene. Journal of Physical Chemistry A, 2014, 118, 4880-4888.	2.5	13
1226	Redox Chemistry of Selenenic Acids and the Insight It Brings on Transition State Geometry in the Reactions of Peroxyl Radicals. Journal of the American Chemical Society, 2014, 136, 1570-1578.	13.7	48
1227	Experimental Investigation of the Low Temperature Oxidation of the Five Isomers of Hexane. Journal of Physical Chemistry A, 2014, 118, 5573-5594.	2.5	44
1228	Ab initio studies of isomerization and dissociation reactions of methyl peroxyxynitrate. Structural Chemistry, 2014, 25, 859-871.	2.0	1
1229	Mechanism of Fast Pyrolysis of Lignin: Studying Model Compounds. Journal of Physical Chemistry B, 2014, 118, 8524-8531.	2.6	125
1230	Theoretical kinetic study of the unimolecular decomposition of 2-bromopropene. Chemical Physics Letters, 2014, 608, 386-392.	2.6	4
1231	Kinetics and thermodynamics of the decarboxylation of 1,2-glycerol carbonate to produce glycidol: computational insights. Green Chemistry, 2014, 16, 247-252.	9.0	19
1232	The CH ₃ PH ₂ and CH ₃ PH isomers: isomerization, hydrogen release, thermodynamic, and spectroscopy properties. Journal of Molecular Modeling, 2014, 20, 2372.	1.8	8
1233	Theoretical Study of the Oxidation Mechanisms of Naphthalene Initiated by Hydroxyl Radicals: The H Abstraction Pathway. Journal of Physical Chemistry A, 2014, 118, 3625-3636.	2.5	26
1234	Mechanistic and kinetic investigations on the ozonolysis of isopropenyl acetate and propenyl acetate in atmosphere. Computational and Theoretical Chemistry, 2014, 1049, 42-50.	2.5	4
1235	Synchrotron Photoionization Study of Mesitylene Oxidation Initiated by Reaction with Cl(² P) or O(³ P) Radicals. Journal of Physical Chemistry A, 2014, 118, 3735-3748.	2.5	14
1236	Pathways to Soot Oxidation: Reaction of OH with Phenanthrene Radicals. Journal of Physical Chemistry A, 2014, 118, 8606-8613.	2.5	43
1237	Activation of Methane by FeO ⁺ : Determining Reaction Pathways through Temperature-Dependent Kinetics and Statistical Modeling. Journal of Physical Chemistry A, 2014, 118, 2029-2039.	2.5	46
1238	Predicting pKa in Implicit Solvents: Current Status and Future Directions. Australian Journal of Chemistry, 2014, 67, 1441.	0.9	91
1239	Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates. Journal of Physical Chemistry A, 2014, 118, 9310-9318.	2.5	34
1240	Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part III: 2,5-Dimethylfuran. Combustion and Flame, 2014, 161, 780-797.	5.2	127
1241	On the stability and dynamics of (sulfuric acid)(ammonia) and (sulfuric acid)(dimethylamine) clusters: A first-principles molecular dynamics investigation. Chemical Physics, 2014, 428, 164-174.	1.9	22

#	ARTICLE	IF	CITATIONS
1242	Thermochemical Properties and Bond Dissociation Enthalpies of 3- to 5-Member Ring Cyclic Ether Hydroperoxides, Alcohols, and Peroxy Radicals: Cyclic Ether Radical + 3O ₂ Reaction Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3147-3167.	2.5	20
1243	MR-ccCA: A route for accurate ground and excited state potential energy curves and spectroscopic properties for third-row diatomic molecules. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 72-83.	2.5	9
1244	Theoretical insight into the pyrolytic deformylation of levoglucosenone and isolevoglucosenone. <i>Carbohydrate Research</i> , 2014, 390, 76-80.	2.3	16
1245	The theoretical assessment and prediction of CBr bond dissociation enthalpies. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 116-124.	2.5	14
1246	Combustion chemistry and flame structure of furan group biofuels using molecular-beam mass spectrometry and gas chromatography – Part I: Furan. <i>Combustion and Flame</i> , 2014, 161, 748-765.	5.2	117
1247	Development of a reaction mechanism for liquid-phase decomposition of guanidinium 5-amino tetrazolate. <i>Thermochimica Acta</i> , 2014, 582, 25-34.	2.7	18
1248	Thermochemistry of N-heterocyclic carbenes with 5-, 4-, 3-, and 2-membered rings. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 675-687.	2.0	2
1249	Shock wave and modeling study of the thermal decomposition reactions of pentafluoroethane and 2-H-heptafluoropropane. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9797-9807.	2.8	11
1250	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	74
1251	Theoretical calculations of the pK _a values of 1-aryl-4-propylpiperazine drugs in aqueous solution. <i>Chemical Research in Chinese Universities</i> , 2014, 30, 455-460.	2.6	2
1252	Thermochemistry, Reaction Paths, and Kinetics on the <i>tert</i> -Isooctane Radical Reaction with O ₂ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 4631-4646.	2.5	25
1255	Identification of liquid-phase decomposition species and reactions for guanidinium azotetrazolate. <i>Thermochimica Acta</i> , 2014, 590, 51-65.	2.7	13
1256	Experimental and theoretical study on the dissociative photoionization of trans-2-methyl-2-butenal. <i>Journal of Molecular Structure</i> , 2014, 1068, 130-139.	3.6	2
1257	Shock Wave Study of the Thermal Dissociations of C ₃ F ₆ and c-C ₃ F ₆ . II. Dissociation of Hexafluorocyclopropane and Dimerization of CF ₂ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 4873-4879.	2.5	12
1258	Quantum chemistry structures and properties of 134 kilo molecules. <i>Scientific Data</i> , 2014, 1, 140022.	5.3	887
1259	Kinetics of Hydrogen Abstraction Reactions from Fluoromethanes and Fluoroethanes. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 890-901.	3.2	30
1260	The Unimolecular Chemistry of Protonated and Deprotonated 2,2-Dinitroethene-1,1-Diamine (FOX-7) Studied by Tandem Mass Spectrometry and Computational Chemistry. <i>European Journal of Mass Spectrometry</i> , 2014, 20, 233-247.	1.0	4
1261	Dissociative Photoionization of ¹² C-Pinene: An Experimental and Theoretical Study. <i>European Journal of Mass Spectrometry</i> , 2014, 20, 419-428.	1.0	6

#	ARTICLE	IF	CITATIONS
1262	Electrical charging changes the composition of sulfuric acid–ammonia/dimethylamine clusters. <i>Atmospheric Chemistry and Physics</i> , 2014, 14, 7995-8007.	4.9	59
1263	Resolving the strange behavior of extraterrestrial potassium in the upper atmosphere. <i>Geophysical Research Letters</i> , 2014, 41, 4753-4760.	4.0	43
1265	One-Pot Cannizzaro Cascade Synthesis of <i>ortho</i> -Fused Cycloocta-2,5-dien-1-ones from 2-Bromo(hetero)aryl Aldehydes. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 10648-10651.	13.8	10
1267	A density functional for core-valence correlation energy. <i>Journal of Chemical Physics</i> , 2015, 143, 214111.	3.0	9
1268	First-principles based group additivity values for thermochemical properties of substituted aromatic compounds. <i>AIChE Journal</i> , 2015, 61, 3858-3870.	3.6	27
1269	Initiation Chemistries in Hydrocarbon (Aut)Oxidation. <i>Chemistry - A European Journal</i> , 2015, 21, 14060-14067.	3.3	14
1270	Electron-Induced Chemistry of Cobalt Tricarbonyl Nitrosyl (Co(CO) ₃ NO) in Liquid Helium Nanodroplets. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20917-20922.	3.1	8
1271	Unimolecular Reaction Properties for the Long-Chain Alkenyl Radicals. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 685-694.	1.6	12
1272	<i>In Silico</i> Study on Chemical Properties and Reactivity of Enal Derivatives. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 6615-6623.	2.4	0
1273	Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. <i>Journal of Computational Chemistry</i> , 2015, 36, 2158-2167.	3.3	10
1274	Multi-Species Multi-Channel (MSMC): An Ab Initio-based Parallel Thermodynamic and Kinetic Code for Complex Chemical Systems. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 564-575.	1.6	59
1275	A Computational Study of the Kinetics and Mechanism for the C ₂ H ₃ +CH ₃ OH Reaction. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 764-772.	1.6	3
1276	Absolute photoionization cross sections of furanic fuels: 2-ethylfuran, 2-acetylfuran and furfural. <i>Journal of Mass Spectrometry</i> , 2015, 50, 1206-1213.	1.6	23
1278	Ammonia-(Dinitramido)boranes: High-Energy-Density Materials. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11730-11734.	13.8	45
1279	Why base-catalyzed isomerization of <i>N</i> -propargyl amides yields mostly allenamides rather than ynamides. <i>Beilstein Journal of Organic Chemistry</i> , 2015, 11, 1441-1446.	2.2	6
1281	Low-Temperature Combustion Mechanisms. , 2015, , .		0
1282	Insertion, elimination and isomerisation of olefins at alkylaluminium hydride: an experimental and theoretical study. <i>Dalton Transactions</i> , 2015, 44, 15286-15296.	3.3	8
1283	Critical evaluation of the potential energy surface of the CH ₃ + HO ₂ reaction system. <i>Journal of Chemical Physics</i> , 2015, 142, 054308.	3.0	11

#	ARTICLE	IF	CITATIONS
1284	Revising the Role of a Dioxirane as an Intermediate in the Uncatalyzed Hydroperoxidation of Cyclohexanone in Water. <i>Journal of Organic Chemistry</i> , 2015, 80, 6425-6431.	3.2	11
1285	Theoretical Study on the Dynamics of the Reaction of $\text{HNO}(\text{H}^2)$ with $\text{HO}_2(\text{H}^2)$. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5553-5565.	2.5	6
1286	Azine or hydrazone? The dilemma in amidinohydrazones. <i>RSC Advances</i> , 2015, 5, 55938-55947.	3.6	27
1287	Theoretical Studies on the Kinetics of Hydrogen Abstraction Reactions of H and CH_3 Radicals from CH_3OCH_3 and Some of Their H/D Isotopologues. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4711-4717.	2.5	5
1289	Bicyclic CN_2O_2 as a high-energy density material: promising or not?. <i>RSC Advances</i> , 2015, 5, 46648-46653.	3.6	4
1290	Low- and intermediate-temperature oxidation of ethylcyclohexane: A theoretical study. <i>Combustion and Flame</i> , 2015, 162, 4167-4182.	5.2	39
1291	Theoretical study on the nitrate radical oxidation of methyl vinyl ether. <i>Computational and Theoretical Chemistry</i> , 2015, 1072, 72-78.	2.5	2
1292	Influence of temperature and resonance-stabilization on the ortho -effect in cymene oxidation. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 543-552.	3.9	7
1293	Experimental and computational study of the initial decomposition of gamma-valerolactone. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 515-523.	3.9	17
1294	Chlorine atom-initiated low-temperature oxidation of prenol and isoprenol: The effect of C C double bonds on the peroxy radical chemistry in alcohol oxidation. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 401-408.	3.9	6
1295	Calculation of acidity/basicity values of some fluorinated compounds in gas phase and aqueous solution: A computational approach. <i>Computational and Theoretical Chemistry</i> , 2015, 1054, 71-79.	2.5	10
1296	Investigation on primary decomposition of ethylcyclohexane at atmospheric pressure. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 367-375.	3.9	47
1297	Kinetic studies of the reaction of atomic sulfur with acetylene. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 215-222.	3.9	4
1298	Quantum chemical approach for condensed-phase thermochemistry (II): Applications to formation and combustion reactions of liquid organic molecules. <i>Chemical Physics Letters</i> , 2015, 624, 6-11.	2.6	11
1299	Dissociative Photoionization of Quinoline and Isoquinoline. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1127-1136.	2.5	49
1300	Accurate Standard Hydrogen Electrode Potential and Applications to the Redox Potentials of Vitamin C and NAD/NADH. <i>Journal of Physical Chemistry A</i> , 2015, 119, 369-376.	2.5	102
1301	Unprecedented Inhibition of Hydrocarbon Autoxidation by Diarylamine Radical-Trapping Antioxidants. <i>Journal of the American Chemical Society</i> , 2015, 137, 2440-2443.	13.7	25
1302	Solvation of Actinide Salts in Water Using a Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2015, 119, 689-703.	2.5	11

#	ARTICLE	IF	CITATIONS
1303	Can B3LYP be improved by optimization of the proportions of exchange and correlation functionals?. International Journal of Quantum Chemistry, 2015, 115, 502-509.	2.0	21
1304	Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?. Polyhedron, 2015, 89, 160-167.	2.2	10
1305	Experimental and Theoretical Study on the Thermal Decomposition of C ₃ H ₆ (Propene). Journal of Physical Chemistry A, 2015, 119, 1229-1237.	2.5	13
1306	Glyoxal Oxidation Mechanism: Implications for the Reactions HCO + O ₂ and OCHCHO + HO ₂ . Journal of Physical Chemistry A, 2015, 119, 7305-7315.	2.5	24
1307	Mesospheric Removal of Very Long-Lived Greenhouse Gases SF ₆ and CFC-115 by Metal Reactions, Lyman- α Photolysis, and Electron Attachment. Journal of Physical Chemistry A, 2015, 119, 2016-2025.	2.5	18
1308	Computational Study on the Mechanisms and Rate Constants of the Cl-Initiated Oxidation of Methyl Vinyl Ether in the Atmosphere. Journal of Physical Chemistry A, 2015, 119, 719-727.	2.5	13
1309	Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the <sc>CBS- $\text{M}3$ </sc> composite method and their consequences in <sc>DFT</sc> benchmark studies. Journal of Computational Chemistry, 2015, 36, 622-632.	3.3	124
1310	Can a pentamethylcyclopentadienyl ligand act as a proton-relay in f-element chemistry? Insights from a joint experimental/theoretical study. Dalton Transactions, 2015, 44, 2575-2587.	3.3	25
1311	Automatic Mechanism and Kinetic Model Generation for Gas- and Solution-Phase Processes: A Perspective on Best Practices, Recent Advances, and Future Challenges. International Journal of Chemical Kinetics, 2015, 47, 199-231.	1.6	94
1312	Nitrenium Ion Analogues of Nonclassical Carbocations: Cyclopropylnitrenium, Allylnitrenium, and Azetidenium Ions and Mechanisms for Their Interconversion. Organic Letters, 2015, 17, 484-487.	4.6	4
1313	Intramolecular C \equiv N Bond Activation and Ring-Expansion Reactions of N-Heterocyclic Carbenes. Chemistry - A European Journal, 2015, 21, 1434-1438.	3.3	35
1314	New Mechanism for the Atmospheric Oxidation of Dimethyl Sulfide. The Importance of Intramolecular Hydrogen Shift in a CH ₃ SCH ₂ OO Radical. Journal of Physical Chemistry A, 2015, 119, 112-117.	2.5	52
1315	Origins of the Regioselectivity in the Lutetium Triflate Catalyzed Ketalization of Acetone with Glycerol: A DFT Study. ACS Catalysis, 2015, 5, 1013-1019.	11.2	24
1316	Low energy electron attachment to cyanamide (NH ₂ CN). Journal of Chemical Physics, 2015, 142, 034301.	3.0	12
1317	Ultraviolet photodissociation action spectroscopy of the N-pyridinium cation. Journal of Chemical Physics, 2015, 142, 014301.	3.0	24
1318	Theoretical and kinetic study of reaction C ₂ H ₄ +C ₃ H ₆ on the C ₅ H ₇ potential energy surface. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	12
1320	Dramatic Behavioral Differences of the Copolymerization Reactions of 1,4-Cyclohexadiene and 1,3-Cyclohexadiene Oxides with Carbon Dioxide. Macromolecules, 2015, 48, 1679-1687.	4.8	40
1321	A comparison of the C-H bond dissociation enthalpies of sulfur-containing fused heterocyclic compounds to the C-H bond dissociation enthalpies in other heterocycles. Journal of Sulfur Chemistry, 2015, 36, 155-169.	2.0	7

#	ARTICLE	IF	CITATIONS
1322	On the formation of cyclopentadiene in the $C_3H_5\dot{E} + C_2H_2$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20508-20514.	2.8	24
1323	Quantum Chemical Study of Autoignition of Methyl Butanoate. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7282-7292.	2.5	18
1324	Stability and bonding of new superalkali phosphide species. <i>Dalton Transactions</i> , 2015, 44, 14753-14762.	3.3	13
1325	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles' heel for DFT and standard ab initio procedures. <i>Chemical Physics</i> , 2015, 458, 1-8.	1.9	68
1326	Fe embedded in ice: The impacts of sublimation and energetic particle bombardment. <i>Journal of Atmospheric and Solar-Terrestrial Physics</i> , 2015, 127, 103-110.	1.6	4
1327	Study of <i>tert</i> -Amyl Methyl Ether Low Temperature Oxidation Using Synchrotron Photoionization Mass Spectrometry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8667-8682.	2.5	12
1328	Formation of fulvene in the reaction of C_2H with 1,3-butadiene. <i>International Journal of Mass Spectrometry</i> , 2015, 378, 232-245.	1.5	16
1329	Distortion-Interaction analysis along the reaction pathway to reveal the reactivity of the Alder-ene reaction of enes. <i>RSC Advances</i> , 2015, 5, 61426-61435.	3.6	27
1330	Experimental Study of Tetrahydrofuran Oxidation and Ignition in Low-Temperature Conditions. <i>Energy & Fuels</i> , 2015, 29, 6118-6125.	5.1	33
1331	Multiplexed Photoionization Mass Spectrometry Investigation of the $O(^3P) + Propyne$ Reaction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7388-7403.	2.5	14
1332	Tautomerization of Some Methylacenes and the Role of Reverse Radical Disproportionation. <i>Journal of Organic Chemistry</i> , 2015, 80, 8206-8216.	3.2	7
1333	Benchmarking Continuum Solvent Models for Keto-Enol Tautomerizations. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8724-8733.	2.5	25
1334	Experimental and Theoretical Study on the OH-Reaction Kinetics and Photochemistry of Acetyl Fluoride ($CH_3C(O)F$), an Atmospheric Degradation Intermediate of HFC-161 (C_2H_5F). <i>Journal of Physical Chemistry A</i> , 2015, 119, 7753-7765.	2.5	10
1335	Understanding the Importance of Carbenium Ions in the Conversion of Biomass-Derived Alcohols with First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16139-16147.	3.1	18
1336	Group Additive Kinetics for Hydrogen Transfer Between Oxygenates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6961-6980.	2.5	16
1337	Ring strain energy in ether- and lactone-containing spiro compounds. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 298-303.	1.9	10
1338	Arsenic(III) chloride ammonolysis. <i>Russian Journal of Inorganic Chemistry</i> , 2015, 60, 589-594.	1.3	0
1339	Thermal Decomposition of 2(3H) and 2(5H) Furanones: Theoretical Aspects. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6919-6927.	2.5	6

#	ARTICLE	IF	CITATIONS
1340	Ultraviolet photodissociation action spectroscopy of gas-phase protonated quinoline and isoquinoline cations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25882-25890.	2.8	23
1341	Controlling Factors in the Rates of Oxidation of Anilines and Phenols by Triplet Methylene Blue in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3233-3243.	2.5	48
1342	Experimental and kinetic modeling study of exo-TCD pyrolysis under low pressure. <i>Combustion and Flame</i> , 2015, 162, 2177-2190.	5.2	27
1343	Pressure-Dependent Kinetics of Initial Reactions in Iso-octane Pyrolysis. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4093-4107.	2.5	25
1344	Theoretical Study of the Reactions of Ethanol with Aluminum and Aluminum Oxide. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3897-3904.	2.5	15
1345	Active Thermochemical Tables: Sequential Bond Dissociation Enthalpies of Methane, Ethane, and Methanol and the Related Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7810-7837.	2.5	180
1346	Theoretical study on the thermal decomposition and isomerization of 3-Me-1-heptyl radical. <i>Computational and Theoretical Chemistry</i> , 2015, 1063, 10-18.	2.5	2
1347	Homolytic C=O Cleavage in Phosphates and Sulfonates. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3488-3499.	2.5	7
1348	Water-assisted isomerization of the [H, C, N, O] system. <i>Journal of Molecular Modeling</i> , 2015, 21, 66.	1.8	3
1349	Pyrolysis study of pectin by tunable synchrotron vacuum ultraviolet photoionization mass spectrometry. <i>Journal of Thermal Analysis and Calorimetry</i> , 2015, 120, 1399-1405.	3.6	13
1350	Atmospheric nucleation precursors catalyzed isomerization of CH ₂ SH to CH ₃ S: mechanisms and topological analysis. <i>Structural Chemistry</i> , 2015, 26, 261-268.	2.0	4
1351	Kinetics of ethylcyclohexane pyrolysis and oxidation: An experimental and detailed kinetic modeling study. <i>Combustion and Flame</i> , 2015, 162, 2873-2892.	5.2	70
1352	The origin of the anomeric effect: probing the impacts of stereoelectronic interactions. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 6965-6976.	2.8	19
1353	The origin and magnitude of intramolecular quasi-cyclic S=O and S=S interactions revisited: A computational study. <i>Chemical Physics Letters</i> , 2015, 631-632, 6-11.	2.6	25
1354	HO + OCLO Reaction System: Featuring a Barrierless Entrance Channel with Two Transition States. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5723-5731.	2.5	20
1355	The substituent effect from the perspective of local hyper-softness. An example applied on normeloxicam, meloxicam and 4-meloxicam: Non-steroidal anti-inflammatory drugs. <i>Chemical Physics Letters</i> , 2015, 618, 162-167.	2.6	7
1356	Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. <i>Journal of Computational Chemistry</i> , 2015, 36, 1370-1389.	3.3	14
1357	Molecular Mechanism of NDMA Formation from N,N-Dimethylsulfamide During Ozonation: Quantum Chemical Insights into a Bromide-Catalyzed Pathway. <i>Environmental Science & Technology</i> , 2015, 49, 4163-4175.	10.0	53

#	ARTICLE	IF	CITATIONS
1358	A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. Journal of Physical Chemistry A, 2015, 119, 4214-4223.	2.5	28
1359	Threshold Photoelectron Spectra of Combustion Relevant C ₄ H ₅ and C ₄ H ₇ Isomers. Journal of Physical Chemistry A, 2015, 119, 3995-4000.	2.5	28
1360	A kinetic and thermochemical database for organic sulfur and oxygen compounds. Physical Chemistry Chemical Physics, 2015, 17, 13625-13639.	2.8	16
1361	Temperature and Pressure Dependent Rate Coefficients for the Reaction of C ₂ H ₄ + HO ₂ on the C ₂ H ₄ O ₂ H Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 3161-3170.	2.5	14
1362	Mechanism and Kinetics of Low-Temperature Oxidation of a Biodiesel Surrogate: Methyl Propanoate Radicals with Oxygen Molecule. Journal of Physical Chemistry A, 2015, 119, 3689-3703.	2.5	24
1363	The Atmospheric Oxidation Mechanism of Benzyl Alcohol Initiated by OH Radicals: The Addition Channels. ChemPhysChem, 2015, 16, 1542-1550.	2.1	14
1364	The ONIOM Method and Its Applications. Chemical Reviews, 2015, 115, 5678-5796.	47.7	936
1365	Accurate Composite and Fragment-Based Quantum Chemical Models for Large Molecules. Chemical Reviews, 2015, 115, 5643-5677.	47.7	225
1366	Theoretical Chemical Kinetics in Tropospheric Chemistry: Methodologies and Applications. Chemical Reviews, 2015, 115, 4063-4114.	47.7	164
1367	Solvatochromism of a tricycloquinazoline based disk-shaped liquid crystal: a potential molecular probe for fluorescence imaging. RSC Advances, 2015, 5, 84592-84600.	3.6	8
1368	Structures and relative stabilities of ammonia clusters at different temperatures: DFT vs. ab initio. Physical Chemistry Chemical Physics, 2015, 17, 29226-29242.	2.8	60
1369	Theoretical study of the oxidation mechanisms of thiophene initiated by hydroxyl radicals. Journal of Molecular Modeling, 2015, 21, 301.	1.8	16
1370	Effects of an acid–alkaline environment on the reactivity of 5-carboxycytosine with hydroxyl radicals. RSC Advances, 2015, 5, 87364-87376.	3.6	2
1371	Theoretical Investigation of Intramolecular Hydrogen Shift Reactions in 3-Methyltetrahydrofuran (3-MTHF) Oxidation. Journal of Physical Chemistry A, 2015, 119, 10917-10928.	2.5	12
1372	Are the three hydroxyphenyl radical isomers created equal? – The role of the phenoxy radical –. Physical Chemistry Chemical Physics, 2015, 17, 30076-30083.	2.8	35
1373	Isomerism of Cyanomethanimine: Accurate Structural, Energetic, and Spectroscopic Characterization. Journal of Physical Chemistry A, 2015, 119, 11614-11622.	2.5	22
1374	Monocyclic and bicyclic CO ₄ : how stable are they?. RSC Advances, 2015, 5, 91581-91586.	3.6	1
1375	Threshold photoelectron spectroscopy of unstable N-containing compounds: Resolution of \hat{I}° K subbands in HNCO ⁺ and vibrational resolution in NCO ⁺ . Journal of Chemical Physics, 2015, 142, 184306.	3.0	9

#	ARTICLE	IF	CITATIONS
1376	Formation of H ₂ from internally heated polycyclic aromatic hydrocarbons: Excitation energy dependence. <i>Journal of Chemical Physics</i> , 2015, 142, 144305.	3.0	43
1377	The growth of phenanthrene from naphthalene by C ₂ H ₂ additions. <i>Molecular Physics</i> , 2015, 113, 1834-1838.	1.7	3
1378	The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2015, 211, 506-514.	4.9	69
1379	Quantum Chemical Study of the Thermochemical Properties of Organophosphorous Compounds. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10527-10539.	2.5	29
1380	Estimating Ring Strain Energies of Highly Substituted Cyclohexanes with the Semi-homodesmotic Approach: Why Substantial Ring Strain Exists for Nominally Tetrahedral Ring Carbon Atoms. <i>Journal of Organic Chemistry</i> , 2015, 80, 10234-10243.	3.2	6
1381	Synergy of Vicinal Oxygenated Groups of Catalysts for Hydrolysis of Cellulosic Molecules. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20993-20999.	3.1	50
1382	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.	3.6	23
1383	Mechanism of the Intramolecular Hexadehydro-Diels-Alder Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 11744-11754.	3.2	49
1384	Computational Study and Kinetic Analysis of the Aminolysis of Thiolactones. <i>Journal of Organic Chemistry</i> , 2015, 80, 8520-8529.	3.2	18
1385	DFT Study of Oxygen Dissociation in Molten Carbonate. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8806-8812.	2.5	10
1386	Theoretical kinetic study for methyl levulinate: oxidation by OH and CH ₃ radicals and further unimolecular decomposition pathways. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23384-23391.	2.8	19
1387	Theoretical study on homolytic C(sp ²)=O cleavage in ethers and phenols. <i>New Journal of Chemistry</i> , 2015, 39, 6935-6943.	2.8	7
1388	Bond Energies and Thermochemical Properties of Ring-Opened Diradicals and Carbenes of <i>exo</i> -Tricyclo[5.2.1.0 ^{2,6}]decane. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9857-9878.	2.5	15
1389	Exploring physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs). <i>Journal of Molecular Liquids</i> , 2015, 209, 14-24.	4.9	17
1390	Low temperature (550-700 K) oxidation pathways of cyclic ketones: dominance of HO ₂ -elimination channels yielding conjugated cyclic coproducts. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12124-12134.	2.8	17
1391	Kinetic and mechanistic investigations of the thermal decomposition of methyl-substituted cycloalkyl radicals. <i>RSC Advances</i> , 2015, 5, 28044-28053.	3.6	1
1392	Pyrolysis and combustion chemistry of tetrahydropyran: Experimental and modeling study. <i>Combustion and Flame</i> , 2015, 162, 4283-4303.	5.2	19
1393	The threshold photoelectron spectrum of cyanovinylacetylene leads to an upward revision of the ionization energy. <i>Chemical Physics Letters</i> , 2015, 638, 201-204.	2.6	3

#	ARTICLE	IF	CITATIONS
1394	Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism – a gas-phase <i>ab initio</i> study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4054-4066.	2.8	14
1395	Pyrolysis Pathways of the Furanic Ether 2-Methoxyfuran. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9962-9977.	2.5	9
1396	Smallest deltahedra silicon dicarbide: C ₂ Si ₃₂ . <i>RSC Advances</i> , 2015, 5, 101193-101199.	3.6	5
1397	Theoretical Investigation of the Radical–Radical Reaction of O(³ P) + C ₂ H ₃ and Comparison with Gas-Phase Crossed-Beam Experiments. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11761-11771.	2.5	6
1398	A Computational Re-examination of the Criegee Intermediate–Sulfur Dioxide Reaction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10316-10335.	2.5	60
1399	Correlations between hardness, electrostatic interactions, and thermodynamic parameters in the decomposition reactions of 3-buten-1-ol, 3-methoxy-1-propene, and ethoxyethene. <i>Structural Chemistry</i> , 2015, 26, 547-554.	2.0	3
1400	An assessment of theoretical procedures for π -conjugation stabilisation energies in enones. <i>Molecular Physics</i> , 2015, 113, 1284-1296.	1.7	19
1401	Dissociative VUV photoionization of butanediol isomers. <i>International Journal of Mass Spectrometry</i> , 2015, 376, 46-53.	1.5	4
1402	Kinetics of the (salen)Cr(III)- and (salen)Co(III)-catalyzed copolymerization of epoxides with CO ₂ , and of the accompanying degradation reactions. <i>Polymer Chemistry</i> , 2015, 6, 1103-1117.	3.9	37
1403	Structure, stability, energy barrier and ionization energies of chemically modified DNA-bases: Quantum chemical calculations on 37 favored and rare tautomeric forms of tetraphosphoadenine. <i>Computational and Theoretical Chemistry</i> , 2015, 1052, 35-41.	2.5	4
1404	Elucidating the Thermal Decomposition of Dimethyl Methylphosphonate by Vacuum Ultraviolet (VUV) Photoionization: Pathways to the PO Radical, a Key Species in Flame Retardant Mechanisms. <i>Chemistry - A European Journal</i> , 2015, 21, 1073-1080.	3.3	102
1405	Synthesis and Characterization of Fluorodinitroamine, FN(NO ₂) ₂ . <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1316-1320.	13.8	20
1406	Computational study of unsaturated and saturated cyclic (alkyl) (amino) carbene borane complexes. <i>Computational and Theoretical Chemistry</i> , 2015, 1051, 17-23.	2.5	3
1407	Integrated data-model analysis facilitated by an Instrumental Model. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 597-605.	3.9	14
1408	Calculations of pK _a ™s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5134-5144.	2.5	111
1409	Molecular Orbital Based Design Guideline for Hypergolic Ionic Liquids. <i>Propellants, Explosives, Pyrotechnics</i> , 2015, 40, 144-149.	1.6	15
1410	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.	2.0	13
1411	Unimolecular decomposition of tetrahydrofuran: Carbene vs. diradical pathways. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 533-541.	3.9	30

#	ARTICLE	IF	CITATIONS
1412	A theoretical kinetics study of the reactions of methylbutanoate with hydrogen and hydroxyl radicals. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 481-489.	3.9	40
1413	A computational study on the kinetics of unimolecular reactions of ethoxyethylperoxy radicals employing CTST and VTST. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 161-169.	3.9	34
1414	Coordination and electronic characteristics of a nitrogen heterocycle pincer ligand. <i>Inorganica Chimica Acta</i> , 2016, 451, 82-91.	2.4	27
1415	A high-level theoretical study into the atmospheric phase hydration, bond dissociation enthalpies, and acidity of aldehydes. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 336-345.	1.9	5
1416	Computational characterization of isomeric C ₄ H ₂ O systems: Thermochemistry, vibrational frequencies, and optical spectra for butatrienone, ethynyl ketene, butadiynol, and triafulvenone. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 444-451.	2.0	5
1417	A computational chemist's guide to accurate thermochemistry for organic molecules. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 292-310.	14.6	185
1418	Hydrogen bonding in the hydroxysulfinyl radical-formic acid-water system: A theoretical study. <i>Journal of Computational Chemistry</i> , 2016, 37, 1611-1625.	3.3	3
1419	Chemical Reaction CO+OH ⁺ →CO ₂ +H ⁺ Autocatalyzed by Carbon Dioxide: Quantum Chemical Study of the Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6023-6028.	2.5	26
1420	Analysis of Geologically Relevant Metal Porphyrins Using Trapped Ion Mobility Spectrometry–Mass Spectrometry and Theoretical Calculations. <i>Energy & Fuels</i> , 2016, 30, 10341-10347.	5.1	21
1421	Assessment of a composite CC2/DFT procedure for calculating O ⁺ O excitation energies of organic molecules. <i>Molecular Physics</i> , 2016, 114, 3448-3463.	1.7	20
1422	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. <i>Journal of Chemical Physics</i> , 2016, 145, .	3.0	60
1423	A dataset of highly accurate homolytic Ni–Br bond dissociation energies obtained by Means of W2 theory. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 52-60.	2.0	28
1424	Acid Is Key to the Radical-Trapping Antioxidant Activity of Nitroxides. <i>Journal of the American Chemical Society</i> , 2016, 138, 5290-5298.	13.7	61
1425	Reaction between propargyl radical and 1,3-butadiene to form five to seven membered rings. Theoretical study. <i>Combustion and Flame</i> , 2016, 168, 331-341.	5.2	10
1426	Hydrogen transfer between dimethyl ether and the methoxy radical: Understanding and kinetic modeling with anharmonic torsions. <i>Computational and Theoretical Chemistry</i> , 2016, 1089, 43-53.	2.5	6
1427	Theoretical calculations on the mechanism of the elimination kinetics of allyl cyclohexyl-, -amine, -sulfide, -ether, and allyl ethyl ether in the gas phase. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 6-16.	2.5	3
1428	Water mediated hydrogen abstraction mechanism in the radical reaction between HOSO and NO ₂ . <i>Chemical Physics Letters</i> , 2016, 651, 209-215.	2.6	12
1429	Removal of oxygen functional groups in lignite by hydrothermal dewatering: An experimental and DFT study. <i>Fuel</i> , 2016, 178, 85-92.	6.4	77

#	ARTICLE	IF	CITATIONS
1430	Thermal Decomposition of 3-Bromopropene. A Theoretical Kinetic Investigation. Journal of Physical Chemistry A, 2016, 120, 2285-2294.	2.5	6
1431	Comparative Study of Cl-Atom Reactions in Solution Using Time-Resolved Vibrational Spectroscopy. Journal of Physical Chemistry B, 2016, 120, 3920-3931.	2.6	3
1432	Preparation of the Cyclopentazole Anion in the Bulk: A Computational Study. Journal of Physical Chemistry B, 2016, 120, 6208-6214.	2.6	13
1433	Skeletal chemical mechanism of high-temperature TEOS oxidation in hydrogen-oxygen environment. Combustion and Flame, 2016, 166, 243-254.	5.2	13
1434	Real-Time Detection of Arsenic Cations from Ambient Air in Boreal Forest and Lake Environments. Environmental Science and Technology Letters, 2016, 3, 42-46.	8.7	12
1435	Acidity of Strong Acids in Water and Dimethyl Sulfoxide. Journal of Physical Chemistry A, 2016, 120, 3663-3669.	2.5	140
1436	Relationship between Electron Affinity and Half-Wave Reduction Potential: A Theoretical Study on Cyclic Electron-Acceptor Compounds. ChemPhysChem, 2016, 17, 3881-3890.	2.1	15
1437	Relative Rate and Product Studies of the Reactions of Atomic Chlorine with Tetrafluoroethylene, 1,2-Dichloro-1,2-difluoroethylene, 1,1-Dichloro-2,2-difluoroethylene, and Hexafluoro-1,3-butadiene in the Presence of Oxygen. Journal of Physical Chemistry A, 2016, 120, 7311-7319.	2.5	4
1438	On calculating HR bond enthalpies using computational data. Computational and Theoretical Chemistry, 2016, 1096, 89-93.	2.5	1
1439	Comparative Kinetic Analysis of Ethane Pyrolysis at 0.1 and 2.0 MPa. Energy & Fuels, 2016, 30, 9703-9711.	5.1	8
1440	Benchmarking the DFT methodology for assessing antioxidant-related properties: quercetin and edaravone as case studies. Journal of Molecular Modeling, 2016, 22, 250.	1.8	24
1441	Understanding and modeling the hydrogen-abstraction from dimethyl ether by the methyl radical with torsional anharmonicity. Computational and Theoretical Chemistry, 2016, 1096, 7-16.	2.5	3
1442	Air-water partition coefficients for a suite of polycyclic aromatic and other C ₁₀ through C ₂₀ unsaturated hydrocarbons. Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering, 2016, 51, 938-953.	1.7	2
1443	High-temperature unimolecular decomposition of ethyl propionate. Chemical Physics Letters, 2016, 664, 184-190.	2.6	11
1444	Proton-coupled electron transfer in the reduction of carbonyls using Sml ₂ -H ₂ O: implications for the reductive coupling of acyl-type ketyl radicals with Sml ₂ -H ₂ O. Organic and Biomolecular Chemistry, 2016, 14, 9151-9157.	2.8	19
1445	Mutagenicity of heteroaromatic amines: Computational study on the influence of methyl substituents. Journal of Molecular Graphics and Modelling, 2016, 69, 92-102.	2.4	1
1446	The 1,2-hydrogen shift reaction for monohalogenophosphanes PH ₂ X and HPX (X = F, Cl). Molecular Physics, 2016, 114, 2999-3014.	1.7	3
1447	Thermochemistry of icosahedral closo-dicarbaboranes: a composite ab initio quantum-chemical perspective. Canadian Journal of Chemistry, 2016, 94, 1082-1089.	1.1	4

#	ARTICLE	IF	CITATIONS
1448	The Effect of Alcohol and Carbonyl Functional Groups on the Competition between Unimolecular Decomposition and Isomerization in C ₄ and C ₅ Alkoxy Radicals. International Journal of Chemical Kinetics, 2016, 48, 544-555.	1.6	1
1449	Understanding the reactivity of unsaturated alcohols: Experimental and kinetic modeling study of the pyrolysis and oxidation of 3-methyl-2-butenol and 3-methyl-3-butenol. Combustion and Flame, 2016, 171, 237-251.	5.2	24
1450	A comparative examination of density functional performance against the ISOL24/11 isomerization energy benchmark. Computational and Theoretical Chemistry, 2016, 1090, 147-152.	2.5	23
1451	Exploration of Unimolecular Gas-Phase Detoxication Pathways of Sarin and Soman: A Computational Study from the Perspective of Reaction Energetics and Kinetics. Chemical Research in Toxicology, 2016, 29, 1439-1457.	3.3	11
1452	Detailed Kinetic Modeling of Lignin Pyrolysis for Process Optimization. Industrial & Engineering Chemistry Research, 2016, 55, 9147-9153.	3.7	40
1453	Potential Energy Surfaces for the Reactions of HO ₂ Radical with CH ₂ O and HO ₂ in CO ₂ Environment. Journal of Physical Chemistry A, 2016, 120, 7681-7688.	2.5	17
1454	Atmospheric oxidation mechanism of OH-initiated reactions of diethyl ether – the fate of the 1-ethoxy ethoxy radical. RSC Advances, 2016, 6, 81354-81363.	3.6	7
1455	Tautomerization lowers the activation barriers for N-glycosidic bond cleavage of protonated uridine and 2'-deoxyuridine. Physical Chemistry Chemical Physics, 2016, 18, 24451-24459.	2.8	15
1456	An adaptive distance-based group contribution method for thermodynamic property prediction. Physical Chemistry Chemical Physics, 2016, 18, 23822-23830.	2.8	16
1457	The outlook for platonic and cubic gauche nitrogens. Computational Materials Science, 2016, 123, 31-39.	3.0	5
1458	Dissociative electron transfer in polychlorinated aromatics. Reduction potentials from convolution analysis and quantum chemical calculations. Physical Chemistry Chemical Physics, 2016, 18, 22573-22582.	2.8	20
1459	Theoretical Analysis of the Effect of C=C Double Bonds on the Low-Temperature Reactivity of Alkenylperoxy Radicals. Journal of Physical Chemistry A, 2016, 120, 5969-5978.	2.5	21
1460	Low-Temperature Reactivity of C ₂ N ₂ ⁺ Anions with Polar Molecules. Journal of Physical Chemistry Letters, 2016, 7, 2957-2961.	4.6	12
1461	Formation and emission of large furans and oxygenated hydrocarbons from flames. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8374-8379.	7.1	76
1462	Resonance Stabilization Effects on Ketone Autoxidation: Isomer-Specific Cyclic Ether and Ketohydroperoxide Formation in the Low-Temperature (400–625 K) Oxidation of Diethyl Ketone. Journal of Physical Chemistry A, 2016, 120, 8625-8636.	2.5	11
1463	Electron-Induced Fragmentation of Methylated Formamides. International Journal of Mass Spectrometry, 2016, 410, 36-46.	1.5	4
1464	Prediction of heat of formation for exo -Dicyclopentadiene. Journal of Loss Prevention in the Process Industries, 2016, 44, 433-439.	3.3	7
1465	Ruthenium-Catalyzed Azide Alkyne Cycloaddition Reaction: Scope, Mechanism, and Applications. Chemical Reviews, 2016, 116, 14726-14768.	47.7	286

#	ARTICLE	IF	CITATIONS
1466	Kinetics and Thermodynamics of Reversible Thiol Additions to Mono- and Diactivated Michael Acceptors: Implications for the Design of Drugs That Bind Covalently to Cysteines. <i>Journal of Organic Chemistry</i> , 2016, 81, 11726-11733.	3.2	106
1467	Towards first-principles molecular design of liquid crystal-based chemoresponsive systems. <i>Nature Communications</i> , 2016, 7, 13338.	12.8	34
1468	Group additive kinetic modeling for carbon-centered radical addition to oxygenates and β -scission of oxygenates. <i>AIChE Journal</i> , 2016, 62, 802-814.	3.6	15
1469	Mechanisms and energetics for N-glycosidic bond cleavage of protonated adenine nucleosides: N3 protonation induces base rotation and enhances N-glycosidic bond stability. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16021-16032.	2.8	23
1470	Polysulfide-1-oxides react with peroxy radicals as quickly as hindered phenolic antioxidants and do so by a surprising concerted homolytic substitution. <i>Chemical Science</i> , 2016, 7, 6347-6356.	7.4	36
1471	Rotamers and Migration: Investigating the Dissociative Photoionization of Ethylenediamine. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3906-3916.	2.5	9
1472	The strength of multi-scale modeling to unveil the complexity of radical polymerization. <i>Progress in Polymer Science</i> , 2016, 58, 59-89.	24.7	174
1473	O2 Protonation Controls Threshold Behavior for N-Glycosidic Bond Cleavage of Protonated Cytosine Nucleosides. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4803-4811.	2.6	25
1474	Formation of persistent organic pollutants from 2,4,5-trichlorothiophenol combustion: a density functional theory investigation. <i>Journal of Molecular Modeling</i> , 2016, 22, 128.	1.8	8
1475	The exceptionally high reactivity of Cys 621 is critical for electrophilic activation of the sensory nerve ion channel TRPA1. <i>Journal of General Physiology</i> , 2016, 147, 451-465.	1.9	47
1476	Energetic Properties of Rocket Propellants Evaluated through the Computational Determination of Heats of Formation of Nitrogen-Rich Compounds. <i>Chemistry - an Asian Journal</i> , 2016, 11, 730-744.	3.3	6
1477	Tunneling effect in 1,5 H-migration of a prototypical OOQOOH. <i>Chemical Physics Letters</i> , 2016, 646, 153-157.	2.6	9
1478	Mechanisms and energetics for N-glycosidic bond cleavage of protonated 2'-deoxyguanosine and guanosine. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2968-2980.	2.8	19
1479	A mechanistic study of carbonyl activation under solvent-free conditions: evidence drawn from the synthesis of imidazoles. <i>RSC Advances</i> , 2016, 6, 10743-10749.	3.6	17
1480	Direct ab initio study of the C ₆ H ₆ + CH ₃ /C ₂ H ₅ = C ₆ H ₅ + CH ₄ /C ₂ H ₆ reactions. <i>Chemical Physics Letters</i> , 2016, 646, 102-109.	2.6	9
1481	Atomistic Molecular Dynamics Simulations of Charged Latex Particle Surfaces in Aqueous Solution. <i>Langmuir</i> , 2016, 32, 428-441.	3.5	23
1482	Study of the Formation of the First Aromatic Rings in the Pyrolysis of Cyclopentene. <i>Journal of Physical Chemistry A</i> , 2016, 120, 668-682.	2.5	19
1483	The multi-channel reaction of the OH radical with 5-hydroxymethylcytosine: a computational study. <i>RSC Advances</i> , 2016, 6, 13349-13357.	3.6	1

#	ARTICLE	IF	CITATIONS
1484	Low cost estimation of the contribution of post-CCSD excitations to the total atomization energy using density functional theory calculations. <i>Chemical Physics Letters</i> , 2016, 649, 68-72.	2.6	0
1485	Gas Phase Mercury Oxidation by Halogens (Cl, Br, I) in Combustion Effluents: Influence of Operating Conditions. <i>Energy & Fuels</i> , 2016, 30, 603-615.	5.1	19
1486	Ab Initio Chemical Kinetics for the HCCO + H Reaction. <i>Combustion Science and Technology</i> , 2016, 188, 1095-1114.	2.3	3
1487	Performance of the major semiempirical, ab initio, and DFT methods for isomerization enthalpies of linear to branched heptanes. <i>Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering</i> , 2016, 51, 583-587.	1.7	5
1488	Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. <i>Journal of Computational Chemistry</i> , 2016, 37, 49-58.	3.3	66
1489	Roles of hydroxyls in the noncatalytic and catalyzed formation of levoglucosan from glucose. <i>Catalysis Today</i> , 2016, 269, 110-121.	4.4	26
1490	Possible interstellar formation of glycine through a concerted mechanism: a computational study on the reaction of CH_2NH , CO_2 and H_2 . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20109-20117.	2.8	24
1491	Effect of cis / trans isomerism on selective oxidation of olefins with nitrous oxide. <i>Tetrahedron</i> , 2016, 72, 2501-2506.	1.9	7
1492	Mechanistic Study of Cellulose Hydrolysis by Carbon Catalysts. <i>Springer Theses</i> , 2016, , 77-112.	0.1	2
1493	Isomerization Pathways of ONCNO: Unstable or Metastable?. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4812-4817.	2.5	1
1494	Calculating Free Energy Changes in Continuum Solvation Models. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1319-1329.	2.6	140
1495	The atmospheric oxidation of dimethyl, diethyl, and diisopropyl ethers. The role of the intramolecular hydrogen shift in peroxy radicals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7707-7714.	2.8	24
1496	Theoretical kinetics studies on the unimolecular degradation of trifluoromethyl sulfur pentafluoride, SF_5CF_3 . <i>Journal of Fluorine Chemistry</i> , 2016, 184, 16-21.	1.7	0
1497	Pyrolysis of 3-Methoxypyridine. Detection and Characterization of the Pyrrolyl Radical by Threshold Photoelectron Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4702-4710.	2.5	18
1498	Additional chain-branching pathways in the low-temperature oxidation of branched alkanes. <i>Combustion and Flame</i> , 2016, 164, 386-396.	5.2	94
1499	Binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives as potential high energy materials. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 10-15.	2.5	5
1500	A Study on Catalytic Conversion of Non-Food Biomass into Chemicals. <i>Springer Theses</i> , 2016, , .	0.1	5
1501	Computational benchmark for calculation of silane and siloxane thermochemistry. <i>Journal of Molecular Modeling</i> , 2016, 22, 35.	1.8	21

#	ARTICLE	IF	CITATIONS
1502	Cyclometalated Iridium(III) Complexes Containing 4,4'-Conjugated 2,2'-Bipyridine Derivatives as the Ancillary Ligands: Synthesis, Photophysics, and Computational Studies. <i>Inorganic Chemistry</i> , 2016, 55, 3530-3540.	4.0	27
1503	Understanding anionic Chugaev elimination in pericyclic tetracene formation. <i>Tetrahedron</i> , 2016, 72, 1686-1689.	1.9	3
1504	Low Temperature Chlorine-Initiated Oxidation of Small-Chain Methyl Esters: Quantification of Chain-Terminating HO ₂ -Elimination Channels. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1677-1690.	2.5	6
1505	Computational Study on the Effect of Hydration on New Particle Formation in the Sulfuric Acid/Ammonia and Sulfuric Acid/Dimethylamine Systems. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1886-1896.	2.5	68
1506	On the absolute photoionization cross section and dissociative photoionization of cyclopropenylidene. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 9240-9247.	2.8	20
1507	Ethylbenzene Dehydrogenase and Related Molybdenum Enzymes Involved in Oxygen-Independent Alkyl Chain Hydroxylation. <i>Journal of Molecular Microbiology and Biotechnology</i> , 2016, 26, 45-62.	1.0	50
1508	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.	2.6	18
1509	An experimental and kinetic modeling study of Î³-valerolactone pyrolysis. <i>Combustion and Flame</i> , 2016, 164, 183-200.	5.2	11
1510	Cyclopentadienone Oxidation Reaction Kinetics and Thermochemistry for the Alcohols, Hydroperoxides, and Vinylic, Alkoxy, and Alkylperoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 433-451.	2.5	12
1511	Quantum chemical theory calculations on the mechanism of the homogeneous, unimolecular gas-phase elimination kinetics of selected diazirines. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 23-29.	2.5	4
1512	Density functional theory study of oxygen migration in molten carbonate. <i>Journal of Power Sources</i> , 2016, 305, 161-166.	7.8	11
1513	Can Highly Oxidized Organics Contribute to Atmospheric New Particle Formation?. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1452-1458.	2.5	32
1514	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	1.7	21
1515	Comparison of Relative Activation Energies Obtained by Density Functional Theory and the Random Phase Approximation for Several Claisen Rearrangements. <i>Journal of Physical Chemistry B</i> , 2016, 120, 1486-1496.	2.6	10
1516	Formation and stability of gas-phase o-benzoquinone from oxidation of ortho-hydroxyphenyl: a combined neutral and distonic radical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4320-4332.	2.8	24
1517	Reaction Kinetics of Meteoric Sodium Reservoirs in the Upper Atmosphere. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1330-1346.	2.5	18
1518	Chemical bonding in carborane/aromatic co-polymers: a first-principles analysis of experimental photoemission spectra. <i>Molecular Simulation</i> , 2016, 42, 39-46.	2.0	5
1519	Measuring hydroperoxide chain-branching agents during n-pentane low-temperature oxidation. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 333-342.	3.9	66

#	ARTICLE	IF	CITATIONS
1520	Thiol-Michael addition in polar aprotic solvents: nucleophilic initiation or base catalysis?. Polymer Chemistry, 2017, 8, 1341-1352.	3.9	22
1521	A new type of two-dimensional carbon crystal prepared from 1,3,5-trihydroxybenzene. Scientific Reports, 2017, 7, 40796.	3.3	57
1522	A kinetic mechanism for the thermal decomposition of titanium tetraisopropoxide. Proceedings of the Combustion Institute, 2017, 36, 1019-1027.	3.9	33
1523	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754.	47.7	181
1524	Bottom-up design of high-energy-density molecules (N ₂ CO) _n (n = 2-8). RSC Advances, 2017, 7, 8533-8541.	3.6	2
1525	Development of Predictive Models of the Kinetics of a Hydrogen Abstraction Reaction Combining Quantum-Mechanical Calculations and Experimental Data. Industrial & Engineering Chemistry Research, 2017, 56, 815-831.	3.7	8
1526	Stripping off hydrogens in imidazole triggered by the attachment of a single electron. Physical Chemistry Chemical Physics, 2017, 19, 6406-6415.	2.8	19
1527	Theoretical investigation on the reaction of Methylidyne Radical (CH) with acetaldehyde (CH ₃ CHO). Computational and Theoretical Chemistry, 2017, 1103, 56-62.	2.5	1
1528	Hydroxyl Radicals via Collision-Induced Dissociation of Trimethylammonium Benzyl Alcohols. Australian Journal of Chemistry, 2017, 70, 397.	0.9	5
1529	Hydroperoxide Measurements During Low-Temperature Gas-Phase Oxidation of <i>n</i> -Heptane and <i>n</i> -Decane. Journal of Physical Chemistry A, 2017, 121, 1861-1876.	2.5	31
1530	Catalytic intermolecular hydroaminations of unactivated olefins with secondary alkyl amines. Science, 2017, 355, 727-730.	12.6	282
1531	An investigation on the physicochemical properties of the nanostructured [(4-X)PMAT][N(CN) ₂] ion pairs as energetic and tunable aryl alkyl amino tetrazolium based ionic liquids. Journal of Molecular Structure, 2017, 1137, 530-542.	3.6	14
1532	Theoretical study of the hydrolysis of HOSO+NO ₂ as a source of atmospheric HONO: effects of H ₂ O or NH ₃ . Environmental Chemistry, 2017, 14, 19.	1.5	10
1533	Absorption cross sections and kinetics of formation of AlO at 298 K. Chemical Physics Letters, 2017, 675, 56-62.	2.6	11
1534	On the Mechanism of Cytoprotection by Ferrostatin-1 and Liproxstatin-1 and the Role of Lipid Peroxidation in Ferroptotic Cell Death. ACS Central Science, 2017, 3, 232-243.	11.3	583
1535	Reactivity of 5-carboxycytosine toward addition and hydrogen abstraction by •OH in acetonitrile: a computational study. Molecular Simulation, 2017, 43, 563-567.	2.0	0
1536	Hydrogen Abstraction from Hydrocarbons by NH ₂ . Journal of Physical Chemistry A, 2017, 121, 2221-2231.	2.5	33
1537	Synchrotron Photoionization Investigation of the Oxidation of Ethyl <i>tert</i> -Butyl Ether. Journal of Physical Chemistry A, 2017, 121, 1460-1469.	2.5	7

#	ARTICLE	IF	CITATIONS
1538	Exploring the possibility to store the mixed oxygen-hydrogen cluster in clathrate hydrate in molar ratio 1:2 (O ₂ + 2H ₂). Journal of Molecular Graphics and Modelling, 2017, 73, 1-7.	2.4	2
1539	Formation of glycine from HCN and H ₂ O: A computational mechanistic study. Chemical Physics Letters, 2017, 675, 6-10.	2.6	16
1540	The reactivity of the 5'-formylcytosine with hydroxyl radical: A theoretical perspective. Journal of Physical Organic Chemistry, 2017, 30, e3691.	1.9	3
1541	Accurate alkynyl radical structures from density functional calculations without Hartree-Fock exchange. Journal of Chemical Physics, 2017, 146, 054109.	3.0	5
1542	Computational study of the hydrolysis of carbonyl sulphide: Thermodynamics and kinetic constants estimation using ab initio calculations. Journal of Chemical Thermodynamics, 2017, 110, 154-161.	2.0	3
1543	Catalysis of the Diels-Alder Reaction of Furan and Methyl Acrylate in Lewis Acidic Zeolites. ACS Catalysis, 2017, 7, 2240-2246.	11.2	39
1544	Charge-tagged N-heterocyclic carbenes (NHC): Direct transfer from ionic liquid solutions and long-lived nature in the gas phase. Journal of the American Society for Mass Spectrometry, 2017, 28, 1021-1029.	2.8	4
1545	Low-Temperature Synchrotron Photoionization Study of 2-Methyl-3-buten-2-ol (MBO) Oxidation Initiated by O(³ P) Atoms in the 298-650 K Range. Journal of Physical Chemistry A, 2017, 121, 2936-2950.	2.5	7
1546	Explaining the antioxidant activity of some common non-phenolic components of essential oils. Food Chemistry, 2017, 232, 656-663.	8.2	98
1547	Kinetic Modeling of the Thermal Destruction of Nitrogen Mustard Gas. Journal of Physical Chemistry A, 2017, 121, 3254-3262.	2.5	4
1548	Fragmentation of 1,4,2-oxaselenazoles as a route to isoselenocyanates-A high-level CBS-QB3 study. Chemical Data Collections, 2017, 9-10, 98-103.	2.3	2
1549	Comparative experimental and modeling study of the low- to moderate-temperature oxidation chemistry of 2,5-dimethylfuran, 2-methylfuran, and furan. Combustion and Flame, 2017, 181, 251-269.	5.2	61
1550	Does a Nitrogen Lone Pair Lead to Two Centered-Three Electron (2c-3e) Interactions in Pyridyl Radical Isomers?. Journal of Physical Chemistry A, 2017, 121, 3781-3791.	2.5	9
1551	Furfural: The Unimolecular Dissociative Photoionization Mechanism of the Simplest Furanic Aldehyde. Journal of Physical Chemistry A, 2017, 121, 3401-3410.	2.5	8
1552	Hydropersulfides: H-Atom Transfer Agents Par Excellence. Journal of the American Chemical Society, 2017, 139, 6484-6493.	13.7	85
1553	Impact of Conjugation and Hyperconjugation on the Radical Stability of Allylic and Benzylic Systems: A Theoretical Study. Journal of Organic Chemistry, 2017, 82, 5731-5742.	3.2	9
1554	Catalytic influence of water and formic acid molecules on hydration of methylglyoxal in atmosphere. Computational and Theoretical Chemistry, 2017, 1112, 71-81.	2.5	6
1555	A Comparison of Quantum and Molecular Mechanical Methods to Estimate Strain Energy in Druglike Fragments. Journal of Chemical Information and Modeling, 2017, 57, 1265-1275.	5.4	50

#	ARTICLE	IF	CITATIONS
1556	A Chemical Kinetic Investigation on Butyl Formate Oxidation: <i>Ab Initio</i> Calculations and Experiments in a Jet-Stirred Reactor. <i>Energy & Fuels</i> , 2017, 31, 6194-6205.	5.1	7
1557	Thermochemistry of Hydroxyl and Hydroperoxide Substituted Furan, Methylfuran, and Methoxyfuran. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4523-4544.	2.5	19
1558	Dual-Level Method for Estimating Multistructural Partition Functions with Torsional Anharmonicity. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2511-2522.	5.3	29
1559	Anomalous effect of non-alternant hydrocarbons on carbocation and carbanion electronic configurations. <i>Chemical Science</i> , 2017, 8, 4231-4241.	7.4	10
1560	Quantum Chemical Study of Supercritical Carbon Dioxide Effects on Combustion Kinetics. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3728-3735.	2.5	19
1561	Formic acid catalyzed isomerization of protonated cytosine: a lower barrier reaction for tautomer production of potential biological importance. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13515-13523.	2.8	5
1562	Exploring cation- π interaction in half sandwiches and sandwiches with X X triple bonds (X C, Si and) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5</i>	2.5	4
1563	Computational Study of H ₂ S Release in Reactions of Diallyl Polysulfides with Thiols. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6359-6366.	2.6	43
1564	DFT and TD-DFT study of the enol and thiol tautomers of 3-thioxopropanal in the ground and first singlet excited states. <i>Journal of Theoretical and Computational Chemistry</i> , 2017, 16, 1750034.	1.8	4
1565	Revisiting the thermochemistry of chlorine fluorides. <i>Journal of Computational Chemistry</i> , 2017, 38, 1930-1940.	3.3	1
1566	Quantum chemical study of small Al _n B _m clusters: Structure and physical properties. <i>Chemical Physics</i> , 2017, 493, 61-76.	1.9	11
1567	Protonation of Nitramines: Where Does the Proton Go?. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9587-9591.	13.8	6
1568	Efficient DLPNO-CCSD(T)-Based Estimation of Formation Enthalpies for C-, H-, O-, and N-Containing Closed-Shell Compounds Validated Against Critically Evaluated Experimental Data. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4379-4387.	2.5	112
1569	Tuning the structural, electronic and electrochemical properties of the 4-methyl-1-phenyl triazolium based [PhMeTAZ][Y ¹⁸] ionic liquids through changing anions: A quantum chemical study. <i>Journal of Molecular Liquids</i> , 2017, 240, 138-151.	4.9	13
1570	Theoretical investigation of the selective dehydration and dehydrogenation of ethanol catalyzed by small molecules. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 521-534.	2.4	4
1571	DFT study on abstraction reaction mechanism of OH radical with 2-methoxyphenol. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3713.	1.9	15
1572	$\langle \text{OH} \rangle$ + Isoprene: A Direct Dynamics Study. <i>Bulletin of the Korean Chemical Society</i> , 2017, 38, 651-660.	1.9	4
1573	Mechanistic Description of Photochemical Oligomer Formation from Aqueous Pyruvic Acid. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4272-4282.	2.5	50

#	ARTICLE	IF	CITATIONS
1574	Time-resolved measurements of product formation in the low-temperature (550–675 K) oxidation of neopentane: a probe to investigate chain-branching mechanism. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13731-13745.	2.8	20
1575	Intramolecular Nitrofuran Diels–Alder Reactions: Extremely Substituent-Tolerant Cycloadditions via Asynchronous Transition States. <i>Journal of Organic Chemistry</i> , 2017, 82, 6656-6670.	3.2	10
1576	Theoretical investigation of the molecular structure and spectroscopic properties of oxicams. <i>Journal of Structural Chemistry</i> , 2017, 58, 261-267.	1.0	1
1577	Theoretical studies of unimolecular thermal decomposition reactions of n -hexane and n -hexene isomers. <i>Computational and Theoretical Chemistry</i> , 2017, 1115, 45-55.	2.5	11
1578	Strategy for designing stable and powerful nitrogen-rich high-energy materials by introducing boron atoms. <i>Journal of Molecular Modeling</i> , 2017, 23, 191.	1.8	4
1579	Theoretical Study of Epoxidation Reactions Relevant to Hydrocarbon Oxidation. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 7454-7461.	3.7	13
1580	The mechanism of the gas-phase elimination kinetics of the $\hat{1}^2, \hat{1}^3$ -unsaturated aldehyde 2,2-dimethyl-3-butenal: a theoretical study. <i>Molecular Physics</i> , 2017, 115, 1624-1632.	1.7	2
1581	Probing Phosphorus Nitride ($P\hat{1}\%_{10}N$) and Other Elusive Species Formed upon Pyrolysis of Dimethyl Phosphoramidate. <i>Chemistry - A European Journal</i> , 2017, 23, 5595-5601.	3.3	26
1582	Kinetic barriers, rate constants and branching ratios for unimolecular reactions of methyl octanoate peroxy radicals: A computational study of a mid-sized biodiesel fuel surrogate. <i>Combustion and Flame</i> , 2017, 180, 148-157.	5.2	15
1583	Computational study on the mechanism and kinetics for the reaction between $HCHO$ and HO_{2} . <i>Molecular Simulation</i> , 2017, 43, 900-907.	2.0	3
1584	Kinetics of Thermal Unimolecular Decomposition of Acetic Anhydride: An Integrated Deterministic and Stochastic Model. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3028-3036.	2.5	11
1585	Initial Decomposition Pathways of Aqueous Hydroxylamine Solutions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4502-4511.	2.6	12
1586	How Inter- and Intramolecular Reactions Dominate the Formation of Products in Lignin Pyrolysis. <i>Chemistry - A European Journal</i> , 2017, 23, 8658-8668.	3.3	10
1587	Rate constant calculations of the $C_2 + HCN \hat{1}^+ CCCN + H$ addition via the Master Equation. <i>Journal of Molecular Modeling</i> , 2017, 23, 143.	1.8	2
1588	Catalytic effect of water, water dimer, water trimer, $HCOOH$, H_2SO_4 , CH_3CH_2COOH and $HN(NO_2)_2$ on the isomerisation of $HN(NO_2)_2$ to $O_2NNN(O)OH$: a mechanism study. <i>Molecular Physics</i> , 2017, 115, 1493-1501.	1.7	3
1589	Absolute photoionization cross sections of two cyclic ketones: cyclopentanone and cyclohexanone. <i>Journal of Mass Spectrometry</i> , 2017, 52, 259-270.	1.6	8
1590	Surface-enhanced Raman scattering properties of Lewis acid–base complexes of <i>p</i> -hydroxybenzoic and <i>p</i> -mercaptobenzoic acids with CO_{2} in the presence of silver. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 73-81.	2.5	2
1591	Aminyl Radical Generation via Tandem Norrish Type I Photocleavage, $\hat{1}^2$ -Fragmentation: Independent Generation and Reactivity of the $2\hat{1}^2$ -Deoxyadenosin- <i>N</i> -yl Radical. <i>Journal of Organic Chemistry</i> , 2017, 82, 3571-3580.	3.2	21

#	ARTICLE	IF	CITATIONS
1592	Unimolecular rearrangement of the simplest compound models with a selenium–oxygen, selenium–sulphur and selenium–selenium bond: SeXH and HSeXH (X = O,S,Se). <i>Molecular Physics</i> , 2017, 115, 1004-1013.	1.7	4
1593	Theoretical pK prediction of the Î±-phosphate moiety of uridine 5- ² -diphosphate-GlcNAc. <i>Chemical Physics Letters</i> , 2017, 667, 220-225.	2.6	7
1594	Computational study on C–B homolytic bond dissociation enthalpies of organoboron compounds. <i>New Journal of Chemistry</i> , 2017, 41, 1346-1362.	2.8	12
1595	Experimental and modeling study of the pyrolysis and combustion of 2-methyl-tetrahydrofuran. <i>Combustion and Flame</i> , 2017, 176, 409-428.	5.2	28
1596	Equilibria and Speciation of Chloramines, Bromamines, and Bromochloramines in Water. <i>Environmental Science & Technology</i> , 2017, 51, 128-140.	10.0	26
1597	Identification of Thermal Decomposition Products and Reactions for Liquid Ammonium Nitrate on the Basis of Ab Initio Calculation. <i>International Journal of Chemical Kinetics</i> , 2017, 49, 83-99.	1.6	13
1598	Thermal cracking of 1-n-butyldecalin at high pressure (100 bar). <i>Journal of Analytical and Applied Pyrolysis</i> , 2017, 123, 204-215.	5.5	3
1599	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32184-32215.	2.8	1,230
1600	Kinetic Studies on the Reactions of Atomic Oxygen with Furan, 2-Methylfuran, and 2,5-Dimethylfuran at Elevated Temperatures. <i>Chemistry Letters</i> , 2017, 46, 1207-1210.	1.3	8
1601	Can Biomimetic Zinc Compounds Assist a (3 + 2) Cycloaddition Reaction? A Theoretical Perspective. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6382-6390.	5.3	0
1602	Theoretical study on homolytic B–B cleavages of diboron(4) compounds. <i>RSC Advances</i> , 2017, 7, 49251-49272.	3.6	8
1603	Ab initio coverage-dependent microkinetic modeling of benzene hydrogenation on Pd(111). <i>Catalysis Science and Technology</i> , 2017, 7, 5267-5283.	4.1	19
1604	Unpicking the determinants of amide NH–O hydrogen bond strength with diphenylacetylene molecular balances. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 9156-9163.	2.8	15
1605	Nucleophilic Addition of Ketones To Acetylenes and Allenes: A Quantum-Chemical Insight. <i>Journal of Organic Chemistry</i> , 2017, 82, 12467-12476.	3.2	37
1606	Quantum chemical and kinetic study of the CCl ₂ self-recombination reaction. <i>Computational and Theoretical Chemistry</i> , 2017, 1121, 1-10.	2.5	2
1607	Ab initio dynamics of unimolecular decomposition of Î²-propiolactone and Î²-propiolactam. <i>Chemical Physics Letters</i> , 2017, 686, 55-59.	2.6	6
1608	Theoretical Studies on the Kinetics of Multi-Channel Gas-Phase Unimolecular Decomposition of Acetaldehyde. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6887-6895.	2.5	7
1609	Study of the Synchrotron Photoionization Oxidation of 2-Methylfuran Initiated by O(³ P) under Low-Temperature Conditions at 550 and 650 K. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6966-6980.	2.5	5

#	ARTICLE	IF	CITATIONS
1610	Modeling Oil Shale Pyrolysis: High-Temperature Unimolecular Decomposition Pathways for Thiophene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7655-7666.	2.5	25
1611	Phenoxazine: A Privileged Scaffold for Radical-Trapping Antioxidants. <i>Journal of Organic Chemistry</i> , 2017, 82, 10523-10536.	3.2	56
1612	Systematic Search for Chemical Reactions in Gas Phase Contributing to Methanol Formation in Interstellar Space. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7393-7400.	2.5	3
1613	Claisen rearrangements of benzyl vinyl ethers: theoretical investigation of mechanism, substituent effects, and regioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 7887-7893.	2.8	7
1614	Reaction Paths and Chemical Activation Reactions of 2-Methyl-5-Furanyl Radical with O_3 . <i>Journal of Physical Chemistry A</i> , 2017, 121, 7309-7323.	2.5	3
1615	Investigation on the absolute and relative photoionization cross sections of 3 potential propargylic fuels. <i>Journal of Mass Spectrometry</i> , 2017, 52, 799-808.	1.6	1
1616	Assessment of Methodology and Chemical Group Dependences in the Calculation of the $\text{p}K_a$ for Several Chemical Groups. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4791-4803.	5.3	25
1617	Parent Thioketene Sulfine Oxide H_2CCSO : Gas-Phase Generation, Structure, and Bonding Analysis. <i>Chemistry - A European Journal</i> , 2017, 23, 16566-16573.	3.3	39
1618	Theoretical Designs for Organoaluminum $\text{C}_2\text{Al}_4\text{R}_4$ with Well-Separated Al(I) and Al(III). <i>ACS Omega</i> , 2017, 2, 5407-5414.	3.5	5
1619	Fused 1,2,3-Thiaselenazoles Synthesized from 1,2,3-Dithiazoles through Selective Chalcogen Exchange. <i>Chemistry - A European Journal</i> , 2017, 23, 17037-17047.	3.3	20
1620	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.	2.5	8
1621	Quantum Chemical Study of $\text{CH}_3 + \text{O}_2$ Combustion Reaction System: Catalytic Effects of Additional CO_2 Molecule. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5681-5689.	2.5	18
1622	Polycyclic Aromatic Hydrocarbon Growth by Diradical Cycloaddition/Fragmentation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 5921-5931.	2.5	23
1623	Enthalpy of Formation of N_2H_4 (Hydrazine) Revisited. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6187-6198.	2.5	31
1624	Protonierung von Nitraminen: Bildung des O- oder N-protonierten Kations. <i>Angewandte Chemie</i> , 2017, 129, 9715-9719.	2.0	2
1625	W4-17: A diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. <i>Journal of Computational Chemistry</i> , 2017, 38, 2063-2075.	3.3	120
1626	Enhanced ignition of biomass in presence of NOx. <i>Fire Safety Journal</i> , 2017, 91, 235-242.	3.1	4
1627	VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4382-4396.	5.3	34

#	ARTICLE	IF	CITATIONS
1628	Ab Initio Computations and Active Thermochemical Tables Hand in Hand: Heats of Formation of Core Combustion Species. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6580-6602.	2.5	144
1629	Characterization of Neutral Radicals from a Dissociative Electron Attachment Process. <i>Physical Review Letters</i> , 2017, 119, 053402.	7.8	24
1630	Reduction of carbon dioxide with a superalkali. <i>Dalton Transactions</i> , 2017, 46, 11942-11949.	3.3	36
1631	Decomposition of selected chlorinated volatile organic compounds by ceria (CeO ₂). <i>Catalysis Science and Technology</i> , 2017, 7, 3902-3919.	4.1	64
1632	Reaction of H ₂ with O ₂ in Excited Electronic States: Reaction Pathways and Rate Constants. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9599-9611.	2.5	15
1633	Aryl Nitrenium and Oxenium Ions with Unusual High-Spin $\tilde{\epsilon}, \tilde{\epsilon}^*$ Ground States: Exploiting (Anti)Aromaticity. <i>Journal of Organic Chemistry</i> , 2017, 82, 13550-13556.	3.2	5
1634	Combustion and flammability chemistry for the refrigerant HFO-1234yf (2,3,3,3-tetrafluoropropene). <i>Combustion and Flame</i> , 2017, 184, 176-185.	5.2	38
1635	Experimental and kinetic investigation of 1,2,4-trimethylbenzene oxidation at low temperature. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 909-917.	3.9	31
1636	A computational mechanistic study of the deamination reaction of melamine. <i>International Journal of Quantum Chemistry</i> , 2017, 117, 180-189.	2.0	12
1637	From theoretical reaction dynamics to chemical modeling of combustion. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 77-111.	3.9	199
1638	Kinetics analysis of thermal decomposition of ammonium dinitramide (ADN). <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 127, 255-264.	3.6	36
1639	Reactivity, vibrational spectroscopy, internal rotation and thermochemical aspects of methylarsine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 383-394.	3.9	9
1640	Rate coefficients for fuel + NO ₂ : Predictive kinetics for HONO and HNO ₂ formation. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 617-626.	3.9	64
1641	New insights into the low-temperature oxidation of 2-methylhexane. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 373-382.	3.9	36
1642	Importance of the Hydrogen Isocyanide Isomer in Modeling Hydrogen Cyanide Oxidation in Combustion. <i>Energy & Fuels</i> , 2017, 31, 2156-2163.	5.1	22
1643	A quantum chemical and kinetics modeling study on the autoignition mechanism of diethyl ether. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 195-202.	3.9	55
1644	Theoretical studies on the hydrogen abstraction reactions of methyl esters with HO ₂ radical and the following $\dot{\text{I}}^2$ -scission reactions. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3668.	1.9	10
1645	Theoretical kinetic investigation of thermal decomposition of nitropropane. <i>Structural Chemistry</i> , 2017, 28, 655-666.	2.0	12

#	ARTICLE	IF	CITATIONS
1646	On the high-temperature unimolecular decomposition of ethyl levulinate. Proceedings of the Combustion Institute, 2017, 36, 187-193.	3.9	11
1647	Experimental and RRKM Investigations on the Degradation of Ethyl Formate. ChemistrySelect, 2017, 2, 11603-11614.	1.5	2
1648	Atmospheric chemistry, sources and sinks of carbon suboxide, C ₃ O ₂ . Atmospheric Chemistry and Physics, 2017, 17, 8789-8804.	4.9	6
1649	Quantum mechanical and multichannel RRKM studies of the reaction N ₂ O + O (3P). Arabian Journal of Chemistry, 2017, 10, S3559-S3568.	4.9	0
1650	Theoretical Study of Isoprene Dissociative Photoionization. Chinese Journal of Chemical Physics, 2017, 30, 43-49.	1.3	1
1652	Development of Surrogate Model for Oxygenated Wide-Distillation Fuel with Polyoxymethylene Dimethyl Ether. SAE International Journal of Fuels and Lubricants, 0, 10, .	0.2	16
1653	Reaction kinetics of hydrogen atom abstraction from isopentanol by the H atom and HO ₂ ™ radical. Physical Chemistry Chemical Physics, 2018, 20, 10895-10905.	2.8	6
1654	Detailed kinetic modeling of thermal decomposition of guaiacol – A model compound for biomass lignin. Biomass and Bioenergy, 2018, 112, 45-60.	5.7	21
1655	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. Energy & Fuels, 2018, 32, 3920-3934.	5.1	26
1656	Computational Study on N–N Homolytic Bond Dissociation Enthalpies of Hydrazine Derivatives. Journal of Physical Chemistry A, 2018, 122, 2764-2780.	2.5	10
1657	A wide-range experimental and modeling study of oxidation and combustion of n-propylbenzene. Combustion and Flame, 2018, 191, 53-65.	5.2	25
1658	Environmental Processing of Lipids Driven by Aqueous Photochemistry of ±-Keto Acids. ACS Central Science, 2018, 4, 624-630.	11.3	32
1659	An experimental and modeling study on the low temperature oxidation of surrogate for JP-8 part I: Neat 1,3,5-trimethylbenzene. Combustion and Flame, 2018, 192, 507-516.	5.2	18
1660	Guanidine: A Highly Efficient Stabilizer in Atmospheric New-Particle Formation. Journal of Physical Chemistry A, 2018, 122, 4717-4729.	2.5	32
1661	Rate Coefficient Measurements and Theoretical Analysis of the OH + (<i>E</i>)-CF ₃ CH ₂ CHCF ₃ Reaction. Journal of Physical Chemistry A, 2018, 122, 4635-4646.	2.5	10
1662	Capturing Volatile Organic Compounds Employing Superalkali Species. ChemPhysChem, 2018, 19, 2266-2271.	2.1	3
1663	Theoretical study on complexes and reactions of boron isotopic exchange separation with fluorinated anisoles as novel donors. Journal of Radioanalytical and Nuclear Chemistry, 2018, 316, 587-594.	1.5	3
1664	Structural and thermochemical properties of methyl ethyl sulfide alcohols: HOCH ₂ SCH ₂ CH ₃ , CH ₃ SCH(OH)CH ₃ , CH ₃ SCH ₂ CH ₂ OH, and radicals corresponding to loss of H atom. Journal of Physical Organic Chemistry, 2018, 31, e3836.	1.9	3

#	ARTICLE	IF	CITATIONS
1665	Causal mediation analysis with multiple mediators in the presence of treatment noncompliance. Statistics in Medicine, 2018, 37, 1810-1829.	1.6	4
1666	Theoretical studies on the mechanism and kinetics of the reaction of CF3 radical with oxygen molecule. Journal of Fluorine Chemistry, 2018, 211, 154-158.	1.7	9
1667	Computational study of the decomposition mechanisms of ammonium dinitramide in the gas phase. Molecular Physics, 2018, 116, 1756-1771.	1.7	4
1668	Evolution of π - π^* photoabsorption of the molecular-ion series Si^L H_n^+		

#	ARTICLE	IF	CITATIONS
1683	Methyl Linoleate and Methyl Oleate Bond Dissociation Energies: Electronic Structure Fishing for Wise Crack Products. <i>Energy & Fuels</i> , 2018, 32, 1779-1787.	5.1	7
1684	Through bond and through space interactions in dehydro-diazine radicals: a case study of 3c-5e interactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4386-4395.	2.8	7
1685	The furan microsolvation blind challenge for quantum chemical methods: First steps. <i>Journal of Chemical Physics</i> , 2018, 148, 014301.	3.0	44
1686	The decomposition pathways of ammonium dinitramide on the basis of ab initio calculations. <i>Journal of Energetic Materials</i> , 2018, 36, 302-315.	2.0	11
1687	Vinylsulfonatester: Effiziente Kettenübertragungsreagenzien für verzögerungsfreien 3D-Druck schlagzäher Photopolymere. <i>Angewandte Chemie</i> , 2018, 130, 9305-9310.	2.0	4
1688	Vinyl Sulfonate Esters: Efficient Chain Transfer Agents for the 3D Printing of Tough Photopolymers without Retardation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 9165-9169.	13.8	44
1689	The isomerization of cytosine: Intramolecular hydrogen atom transfer mediated through formic acid. <i>Journal of Physical Organic Chemistry</i> , 2018, 31, e3831.	1.9	4
1690	Mechanistic dichotomy in the gas-phase addition of NO ₃ to polycyclic aromatic hydrocarbons: Theoretical study. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25641.	2.0	0
1691	Furan Fragmentation in the Gas Phase: New Insights from Statistical and Molecular Dynamics Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4153-4166.	2.5	19
1692	Introducing a new methodology for the calculation of local philicity and multiphilic descriptor: an alternative to the finite difference approximation. <i>Molecular Physics</i> , 2018, 116, 1737-1748.	1.7	7
1693	Understanding the kinetics and molecular mechanism of the Curtius rearrangement of 3-oxocyclobutane-1-carbonyl azide. <i>Computational and Theoretical Chemistry</i> , 2018, 1130, 121-129.	2.5	14
1694	Thermal cracking of n-butylbenzene at high pressure: Experimental study and kinetic modelling. <i>Journal of Analytical and Applied Pyrolysis</i> , 2018, 133, 234-245.	5.5	13
1695	Ab Initio Theoretical Studies on the Kinetics of Hydrogen Abstraction Type Reactions of Hydroxyl Radicals with CH ₃ CCl ₂ F and CH ₃ CClF ₂ . <i>Russian Journal of Physical Chemistry A</i> , 2018, 92, 442-448.	0.6	1
1696	Molecular engineering of the electronic, structural, and electrochemical properties of nanostructured 1-methyl-4-phenyl 1,2,4 triazolium-based [PhMTZ][X] ionic liquids through anionic changing. <i>Ionics</i> , 2018, 24, 483-504.	2.4	6
1697	A chemical kinetic mechanism for the low- and intermediate-temperature combustion of Polyoxymethylene Dimethyl Ether 3 (PODE3). <i>Fuel</i> , 2018, 212, 223-235.	6.4	100
1698	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. <i>Combustion and Flame</i> , 2018, 187, 247-256.	5.2	58
1699	Computational study on the molecular conformations of phenolic compounds. <i>Structural Chemistry</i> , 2018, 29, 179-194.	2.0	11
1700	Computational challenges in Astrochemistry. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1349.	14.6	43

#	ARTICLE	IF	CITATIONS
1701	<i>Ab initio</i> analysis on potential superbases of several hyperlithiated species: $\text{Li}_3\text{F}_2\text{O}$ and $\text{Li}_3\text{F}_2\text{OH}_n$ ($n = 1, 2$). Dalton Transactions, 2018, 47, 159-168.	3.3	17
1702	Theoretical studies on the reaction kinetics of methyl crotonate with hydroxyl radical. Sustainable Energy and Fuels, 2018, 2, 392-402.	4.9	24
1703	Effects of C5-substituent group on the hydrogen peroxide-mediated tautomerisation of protonated cytosine: a theoretical perspective. Molecular Physics, 2018, 116, 471-481.	1.7	1
1704	Thermal Decomposition of Phosgene and Diphosgene. Journal of Physical Chemistry A, 2018, 122, 249-257.	2.5	8
1705	Theoretical calculations of homogeneous catalysis in the gas phase: elimination kinetics of 2,2-dimethoxypropane in the presence of HCl, F_3CCOOH and CH_3COOH . Molecular Physics, 2018, 116, 1118-1126.	1.7	3
1706	Synchrotron Photoionization Study of Furan and 2-Methylfuran Reactions with Methylidyne Radical (CH) at 298 K. Journal of Physical Chemistry A, 2018, 122, 280-291.	2.5	7
1707	Activation of Dinitrogen with a Superalkali Species, Li_3F_2 . ChemPhysChem, 2018, 19, 256-260.	2.1	17
1708	Exploring the mechanisms for the radical induced damage of 6- ϵ -thioguanine. International Journal of Quantum Chemistry, 2018, 118, e25544.	2.0	1
1709	Molecular Clusters and Solvation in Volcanic and Hydrothermal Vapors. Reviews in Mineralogy and Geochemistry, 2018, 84, 57-83.	4.8	5
1710	Extrapolation of high-order correlation energies: the WMS model. Physical Chemistry Chemical Physics, 2018, 20, 27375-27384.	2.8	34
1711	Chain-propagation, chain-transfer, and hydride-abstraction by cyclic carbocations on water surfaces. Physical Chemistry Chemical Physics, 2018, 20, 25256-25267.	2.8	11
1712	Detailed kinetics of tetrafluoroethene ozonolysis. Physical Chemistry Chemical Physics, 2018, 20, 28059-28067.	2.8	4
1713	Nitrogen matters: the difference between PANH and PAH formation. Physical Chemistry Chemical Physics, 2018, 20, 29910-29917.	2.8	29
1714	Computational Investigation of $\text{RO}_2 + \text{HO}_2$ and $\text{RO}_2 + \text{RO}_2$ Reactions of Monoterpene Derived First-Generation Peroxy Radicals Leading to Radical Recycling. Journal of Physical Chemistry A, 2018, 122, 9542-9552.	2.5	19
1715	Electrochemical Dimerization of Phenylpropenoids and the Surprising Antioxidant Activity of the Resultant Quinone Methide Dimers. Angewandte Chemie, 2018, 130, 17371-17375.	2.0	6
1716	Electrochemical Dimerization of Phenylpropenoids and the Surprising Antioxidant Activity of the Resultant Quinone Methide Dimers. Angewandte Chemie - International Edition, 2018, 57, 17125-17129.	13.8	26
1717	Catalytic hydrolyses of trifluoroacetyl fluoride by water. Chemical Physics Letters, 2018, 713, 137-144.	2.6	2
1718	Kinetics of Intramolecular Phenyl Migration and Fused Ring Formation in Hexylbenzene Radicals. Journal of Physical Chemistry A, 2018, 122, 9778-9791.	2.5	4

#	ARTICLE	IF	CITATIONS
1719	CAI ₃ X (X = B/Al/Ga/In/Tl) with 16 valence electrons: can planar tetracoordinate carbon be stable?. Physical Chemistry Chemical Physics, 2018, 20, 26266-26272.	2.8	22
1720	Theoretical Study on the Dynamics and Kinetics of the Reaction of CH ₂ OH with OH. Journal of Physical Chemistry A, 2018, 122, 9761-9777.	2.5	2
1721	Tuning Hydrogenated Silicon, Germanium, and SiGe Nanocluster Properties Using Theoretical Calculations and a Machine Learning Approach. Journal of Physical Chemistry A, 2018, 122, 9851-9868.	2.5	9
1722	New insights in conceptual DFT: New model for the calculation of local reactivity indices based on the Sanderson's principle. International Journal of Quantum Chemistry, 2019, 119, e25844.	2.0	8
1723	Umbrella inversion and structure of phosphorus-containing compounds: A quantum chemical study. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850042.	1.8	7
1724	Detailed kinetic model for ammonium dinitramide decomposition. Combustion and Flame, 2018, 198, 222-229.	5.2	23
1725	Ab Initio Simulation of pH-Sensitive Biomarkers in Magnetic Resonance Imaging. Journal of Physical Chemistry A, 2018, 122, 7983-7990.	2.5	0
1726	A reaction kinetics study and model development to predict the formation and destruction of organosulfur species (carbonyl sulfide and mercaptans) in Claus furnace. International Journal of Chemical Kinetics, 2018, 50, 880-896.	1.6	10
1727	Theoretical Study on the Kinetics for the Reactions of Heptyl Radicals with Methanol. Chemical Research in Chinese Universities, 2018, 34, 786-791.	2.6	0
1728	Computational study on the mechanism and kinetics of NO ₃ -initiated atmosphere oxidation of vinyl acetate. Computational and Theoretical Chemistry, 2018, 1144, 18-25.	2.5	11
1729	Atmospheric Fate of Criegee Intermediate Formed During Ozonolysis of Styrene in the Presence of H ₂ O and NH ₃ : The Crucial Role of Stereochemistry. Journal of Physical Chemistry A, 2018, 122, 8377-8389.	2.5	13
1730	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. Journal of Physical Chemistry A, 2018, 122, 8982-8988.	2.5	25
1731	A study of thermal decomposition of bromoethane. Journal of Analytical and Applied Pyrolysis, 2018, 136, 199-207.	5.5	7
1732	Reaction mechanisms and kinetics of the β -elimination processes of compounds CHF ₂ CH ₂ SiF ₃ Me ₃ SiF (n = 1, 2, 3): DFT and CBS-QB3 methods using Rice-Ramsperger-Kassel-Marcus and transition state theories. Journal of Fluorine Chemistry, 2018, 216, 71-80.	2.7	6
1733	A computational study on molecular structure and stability of tautomers of dipyrrole-based phenanthroline analogue. Computational and Theoretical Chemistry, 2018, 1145, 6-14.	2.5	3
1734	Mechanistic and Kinetic Investigations on the Thermal Unimolecular Reaction of Heptafluoroisobutyronitrile. Journal of Physical Chemistry A, 2018, 122, 7704-7715.	2.5	31
1735	[(H ₂ O)Zn(Imidazole) _n] ²⁺ : the vital roles of coordination number and geometry in Zn ²⁺ -OH ₂ acidity and catalytic hydrolysis. Physical Chemistry Chemical Physics, 2018, 20, 24979-24991.	2.8	14
1736	Kinetic Study of the Pyrolysis and Oxidation of Guaiacol. Journal of Physical Chemistry A, 2018, 122, 7894-7909.	2.5	41

#	ARTICLE	IF	CITATIONS
1737	An experimental and chemical kinetic modeling study of 1,3-butadiene combustion: Ignition delay time and laminar flame speed measurements. Combustion and Flame, 2018, 197, 423-438.	5.2	432
1738	Low Temperature Oxidation Kinetics of Biodiesel Molecules: Rate Rules for Concerted HO ₂ Elimination from Alkyl Ester Peroxy Radicals. Journal of Physical Chemistry A, 2018, 122, 8259-8273.	2.5	14
1739	Kinetic modeling for unimolecular β -scission of the methoxymethyl radical from quantum chemical and RRKM analyses. Combustion and Flame, 2018, 197, 243-253.	5.2	8
1740	Computational investigation of LiF containing hypersalts. Dalton Transactions, 2018, 47, 13204-13213.	3.3	2
1741	Generation of methylene by the liquid phase oxidation of isobutene with nitrous oxide. Tetrahedron, 2018, 74, 3589-3595.	1.9	6
1742	Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metal-Organic Framework NU-1000. Journal of Physical Chemistry C, 2018, 122, 12362-12368.	3.1	55
1743	An ab initio CBS-QB3 quantum chemical study of singlet and triplet sulfonylnitrenes insertion into acetylenes and nitriles. Journal of Molecular Structure, 2018, 1172, 8-16.	3.6	1
1744	Deciphering Stability of Five-Membered Heterocyclic Radicals: Balancing Act Between Delocalization and Ring Strain. Journal of Physical Chemistry A, 2018, 122, 5464-5476.	2.5	9
1745	CCSDT(Q)/CBS thermochemistry for the D5h \rightarrow D10h isomerization in the C10 carbon cluster: Getting the right answer for the right reason. Chemical Physics Letters, 2018, 706, 19-23.	2.6	4
1746	Solvation Dynamics of HEHEHP Ligand at the Liquid-Liquid Interface. Journal of Physical Chemistry B, 2018, 122, 5999-6006.	2.6	12
1747	Investigation on pyrolysis mechanism of guaiacol as lignin model compound at atmospheric pressure. Fuel, 2018, 232, 632-638.	6.4	56
1748	Thermochemistry and Kinetic Studies on the Autoignition of 2-Butanone: A Computational Study. Journal of Physical Chemistry A, 2018, 122, 6134-6146.	2.5	5
1749	Decomposition and isomerization of 1-pentanol radicals and the pyrolysis of 1-pentanol. Combustion and Flame, 2018, 196, 500-514.	5.2	23
1750	Study of Methylidyne Radical (CH and CD) Reaction with 2,5-Dimethylfuran Using Multiplexed Synchrotron Photoionization Mass Spectrometry. Journal of Physical Chemistry A, 2018, 122, 6118-6133.	2.5	5
1751	Theoretical study on the acidities of pyrrole, indole, carbazole and their hydrocarbon analogues in DMSO. Canadian Journal of Chemistry, 2018, 96, 1001-1009.	1.1	4
1752	Modeling of thermodynamics of substituted toluene derivatives and benzylic radicals <i>via</i> group additivity. AIChE Journal, 2018, 64, 3649-3661.	3.6	6
1753	The hydrogen atom transfer reactivity of sulfinic acids. Chemical Science, 2018, 9, 7218-7229.	7.4	36
1754	A theoretical study of the thermal stability of the FS(O ₂)OSO ₂ radical and the recombination kinetics with the FSO ₃ radical. Computational and Theoretical Chemistry, 2018, 1123, 87-95.	2.5	1

#	ARTICLE	IF	CITATIONS
1755	Investigation of Oxidation Reaction Products of 2-Phenylethanol Using Synchrotron Photoionization. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6789-6798.	2.5	4
1756	Quantum-chemical and kinetic study of the reactions of the ClSO ₂ radical with H, O, Cl, S, SCl and ClSO ₂ in the atmosphere of Venus. <i>Computational and Theoretical Chemistry</i> , 2018, 1140, 14-23.	2.5	0
1757	Kinetic analysis of the thermal decomposition of liquid ammonium nitrate based on thermal analysis and detailed reaction simulations. <i>Journal of Thermal Analysis and Calorimetry</i> , 2018, 134, 813-823.	3.6	23
1758	The influences of ammonia on aerosol formation in the ozonolysis of styrene: roles of Criegee intermediate reactions. <i>Royal Society Open Science</i> , 2018, 5, 172171.	2.4	21
1759	Acid-catalyzed conversion of caryolan-1-ol to isoclovene: A computational investigation of the multi-step carbocation rearrangement. <i>Tetrahedron</i> , 2018, 74, 3781-3786.	1.9	1
1760	Why Do Bâ€P and Alâ€P Polymers Differ? Structures, Stability, and Electronic Properties of Chain and Ring [H 2 PEH 2] n Oligomers (E=B, Al; n =1 â€ 15). <i>Chemistry - A European Journal</i> , 2018, 24, 17046-17054.	3.3	7
1761	Kinetics of the Reaction of the Cyclopentadienyl Radical with Nitrogen Dioxide. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6978-6984.	2.5	0
1762	Guanine synthesis from 4-aminoimidazole-5-carbonitrile: A computational mechanistic study. <i>Chemical Physics Letters</i> , 2018, 708, 71-76.	2.6	8
1763	Physicochemical Prediction of Metabolite Fragmentation in Tandem Mass Spectrometry. <i>Mass Spectrometry</i> , 2018, 7, A0066-A0066.	0.6	1
1764	Absolute and relative pKa predictions via a DFT approach applied to the SAMPL6 blind challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1179-1189.	2.9	25
1765	Gas Phase OH Radical Reaction with 2â€Chloroethyl Vinyl Ether in the 256â€333â€K Temperature Range: A Combined LPâ€LIF and Computational Study. <i>ChemistrySelect</i> , 2018, 3, 5910-5919.	1.5	3
1766	Ab initio chemical kinetics of the CH ₂ OOâ€+â€C ₂ F ₄ reaction. <i>Chemical Physics Letters</i> , 2018, 706, 280-284.	2.6	10
1767	S₂ + Air Combustion: Reaction Kinetics, Flame Structure, and Laminar Flame Behavior. <i>Energy & Fuels</i> , 2018, 32, 10184-10193.	5.1	8
1768	Inhibition of hydrocarbon autoxidation by nitroxide-catalyzed cross-dismutation of hydroperoxyl and alkylperoxyl radicals. <i>Chemical Science</i> , 2018, 9, 6068-6079.	7.4	38
1769	Combustion and Pyrolysis Kinetics of Chloropicrin. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5735-5741.	2.5	0
1770	Multichannel Gas-Phase Unimolecular Decomposition of Acetone: Theoretical Kinetic Studies. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5895-5904.	2.5	9
1771	Theoretical Studies on Isomerization and Decomposition Reactions of 2-Methyl-1-butanol Radicals. <i>Energy & Fuels</i> , 2018, 32, 7652-7659.	5.1	3
1772	Dissociative electron attachment induced ring opening in five-membered heterocyclic compounds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18271-18278.	2.8	12

#	ARTICLE	IF	CITATIONS
1773	Probing the basis set limit for thermochemical contributions of inner-shell correlation: balance of core-core and core-valence contributions. <i>Molecular Physics</i> , 2019, 117, 1078-1087.	1.7	15
1774	The C ₂ H ₂ + NO ₂ reaction: Implications for high pressure oxidation of C ₂ H ₂ /NO _x mixtures. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 469-476.	3.9	14
1775	Accurate and standard thermochemistry for oxygenated hydrocarbons: A case study of ethyl levulinate. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 337-346.	3.9	4
1776	The thermal decomposition of furfural: molecular chemistry unraveled. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 445-452.	3.9	16
1777	An experimental and modeling study of oxidation of 1,2,4-trimethylcyclohexane with JSR. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 437-444.	3.9	9
1778	The role of guaiacyl moiety in free radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol: thermodynamics of 3H+/3e ⁻ mechanisms. <i>Molecular Physics</i> , 2019, 117, 207-217.	1.7	7
1779	Insights into the oxidation kinetics of a cetane improver “1,2-dimethoxyethane (1,2-DME) with experimental and modeling methods. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 555-564.	3.9	12
1780	HO ₂ -mediated reactions in cyclohexene oxidation. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 323-335.	3.9	21
1781	A simple heuristic approach to estimate the thermochemistry of condensed-phase molecules based on the polarizable continuum model. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18920-18929.	2.8	15
1782	Thermochemistry of Guanine Tautomers Re-Examined by Means of High-Level CCSD(T) Composite Ab Initio Methods. <i>Australian Journal of Chemistry</i> , 2019, 72, 607.	0.9	13
1783	Methods To Improve the Calculations of Solvation Model Density Solvation Free Energies and Associated Aqueous p _K Values: Comparison between Choosing an Optimal Theoretical Level, Solute Cavity Scaling, and Using Explicit Solvent Molecules. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7430-7438.	2.5	39
1784	Theoretical Investigation of the Reaction of Pyrene Formation from Fluoranthene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7491-7498.	2.5	4
1785	Interaction of CH ₄ with Electronically Excited O ₂ : Ab Initio Potential Energy Surfaces and Reaction Kinetics. <i>Plasma Chemistry and Plasma Processing</i> , 2019, 39, 1533-1558.	2.4	13
1786	Trifluoroacetic Acid and Trifluoroacetic Anhydride Radical Cations Dissociate near the Ionization Limit. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6313-6318.	2.5	3
1787	Ab Initio and Quasiclassical Trajectory Study of the O(³ P) + 2-Propanol Hydrogen Abstraction Reaction. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6911-6920.	2.5	6
1788	Reactivity analysis of ammonium dinitramide binary mixtures based on ab initio calculations and thermal analysis. <i>Journal of Thermal Analysis and Calorimetry</i> , 2019, 138, 2615-2622.	3.6	4
1789	Product detection study of the gas-phase oxidation of methylphenyl radicals using synchrotron photoionisation mass spectrometry. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17939-17949.	2.8	8
1790	Chemical Kinetics Approves the Occurrence of C(³ P _j) Reaction with H ₂ O. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5877-5892.	2.5	1

#	ARTICLE	IF	CITATIONS
1791	Low Temperature Kinetics of the Reaction Between Methanol and the CN Radical. Journal of Physical Chemistry A, 2019, 123, 9995-10003.	2.5	7
1792	Reaction of Hydroperoxy Radicals with Primary C ₅ Alcohols: A Profound Effect on Ignition Delay Times. Energy & Fuels, 2019, 33, 11781-11794.	5.1	16
1793	Computational Studies on the Thermodynamic and Kinetic Parameters of Oxidation of 2-Methoxyethanol Biofuel via H-Atom Abstraction by Methyl Radical. Scientific Reports, 2019, 9, 15361.	3.3	17
1794	Characterization of the 2-methylvinoxy radical + O ₂ reaction: A focal point analysis and composite multireference study. Journal of Chemical Physics, 2019, 151, 124302.	3.0	11
1795	Condensed-phase pyrolysis mechanism of ammonium nitrate based on detailed kinetic model. Journal of Analytical and Applied Pyrolysis, 2019, 143, 104671.	5.5	8
1796	Competitive Gas Phase Reactions for the Production of Isomers C ₂ O ₂ H ₄ . Spectroscopic Constants of Methyl Formate. Journal of Physical Chemistry A, 2019, 123, 9658-9668.	2.5	6
1797	Decomposition of Picolyl Radicals at High Temperature: A Mass Selective Threshold Photoelectron Spectroscopy Study. Chemistry - A European Journal, 2019, 25, 16652-16659.	3.3	6
1798	Machine Learning To Predict Standard Enthalpy of Formation of Hydrocarbons. Journal of Physical Chemistry A, 2019, 123, 8305-8313.	2.5	40
1799	Computational investigation on the reaction of dimethyl ether with nitric dioxide. I. Underlying mechanism and accurate energetics. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	4
1800	Thermochemistry of Intermediates and Products in the Oxidation Reaction of 1,1,2-Trifluoroethene via OH Radical. Journal of Physical Chemistry A, 2019, 123, 8017-8027.	2.5	4
1801	Enthalpies of formation of the benzyloxy, benzylperoxy, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
1802	Reaction Pathways, Thermodynamics, and Kinetics of Cyclopentanone Oxidation Intermediates: A Theoretical Approach. Journal of Physical Chemistry A, 2019, 123, 9644-9657.	2.5	6
1803	1-Methyl-1,4-cyclohexadiene as a Traceless Reducing Agent for the Synthesis of Catechols and Hydroquinones. Journal of Organic Chemistry, 2019, 84, 13655-13664.	3.2	17
1804	Theoretical study on desulfurization mechanisms of a coal-based model compound 2-methylthiophene during pyrolysis under inert and oxidative atmospheres. Fuel, 2019, 257, 116028.	6.4	15
1805	Probing the low-temperature chemistry of di-n-butyl ether: Detection of previously unobserved intermediates. Combustion and Flame, 2019, 210, 9-24.	5.2	26
1806	Understanding Carbamate Formation Reaction Thermochemistry of Amino Acids as Solvents for Postcombustion CO ₂ Capture. Journal of Physical Chemistry B, 2019, 123, 8433-8447.	2.6	13
1807	Catalytic Mechanism of Calcium on the Formation of HCN during Pyrolysis of Pyrrole and Indole: A Theoretical Study. Energy & Fuels, 2019, 33, 11516-11523.	5.1	12
1808	Novel Energetic Coordination Polymers Based on 1,5-Di(nitramino)tetrazole With High Oxygen Content and Outstanding Properties: Syntheses, Crystal Structures, and Detonation Properties. Frontiers in Chemistry, 2019, 7, 672.	3.6	6

1810	Correlations between Fukui Indices and Reactivity Descriptors Based on Sanderson's Principle. Journal of Physical Chemistry A, 2019, 123, 8571-8582.	2.5	13
1811	Ab Initio/Transition-State Theory Study of the Reactions of H^+ Species of Relevance to 1,3-Pentadiene, Part I: Potential Energy Surfaces, Thermochemistry, and High-Pressure Limiting Rate Constants. Journal of Physical Chemistry A, 2019, 123, 9019-9052.	2.5	19
1812	Kinetics and mechanism of the $\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{CO} + \text{CH}_4$ reaction. Chemical Physics Letters, 2019, 734, 136699.	2.6	1
1813	A thermochemical computational study on hydroxyquinolines and their azulene analogues. Journal of Molecular Structure, 2019, 1183, 70-77.	3.6	4
1814	Imaging the infrared multiphoton excitation and dissociation of propargyl chloride. Physical Chemistry Chemical Physics, 2019, 21, 1528-1535.	2.8	2
1815	Assessment of a composite method based on selected density functional theory methods and complete basis set extrapolation formulas. International Journal of Quantum Chemistry, 2019, 119, e25892.	2.0	6
1816	Conserved Vibrational Coherence in the Ultrafast Rearrangement of 2-Nitrotoluene Radical Cation. Journal of Physical Chemistry A, 2019, 123, 1140-1152.	2.5	24
1817	Experimental and Computational Study of the Group 1 Metal Cation Chelates with Lysine: Bond Dissociation Energies, Structures, and Structural Trends. Journal of Physical Chemistry B, 2019, 123, 1983-1997.	2.6	11
1818	Combustion study of a surrogate jet fuel. Combustion and Flame, 2019, 202, 252-261.	5.2	37
1819	Proton Abstraction from DME O_2 by OH^+ , O_2^+ , and XO_2^+ , for X = Li, Na, and K: Implications for Li O_2 Batteries. Journal of Physical Chemistry A, 2019, 123, 4942-4947.	2.5	4
1820	The deamination mechanism of 5,6-dihydrocytosine and 5,6-dihydro-5-methylcytosine under typical bisulfite condition. Journal of Physical Organic Chemistry, 2019, 32, e3990.	1.9	0
1821	Accurate quantum chemical energies for 133,000 organic molecules. Chemical Science, 2019, 10, 7449-7455.	7.4	53
1822	Tunable electron transfer rate in a CdSe/ZnS-based complex with different anthraquinone chloride substitutes. Scientific Reports, 2019, 9, 7756.	3.3	5
1823	Thermochemistry. Computer Aided Chemical Engineering, 2019, 45, 3-114.	0.5	31
1824	Ab initio kinetics for pyrolysis and combustion systems. Computer Aided Chemical Engineering, 2019, , 115-167.	0.5	27
1825	Thermochemistry of phosphorus sulfide cages: an extreme challenge for high-level ab initio methods. Structural Chemistry, 2019, 30, 1665-1675.	2.0	4
1826	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. Journal of Physical Chemistry A, 2019, 123, 5129-5143.	2.5	262

#	ARTICLE	IF	CITATIONS
1827	As ⁺ P vs. P ⁺ P Insertion in AsP ₃ : Kinetic Control of the Formation of [AsP ₃ NO] ⁺ . European Journal of Inorganic Chemistry, 2019, 2019, 2607-2612.	2.0	6
1828	A detailed kinetic study on oxidation of benzyl alcohol. Combustion and Flame, 2019, 207, 10-19.	5.2	11
1829	Pressure-Dependent Rate Rules for the Intramolecular H-Shift Reactions of Hydroperoxy-Alkenyl-Peroxy Radicals in Low Temperature. Energy & Fuels, 2019, 33, 5597-5609.	5.1	6
1830	To Boldly Look Where No One Has Looked Before: Identifying the Primary Photoproducts of Acetylacetone. Journal of Physical Chemistry A, 2019, 123, 5472-5490.	2.5	22
1831	Accuracy and Interpretability: The Devil and the Holy Grail. New Routes across Old Boundaries in Computational Spectroscopy. Chemical Reviews, 2019, 119, 8131-8191.	47.7	167
1832	Kinetic Investigations of the CH (X ²⁺) Radical Reaction with Cyclopentadiene. Journal of Physical Chemistry A, 2019, 123, 5692-5703.	2.5	7
1833	New global minima of 6-vertex dicarboranes: classical but unexpected. Chemical Communications, 2019, 55, 6373-6376.	4.1	4
1834	Structurally uneasy but kinetically stable nitrogens in 1,3-disubstituted cyclotetrazenes: Viable high-energy-density materials. International Journal of Quantum Chemistry, 2019, 119, e25976.	2.0	3
1835	Reaction kinetics and thermochemistry of the chemically activated and stabilized primary ethyl radical of methyl ethyl sulfide, CH ₃ SCH ₂ CH ₂ •, with O ₂ to CH ₃ SCH ₂ CH ₂ OO•. International Journal of Chemical Kinetics, 2019, 51, 618-633.	1.6	0
1836	Auto-ignition control using an additive with adaptable chemical structure. Part I: Development of a kinetic model for 1,3-cyclohexadiene and 1,3,5-hexatriene combustion. Combustion and Flame, 2019, 205, 466-483.	5.2	13
1837	First Study of the Pyrolysis of a Halogenated Ester: Methyl Chloroacetate. Industrial & Engineering Chemistry Research, 2019, 58, 9331-9338.	3.7	4
1838	Electrochemical performance of L-tryptophan picrate as an efficient electrode material for supercapacitor application. Physical Chemistry Chemical Physics, 2019, 21, 11829-11838.	2.8	22
1839	Aqueous reactions of organic triplet excited states with atmospheric alkenes. Atmospheric Chemistry and Physics, 2019, 19, 5021-5032.	4.9	16
1840	New advances in conceptual-DFT: an alternative way to calculate the Fukui function and dual descriptor. Journal of Molecular Modeling, 2019, 25, 123.	1.8	17
1841	A structural comparative study of charge transfer compounds: Synthesis, crystal structure, IR, Raman-spectroscopy, DFT computation and hirshfeld surface analysis. Journal of Molecular Structure, 2019, 1192, 132-144.	3.6	18
1842	Gas-Phase Deprotonation of Benzhydryl Cations: Carbene Basicity, Multiplicity, and Rearrangements. Journal of Organic Chemistry, 2019, 84, 7685-7693.	3.2	3
1843	Mechanism study of ammonium nitrate decomposition with chloride impurity using experimental and molecular simulation approach. Journal of Hazardous Materials, 2019, 378, 120585.	12.4	18
1844	Thermochemistry and kinetics of the 2-butanone + C ₃ H ₂ reaction system. International Journal of Chemical Kinetics, 2019, 51, 541-562.	1.6	7

#	ARTICLE	IF	CITATIONS
1845	A theoretical study on one-electron redox potentials of organotrifluoroborate anions. <i>New Journal of Chemistry</i> , 2019, 43, 8590-8605.	2.8	0
1846	Global Isomeric Survey of Elusive Cyclopropanetrione: Unknown but Viable Isomers. <i>Frontiers in Chemistry</i> , 2019, 7, 193.	3.6	4
1847	The antioxidant activity of polysulfides: it's radical!. <i>Chemical Science</i> , 2019, 10, 4999-5010.	7.4	38
1848	Peroxy self-reaction leading to the formation of furfural. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10228-10237.	2.8	2
1849	Theoretical study of the microhydration of 1-chloro and 2-chloro ethanol as a clue for their relative propensity toward dehalogenation. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25931.	2.0	5
1850	Enthalpy of Formation of $C_2H_2O_4$ (Oxalic Acid) from High-Level Calculations and the Active Thermochemical Tables Approach. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3481-3496.	2.5	9
1851	Concise Synthesis of a New Chiral Cyclopentenone Building Block for Prostaglandins and their Derivatives. <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2612-2620.	2.4	1
1852	Thermochemistry and Kinetics of the Thermal Degradation of 2-Methoxyethanol as Possible Biofuel Additives. <i>Scientific Reports</i> , 2019, 9, 4535.	3.3	20
1853	Product Detection of the CH Radical Reactions with Ammonia and Methyl-Substituted Amines. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2178-2193.	2.5	4
1854	An Ab Initio Investigation of the 4,4'-Methylene Diphenyl Diamine (4,4'-MDA) Formation from the Reaction of Aniline with Formaldehyde. <i>Polymers</i> , 2019, 11, 398.	4.5	7
1855	Theoretical study of hydrogen abstraction by small radicals from cyclohexane-carbonyl-hydroperoxide. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	1.4	1
1856	Thermodynamics and Reaction Mechanisms for Decomposition of a Simple Protonated Tripeptide, H^+GAG : a Guided Ion Beam and Computational Study. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 1013-1027.	2.8	8
1857	Pressure-dependent rate rules for intramolecular H-migration reactions of normal-alkyl cyclohexylperoxy radicals. <i>Combustion and Flame</i> , 2019, 204, 176-188.	5.2	24
1858	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. <i>Journal of the American Chemical Society</i> , 2019, 141, 6234-6246.	13.7	42
1859	Alternated Branching Ratios by Anomaly in Collision-Induced Dissociation of Proton-Bound Hoogsteen Base Pairs of 1-Methylcytosine with 1-Methylguanine and 9-Methylguanine. <i>Journal of the American Society for Mass Spectrometry</i> , 2019, 30, 846-854.	2.8	10
1860	Experimental and Computational Studies of Unimolecular 1,1-HX (X = F, Cl) Elimination Reactions of $C_2D_5CH_2Cl$: Role of Carbene:HF and HCl Adducts in the Exit Channel of RCH_2Cl and RCH_2Cl Reactions. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2621-2633.	2.5	4
1861	Exploring hydroperoxides in combustion: History, recent advances and perspectives. <i>Progress in Energy and Combustion Science</i> , 2019, 73, 132-181.	31.2	119
1862	Spectroscopic Characterization of Nicotinoyl and Isonicotinoyl Nitrenes and the Photointerconversion of 4-Pyridyl Nitrene with Diazacycloheptatetraene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3793-3801.	2.5	5

#	ARTICLE	IF	CITATIONS
1863	Shock wave and modelling study of the dissociation pathways of (C ₂ F ₅) ₃ N. Physical Chemistry Chemical Physics, 2019, 21, 9785-9792.	2.8	3
1864	Theoretical Calculation of Reaction Rates and Combustion Kinetic Modeling Study of Triethyl Phosphate (TEP). Journal of Physical Chemistry A, 2019, 123, 4764-4775.	2.5	15
1865	Dissociative Photoionization of the C ₇ H ₈ Isomers Cycloheptatriene and Toluene: Looking at Two Sides of the Same Coin Simultaneously. Journal of Physical Chemistry A, 2019, 123, 3454-3463.	2.5	16
1866	Oxidation reaction mechanism and kinetics between OH radicals and alkyl-substituted aliphatic thiols: OH-addition pathways. Progress in Reaction Kinetics and Mechanism, 2019, 44, 157-174.	2.1	1
1867	Screening for Improved Nerve Agent Simulants and Insights into Organophosphate Hydrolysis Reactions from DFT and QSAR Modeling. Chemistry - A European Journal, 2019, 25, 9217-9229.	3.3	26
1868	Reactions of aliphatic amines with ozone: Kinetics and mechanisms. Water Research, 2019, 157, 514-528.	11.3	74
1869	Thermochemistry and Group Additivity Values for Fused Two-Ring Species and Radicals. Journal of Physical Chemistry A, 2019, 123, 3418-3428.	2.5	11
1870	Reaction pathways, kinetics and thermochemistry of the chemically-activated and stabilized primary methyl radical of methyl ethyl sulfide, CH ₃ CH ₂ SCH ₂ •, with 3O ₂ to CH ₂ CH ₃ SCH ₂ OO•. Combustion and Flame, 2019, 204, 368-379.	5.2	0
1871	mHDFSâ€”HoF: A generalized multilevel homodesmotic fragmentâ€”separation reaction based program for heatâ€”ofâ€”formation calculation for acyclic hydrocarbons. Journal of Computational Chemistry, 2019, 40, 1360-1373.	3.3	3
1872	Pentadiynylidene and Its Methyl-Substituted Derivates: Threshold Photoelectron Spectroscopy of R ₁ -C ₅ -R ₂ Triplet Carbon Chains. Journal of Physical Chemistry A, 2019, 123, 2008-2017.	2.5	18
1873	The deamination mechanism of the 5,6-dihydro-6-hydroxylcytosine and 5,6-dihydro-5-methyl-6-hydroxylcytosine under typical bisulfite conditions. Molecular Physics, 2019, 117, 759-767.	1.7	0
1874	Partial combination of composite strategy and the B3LYP functional for the calculation of enthalpies of formation. Journal of Molecular Modeling, 2019, 25, 62.	1.8	8
1875	Theoretical study on the gas phase reaction of methyl chavicol with hydroxyl radical. Computational and Theoretical Chemistry, 2019, 1151, 78-90.	2.5	5
1876	Theoretical study of the molecular aspect of the suspected novichok agent A234 of the Skripal poisoning. Royal Society Open Science, 2019, 6, 181831.	2.4	45
1877	Regioselectivity of Hydroxyl Radical Reactions with Arenes in Nonaqueous Solutions. Journal of Organic Chemistry, 2019, 84, 3260-3269.	3.2	7
1878	Experimental and kinetic study on the low-temperature oxidation of pyridine as a representative of fuel-N compounds. Combustion and Flame, 2019, 202, 394-404.	5.2	35
1879	A case study of antiaromaticity: carbomethoxy cyclopropenyl anion. Turkish Journal of Chemistry, 2019, 43, 594-611.	1.2	0
1880	Role of hydrogen migrations in carbonyl peroxy radicals in the atmosphere. Chinese Journal of Chemical Physics, 2019, 32, 457-466.	1.3	4

#	ARTICLE	IF	CITATIONS
1881	Decomposition characteristics of C4F7N/CO2 mixture under AC discharge breakdown. AIP Advances, 2019, 9, .	1.3	40
1882	Computer-Assisted Design of Environmentally Friendly and Light-Stable Fluorescent Dyes for Textile Applications. International Journal of Molecular Sciences, 2019, 20, 5971.	4.1	2
1883	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. Molecules, 2019, 24, 3810.	3.8	14
1884	DFT Modeling of Organocatalytic Ring-Opening Polymerization of Cyclic Esters: A Crucial Role of Proton Exchange and Hydrogen Bonding. Polymers, 2019, 11, 2078.	4.5	23
1885	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> -PyrrylNitrene. European Journal of Organic Chemistry, 2019, 2019, 401-411.	2.4	5
1886	Steric Demand and Rate-determining Step for Photoenolization of Di <i>ortho</i> -substituted Acetophenone Derivatives. Photochemistry and Photobiology, 2019, 95, 154-162.	2.5	4
1887	Benson group additivity values of phosphines and phosphine oxides: Fast and accurate computational thermochemistry of organophosphorus species. Journal of Computational Chemistry, 2019, 40, 572-580.	3.3	4
1888	Two symmetric arginine residues play distinct roles in <i>Thermus thermophilus</i> Argonaute DNA guide strand-mediated DNA target cleavage. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 845-853.	7.1	15
1889	Benchmark study of popular density functionals for calculating binding energies of three-center two-electron bonds. Journal of Computational Chemistry, 2019, 40, 657-670.	3.3	11
1890	Theoretical kinetic study of the reaction between dimethyl disulfide and OH radicals. Journal of Sulfur Chemistry, 2019, 40, 185-194.	2.0	2
1891	Hydrogen-Bond-Dependent Conformational Switching: A Computational Challenge from Experimental Thermochemistry. Journal of Organic Chemistry, 2019, 84, 613-621.	3.2	5
1892	DFT Research on Benzothiophene Pyrolysis Reaction Mechanism. Journal of Physical Chemistry A, 2019, 123, 796-810.	2.5	20
1893	Understanding the kinetics and molecular mechanism of unimolecular gas phase thermal decomposition of the β -ketoester methyl benzoylformate using RRKM and BET theories. Journal of Molecular Graphics and Modelling, 2019, 87, 22-29.	2.4	7
1894	A theoretical study of the tautomerism kinetics of 4-amino-6-methyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2 <i>H</i>)-one in the gas phase: NBO population and NICS analysis. Journal of Sulfur Chemistry, 2019, 40, 166-184.	2.0	3
1895	Quantum chemical and master equation study of $\text{OH} + \text{CH}_3\text{O} \rightarrow \text{H}_2\text{O} + \text{CHO}$ reaction rates in supercritical CO_2 environment. International Journal of Chemical Kinetics, 2019, 51, 42-48.	1.6	12
1896	CO_2/O_2 Exchange in Magnesium "Water Clusters $\text{Mg}^+(\text{H}_2\text{O})_n$ ". Journal of Physical Chemistry A, 2019, 123, 73-81.	2.5	11
1897	Boosting Quantum Machine Learning Models with a Multilevel Combination Technique: Pople Diagrams Revisited. Journal of Chemical Theory and Computation, 2019, 15, 1546-1559.	5.3	70
1898	Theoretical Study of Gas-Phase Unimolecular Decomposition of Simulants of the Nerve Agent VX. Journal of Physical Chemistry A, 2019, 123, 59-72.	2.5	10

#	ARTICLE	IF	CITATIONS
1899	Monosaccharide Isomer Interconversions Become Significant at High Temperatures. Journal of Physical Chemistry A, 2019, 123, 120-131.	2.5	6
1900	Theoretical study of the effect of hydrogen radicals on the formation of HCN from pyrrole pyrolysis. Journal of the Energy Institute, 2019, 92, 1468-1475.	5.3	19
1901	Exploring the interactional details between aldose reductase (AKR1B1) and 3-Mercapto-5H-1,2,4-triazino[5,6-b]indole-5-acetic acid through molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1724-1735.	3.5	17
1902	Mechanism study on the effect of alkali metal ions on the formation of HCN as NO _x precursor during coal pyrolysis. Journal of the Energy Institute, 2019, 92, 604-612.	5.3	37
1903	A thermochemical study on the primary oxidation of sulfur. Combustion Science and Technology, 2019, 191, 163-177.	2.3	7
1904	N,N-dimethylformamide (DMF), and N,N-dimethylacetamide (DMA) reactions with NO ₃ , OH and Cl: A theoretical study of the kinetics and mechanisms. Arabian Journal of Chemistry, 2019, 12, 4957-4970.	4.9	7
1905	A theoretical study on the kinetics of multichannel Multiwell reaction of H ₂ S(1A ₁) with HO ₂ (2A ₁). Molecular Physics, 2020, 118, e1583387.	1.7	0
1906	Charge oscillation dynamics in various imidazolium based ion pairs and their time scale. Chemical Physics, 2020, 529, 110572.	1.9	1
1907	First time investigation of the substitution effect at anion part of the ILs on their physicochemical properties using [DMT][4-XPhSO ₃] (X=NH ₂ , OH, H, F, Br, CHO, CF ₃ , CN and NO ₂) as a model ILs: A systematic DFT study. Journal of Molecular Structure, 2020, 1201, 127171.	3.6	17
1908	A never-ending story in the sky: The secrets of chemical evolution. Physics of Life Reviews, 2020, 32, 59-94.	2.8	28
1909	Formation mechanism of HCN and NH ₃ during indole pyrolysis: A theoretical DFT study. Journal of the Energy Institute, 2020, 93, 649-657.	5.3	60
1910	New insight on the combined effects of hydrothermal treatment and FeSO ₄ /Ca(ClO) ₂ oxidation for sludge dewaterability improvement: From experimental to theoretical investigation. Fuel Processing Technology, 2020, 197, 106196.	7.2	22
1911	Simulation, synthesis, characterisation and dyeing properties of a fluorescent hemicyanine dye. Coloration Technology, 2020, 136, 23-33.	1.5	2
1912	Mono-silicon isoelectronic replacement in C ₄ : van't Hoff/le bel carbon or not?. Journal of Computational Chemistry, 2020, 41, 119-128.	3.3	2
1913	Base-Promoted Formation of an Annelated Pyrrolo[1,4-c]oxazine Ensemble from 1 <i>H</i> -pyrrol-2-ylmethanol and Propargyl Chloride: A Theoretical and Experimental Study. ChemPlusChem, 2020, 85, 88-100.	2.8	4
1914	First principle studies on the atmospheric oxidation of HFC-C1436 initiated by the OH radical. New Journal of Chemistry, 2020, 44, 2070-2082.	2.8	8
1915	Calculations on the unimolecular decomposition of the nerve agent VX. Physical Chemistry Chemical Physics, 2020, 22, 564-574.	2.8	3
1916	Phenolic Hydrogen Transfer by Molecular Oxygen and Hydroperoxyl Radicals. Insights into the Mechanism of the Anthraquinone Process. Journal of Organic Chemistry, 2020, 85, 2560-2574.	3.2	20

#	ARTICLE	IF	CITATIONS
1917	Isomer-sensitive characterization of low temperature oxidation reaction products by coupling a jet-stirred reactor to an electron/ion coincidence spectrometer: case of <i>n</i> -pentane. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1222-1241.	2.8	28
1918	Exploring free energy profile of petroleum thermal cracking mechanisms. <i>Journal of Molecular Modeling</i> , 2020, 26, 15.	1.8	5
1919	Benchmark study of DFT and composite methods for bond dissociation energies in argon compounds. <i>Chemical Physics</i> , 2020, 531, 110676.	1.9	8
1920	Atmospheric oxidation mechanism and kinetics of isoprene initiated by chlorine radicals: A computational study. <i>Science of the Total Environment</i> , 2020, 712, 136330.	8.0	24
1921	Domain-based local pair natural orbital methods within the correlation consistent composite approach. <i>Journal of Computational Chemistry</i> , 2020, 41, 800-813.	3.3	14
1922	How Chemical Environment Activates Anthralin and Molecular Oxygen for Direct Reaction. <i>Journal of Organic Chemistry</i> , 2020, 85, 1315-1321.	3.2	2
1923	Thermostimulated luminescence of poly(diphenylenephthalide) films. Kinetics and mechanistic steps of irradiative processes. <i>Journal of Luminescence</i> , 2020, 218, 116869.	3.1	1
1924	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.	2.6	8
1925	Interfacial Water Mediates Oligomerization Pathways of Monoterpene Carbocations. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 67-74.	4.6	14
1926	Ab-initio studies of thermal unimolecular decomposition of furan: A complementary deterministic and stochastic master equation model. <i>Fuel</i> , 2020, 264, 116492.	6.4	14
1927	Kinetics and Thermodynamics of Reactions Involving Criegee Intermediates: An Assessment of Density Functional Theory and Ab Initio Methods Through Comparison with CCSDT(Q)/CBS Data. <i>Journal of Computational Chemistry</i> , 2020, 41, 328-339.	3.3	13
1928	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.	2.1	3
1929	Singlet-diradical character in large PAHs triggers spontaneous-ignition of coal. <i>Combustion and Flame</i> , 2020, 212, 279-281.	5.2	10
1930	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.	1.4	0
1931	Chemical kinetics study of 1,3-butadiene + O ₂ ; implications for combustion modeling and simulation. <i>Combustion and Flame</i> , 2020, 221, 241-255.	5.2	10
1932	Hydrogen migration as a potential driving force in the thermal decomposition of dimethoxymethane: New insights from pyrolysis imaging photoelectron photoion coincidence spectroscopy and computations. <i>Combustion and Flame</i> , 2020, 222, 123-132.	5.2	24
1933	Cope rearrangements in shapeshifting molecules re-examined by means of high-level CCSDT(Q) composite ab initio methods. <i>Chemical Physics Letters</i> , 2020, 759, 138018.	2.6	7
1934	Theoretical investigation of protonated thiophene and two of its nitrile substituted derivatives (2-cyanothiophene and 3-cyanothiophene). <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 24735-24743.	2.8	1

#	ARTICLE	IF	CITATIONS
1935	UV-induced radical formation and isomerization of 4-methoxyindole and 5-methoxyindole. Physical Chemistry Chemical Physics, 2020, 22, 22943-22955.	2.8	5
1936	Prebiotic Cytosine Synthesis from Urea in Interstellar Space: A Computational Mechanistic Study. Astrophysical Journal, 2020, 898, 13.	4.5	8
1937	Multichannel dynamics in the OH+ n-butane reaction revealed by crossed-beam slice imaging and quasiclassical trajectory calculations. Journal of Chemical Physics, 2020, 153, 014302.	3.0	2
1938	The role of potential energy surface in quantum mechanical tunneling: A computational perspective. Computational and Theoretical Chemistry, 2020, 1187, 112920.	2.5	1
1939	Detailed experimental and kinetic modeling study of 3-ethylarene pyrolysis. International Journal of Chemical Kinetics, 2020, 52, 785-795.	1.6	4
1940	Solid-phase chemiluminescent reaction of Eu ₂ (SO ₄) ₃ with XeF ₂ as a possible source of the Eu(IV) highest oxidation state. Journal of Solid State Chemistry, 2020, 290, 121554.	2.9	2
1941	An experimental and kinetic modeling study of phenylacetylene decomposition and the reactions with acetylene/ethylene under shock tube pyrolysis conditions. Combustion and Flame, 2020, 220, 257-271.	5.2	23
1942	Computational Study on Metal-Ion-Decorated Prismane Molecules for Selective Adsorption of CO ₂ from Flue Gas Mixtures. ACS Omega, 2020, 5, 31146-31155.	3.5	4
1943	Globally stabilized bent carbon-carbon triple bond by hydrogen-free inorganic-metallic scaffolding Al ₄ F ₆ . RSC Advances, 2020, 10, 25275-25280.	3.6	0
1944	Kinetic study of the CN radical reaction with 2-methylfuran. International Journal of Chemical Kinetics, 2020, 52, 838-851.	1.6	1
1945	Kinetics and Mechanism of the NH (X ³) + SO (X ³) Reaction: A Theoretical Approach. Journal of Physical Chemistry A, 2020, 124, 6585-6600.	2.5	3
1946	Potent Ferroptosis Inhibitors Can Catalyze the Cross-Dismutation of Phospholipid-Derived Peroxyl Radicals and Hydroperoxyl Radicals. Journal of the American Chemical Society, 2020, 142, 14331-14342.	13.7	30
1947	Catalysis on Pristine 2D Materials via Dispersion and Electrostatic Interactions. Journal of Physical Chemistry A, 2020, 124, 6977-6985.	2.5	17
1948	The Electrolysis of Ammonium Dinitramide in Dimethyl Sulfoxide. Propellants, Explosives, Pyrotechnics, 2020, 45, 1614-1620.	1.6	3
1949	A computational study on the kinetics of pyrolysis of isopropyl propionate as a biodiesel model: DFT and ab initio investigation. Fuel, 2020, 281, 118798.	6.4	18
1950	Kinetic Investigation of the Pyrolysis of Isobutyric Anhydride and Isobutyric Acid. Industrial & Engineering Chemistry Research, 2020, 59, 14747-14757.	3.7	3
1951	Photophysical, kinetic and thermodynamic study of one-component Type II thioxanthone acetic acid photoinitiators. European Polymer Journal, 2020, 136, 109909.	5.4	19
1952	Detailed kinetics of hydrogen abstraction from trans-decalin by OH radicals: the role of hindered internal rotation treatment. Physical Chemistry Chemical Physics, 2020, 22, 25740-25746.	2.8	12

#	ARTICLE	IF	CITATIONS
1953	Kinetic Study of the Reactions $\text{PO} + \text{O}_{2\text{}}$ and $\text{PO}_{2\text{}} + \text{O}_{3\text{}}$ and Spectroscopy of the PO Radical. Journal of Physical Chemistry A, 2020, 124, 7911-7926.	2.5	10
1954	Soot formation of n-decane pyrolysis: A mechanistic view from ReaxFF molecular dynamics simulation. Chemical Physics Letters, 2020, 760, 137983.	2.6	21
1955	Unraveling the kinetics and molecular mechanism of gas phase pyrolysis of cubane to [8]annulene. RSC Advances, 2020, 10, 32730-32739.	3.6	2
1956	Gas-phase reaction mechanism in chemical dry etching using $\text{NF}_{3\text{}}$ and remotely discharged $\text{NH}_{3\text{}}/\text{N}_{2\text{}}$ mixture. RSC Advances, 2020, 10, 30806-30814.	3.6	1
1957	Pressure-dependent kinetics of peroxy radicals formed in isobutanol combustion. Physical Chemistry Chemical Physics, 2020, 22, 19802-19815.	2.8	4
1958	A group additivity methodology for predicting the thermochemistry of oxygen-containing organosilanes. International Journal of Chemical Kinetics, 2020, 52, 918-932.	1.6	7
1959	Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Core Valence Correlation, and F12 Alternatives. Journal of Chemical Theory and Computation, 2020, 16, 7507-7524.	5.3	19
1960	Solvent-free Synthesis and Properties of Functionalized Hydrazines and Bishydrazines as Energetic Ingredients for Propulsion Applications. Chemistry - an Asian Journal, 2020, 15, 4347-4357.	3.3	0
1961	Cis-trans isomerization is not rate determining for b2 ion structures: A guided ion beam and computational study of the decomposition of $\text{H}^+(\text{GlyProAla})$. International Journal of Mass Spectrometry, 2020, 458, 116434.	1.5	4
1962	Mechanism and Reaction Energy Landscape for Apiose Cross-Linking by Boric Acid in Rhamnogalacturonan II. Journal of Physical Chemistry B, 2020, 124, 10117-10125.	2.6	5
1963	Theoretical calculation of low-temperature oxidation of heptyl radicals and O_2 . Combustion and Flame, 2020, 217, 274-284.	5.2	14
1964	A Procedure for Computing Hydrocarbon Strain Energies Using Computational Group Equivalents, with Application to 66 Molecules. Chemistry, 2020, 2, 347-360.	2.2	19
1965	Quantum chemical study of the reaction of trichloroethylene with $\text{O}(^3\text{P})$. International Journal of Chemical Kinetics, 2020, 52, 589-598.	1.6	2
1966	Radical Substitution Provides a Unique Route to Disulfides. Journal of the American Chemical Society, 2020, 142, 10284-10290.	13.7	60
1967	The Underlying Chemistry to the Formation of $\text{PO}_{2\text{}}$ Radicals from Organophosphorus Compounds: A Missing Puzzle Piece in Flame Chemistry. Chemistry - A European Journal, 2020, 26, 10795-10800.	3.3	17
1968	OH-Initiated Reactions of <i>p</i> -Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part II. Kinetic Analysis. Journal of Physical Chemistry A, 2020, 124, 4875-4904.	2.5	5
1969	Quinone methide dimers lacking labile hydrogen atoms are surprisingly excellent radical-trapping antioxidants. Chemical Science, 2020, 11, 5676-5689.	7.4	11
1970	A computational study on phenibut lactamization mechanism and the pH effects on the process. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0

#	ARTICLE	IF	CITATIONS
1971	Anti- π -elektrostatische-Halogenbrücken. Angewandte Chemie, 2020, 132, 11244-11251.	2.0	10
1972	Formation of Low-Volatile Products and Unexpected High Formaldehyde Yield from the Atmospheric Oxidation of Methylsiloxanes. Environmental Science & Technology, 2020, 54, 7136-7145.	10.0	27
1973	Facile Preparation of 3-Acetamido-5-acetylfuran from N -Acetylglucosamine by using Commercially Available Aluminum Salts. ChemSusChem, 2020, 13, 3594-3598.	6.8	37
1974	Experimental and kinetic modeling study of the pyrolysis and oxidation of diethylamine. Fuel, 2020, 275, 117744.	6.4	11
1975	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. Journal of Chemical Theory and Computation, 2020, 16, 4238-4255.	5.3	30
1976	Modeling temperature dependent and absolute carbamate stability constants of amines for CO ₂ capture. International Journal of Greenhouse Gas Control, 2020, 98, 103061.	4.6	10
1977	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
1978	Computational investigations on the thermochemistry and kinetics for the autoignition of 2-pentanone. Combustion and Flame, 2020, 219, 147-160.	5.2	4
1979	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The "Hidden" Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
1980	Modeling the Kinetics of Luminescence in the 1,4-Dimethylnaphthalene Endoperoxide/Eu(fod) ₃ System. Bulletin of the Russian Academy of Sciences: Physics, 2020, 84, 572-575.	0.6	0
1981	Investigation of the neutral and cation chloroacetone molecular structures and spectroscopic properties by ab initio and density functional theory methods. Journal of Molecular Structure, 2020, 1220, 128703.	3.6	4
1982	Impact of Quantum Chemistry Parameter Choices and Cluster Distribution Model Settings on Modeled Atmospheric Particle Formation Rates. Journal of Physical Chemistry A, 2020, 124, 5931-5943.	2.5	34
1983	W2SDD theory for computational thermochemistry: study of the addition of hydrogen halide to propene. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	8
1984	The investigation on ibuprofen methyl ester isomerization as a fundamental stage in the preparation of antipyretic medicine (R)-ibuprofen: a computational insight. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
1985	Structure dependency of the reactivity of aromatic hydrocarbons involving the formation of oxygenated polycyclic aromatic hydrocarbons (OPAHs). Chemical Physics Letters, 2020, 754, 137652.	2.6	4
1986	Temperature-dependent rate coefficients for the gas-phase OH + furan-2,5-dione (C ₄ H ₂ O ₃ , maleic anhydride) reaction. International Journal of Chemical Kinetics, 2020, 52, 623-631.	1.6	6
1987	A twist on the reaction of the CN radical with methylamine in the interstellar medium: new hints from a state-of-the-art quantum-chemical study. Monthly Notices of the Royal Astronomical Society, 2020, 496, 4298-4310.	4.4	24
1988	OH-Initiated Reactions of <i>para</i> -Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part III. Kinetics of H-Abstraction by H, OH, and CH ₃ Radicals. Journal of Physical Chemistry A, 2020, 124, 4905-4915.	2.5	3

#	ARTICLE	IF	CITATIONS
1989	Dynamics of imidogen reaction with hydroxyl radical: a theoretical approach. Journal of the Iranian Chemical Society, 2020, 17, 1987-2000.	2.2	2
1990	Theoretical studies on the kinetics of the hydrogen-abstraction reactions from 1,3,5-trioxane and 1,4-dioxane by OH radicals. Progress in Reaction Kinetics and Mechanism, 2020, 45, 146867831989925.	2.1	3
1991	An investigation of pregabalin lactamization process and effect of various pH on reaction: A computational insight. Journal of Molecular Structure, 2020, 1210, 128048.	3.6	2
1992	Interaction of triols with formaldehyde and acetone: Experimental and theoretical study. Journal of the Chinese Chemical Society, 2020, 67, 1144-1151.	1.4	3
1993	The challenging playground of astrochemistry: an integrated rotational spectroscopy “ quantum chemistry strategy. Physical Chemistry Chemical Physics, 2020, 22, 6507-6523.	2.8	36
1994	Liquid-phase decomposition mechanism for bis(triaminoguanidinium) azotetrazolate (TAGzT). Physical Chemistry Chemical Physics, 2020, 22, 7314-7328.	2.8	6
1995	Criegee intermediate decomposition pathways for the formation of o-toluic acid and 2-methylphenylformate. Chemical Physics Letters, 2020, 748, 137399.	2.6	0
1996	Isomer-Selective Threshold Photoelectron Spectra of Phenylnitrene and Its Thermal Rearrangement Products. Journal of Physical Chemistry A, 2020, 124, 3836-3843.	2.5	5
1997	Multi-coefficients correlation methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1474.	14.6	4
1998	Binding energies and isomer distribution of neutral acetonitrile clusters. International Journal of Quantum Chemistry, 2020, 120, e26221.	2.0	31
1999	“Anti“Electrostatic•Halogen Bonding. Angewandte Chemie - International Edition, 2020, 59, 11150-11157.	13.8	59
2000	Electron ionization and photoionization of cyclopropylamine. International Journal of Mass Spectrometry, 2020, 455, 116390.	1.5	0
2001	State-of-the-Art Quantum Chemistry Meets Variable Reaction Coordinate Transition State Theory to Solve the Puzzling Case of the H ₂ S + Cl System. Journal of Chemical Theory and Computation, 2020, 16, 5090-5104.	5.3	27
2002	Global uncertainty analysis for the RRKM/master equation modeling of a typical multi-well and multi-channel reaction system. Combustion and Flame, 2020, 216, 62-71.	5.2	13
2003	Direct oxidation of methane to methanol on Co embedded N-doped graphene: Comparing the role of N ₂ O and O ₂ as oxidants. Applied Catalysis A: General, 2020, 602, 117716.	4.3	11
2004	Theoretical kinetics of the C ₂ H ₄ +NH ₂ reaction. Combustion and Flame, 2020, 215, 193-202.	5.2	5
2005	What a little branching can do “ Dissociative photoionization of two butanol isomers. International Journal of Mass Spectrometry, 2020, 453, 116341.	1.5	1
2006	A piece of the C ₆ H ₉ ⁺ potential energy surface: Rearrangement of spiropentylmethyl cation and an elegant nonclassical spiro[2.3]hex-5-yl cation. Journal of Physical Organic Chemistry, 2020, 33, e4064.	1.9	3

#	ARTICLE	IF	CITATIONS
2007	Exploring the Chemistry of Low-Temperature Ignition by Pressure-Accelerated Dynamics. <i>ChemSystemsChem</i> , 2020, 2, e1900043.	2.6	9
2008	Probing the bent bonds in cyclopropane systems for gas storage and separation process: A computational study. <i>Journal of Computational Chemistry</i> , 2020, 41, 1271-1284.	3.3	4
2009	Thermochemistry of Fluorinated Dimethyl and Ethyl Methyl Ethers and Corresponding Radical Species. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 1594-1616.	1.9	2
2010	Prediction of the tautomer stability and acidity of phenacylpyridines in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	1
2011	Computational Study of the Dissociation Reactions of Secondary Ozonide. <i>Atmosphere</i> , 2020, 11, 100.	2.3	4
2012	Evidence and evolution of Criegee intermediates, hydroperoxides and secondary organic aerosols formed via ozonolysis of α -pinene. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6528-6537.	2.8	14
2013	Synchrotron Photoionization Study of the Diisopropyl Ether Oxidation. <i>ChemPhysChem</i> , 2020, 21, 927-937.	2.1	4
2014	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 403-419.	2.7	9
2015	Extensive Quantum Chemistry Study of Neutral and Charged C_4N Chains: An Attempt To Aid Astronomical Observations. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 434-448.	2.7	8
2016	Base-Promoted C-C Bond Activation Enables Radical Allylation with Homoallylic Alcohols. <i>Journal of the American Chemical Society</i> , 2020, 142, 2609-2616.	13.7	45
2017	Experimental and kinetic modeling investigation on ethylcyclohexane low-temperature oxidation in a jet-stirred reactor. <i>Combustion and Flame</i> , 2020, 214, 211-223.	5.2	31
2018	The reaction of OH radical with the Criegee intermediate propanone oxide: Theoretical investigations. <i>Computational and Theoretical Chemistry</i> , 2020, 1175, 112726.	2.5	2
2019	Quantum-chemical models of $KOH(KOBu^t)/DMSO$ superbasic systems and mechanisms of base-promoted acetylene reactions. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26158.	2.0	27
2020	How does cross-conjugation influence thiol additions to enones? A computational study of thiol trapping by the naturally occurring divinyl ketones zerumbone and β -santonin. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 1426-1435.	2.8	7
2021	Dissociative photoionization of 1,3-dioxolane: We need six channels to fit the elephant. <i>Journal of Mass Spectrometry</i> , 2020, 55, e4522.	1.6	6
2022	Hydrogen Atom Abstraction from Polyolefins: Experimental and Computational Studies of Model Systems. <i>Macromolecules</i> , 2020, 53, 2793-2800.	4.8	6
2023	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. <i>New Journal of Chemistry</i> , 2020, 44, 6543-6552.	2.8	8
2024	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.	1.7	3

#	ARTICLE	IF	CITATIONS
2025	Assessment of property estimation methods for the thermodynamics of carbon dioxide-based products. <i>Energy Conversion and Management</i> , 2020, 211, 112756.	9.2	9
2026	Reaction mechanisms of a cyclic ether intermediate: Ethyloxirane. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 43-59.	1.6	20
2027	Mechanism and kinetics of the reaction $\text{CH}_3 + \text{CH}_3\text{CHO}$: Ab initio semiclassical transition state theory study. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26468.	2.0	2
2028	A comprehensive model for the role of water and silanols in the amine catalyzed aldol reaction. <i>Chemical Engineering Journal</i> , 2021, 404, 127070.	12.7	7
2029	Combustion of ethylamine, dimethylamine and diethylamine: Theoretical and kinetic modeling study. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 585-592.	3.9	12
2030	Probing the fuel-specific intermediates in the low-temperature oxidation of 1-heptene and modeling interpretation. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 385-394.	3.9	8
2031	Probing the antiknock effect of anisole through an ignition, speciation and modeling study of its blends with isooctane. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 739-748.	3.9	9
2032	Thermal decomposition of furans with oxygenated substituents: A combined experimental and quantum chemical study. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 699-707.	3.9	9
2033	Detailed kinetic mechanism of thermal decomposition of furyl radicals: Theoretical insights. <i>Fuel</i> , 2021, 288, 119699.	6.4	4
2034	Reaction modeling study on the combustion of aluminum in gas phase: The $\text{Al} + \text{O}_2$ and related reactions. <i>Combustion and Flame</i> , 2021, 225, 535-550.	5.2	20
2035	Structures, energetics, and kinetics of H-atom abstraction from methyl propionate by molecular oxygen: Ab initio and DFT investigations. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113119.	2.5	15
2036	Theoretical study of the hydrogen abstraction reactions from substituted phenolic species. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113120.	2.5	6
2037	Structure of premixed flames of propylene oxide: Molecular beam mass spectrometric study and numerical simulation. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 2467-2475.	3.9	7
2038	Investigation of the molecular structure and VUV-induced ion dissociation dynamics of 2-azetidinone ($\text{C}_3\text{H}_5\text{NO}$). <i>Rapid Communications in Mass Spectrometry</i> , 2021, 35, e8988.	1.5	1
2039	Threshold photoionization shows no sign of nitril hydride in methane oxidation with nitric oxide. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1265-1272.	2.8	8
2040	"Catalysis in Carbon Flatland" Flipping [8]Annulene on Graphene. <i>Chemistry - A European Journal</i> , 2021, 27, 3420-3426.	3.3	12
2041	CBS-QB3 study on the pyrolysis mechanism of 3-ethynylbenzo[b]thiophene. <i>Chemical Physics Letters</i> , 2021, 762, 138120.	2.6	5
2042	Can density functional theory "Cope" with highly fluxional shapeshifting molecules?. <i>Chemical Physics</i> , 2021, 540, 111013.	1.9	15

#	ARTICLE	IF	CITATIONS
2043	Bond additivity corrections for CBS-QB3 calculated standard enthalpies of formation of H, C, O, N, and S containing species. International Journal of Chemical Kinetics, 2021, 53, 345-355.	1.6	5
2044	Five <i>vs.</i> six membered-ring PAH products from reaction of <i>o</i> -methylphenyl radical and two C ₃ H ₄ isomers. Physical Chemistry Chemical Physics, 2021, 23, 14913-14924.	2.8	0
2045	Insights into the kinetics and molecular mechanism of the Newman-Kwart rearrangement. New Journal of Chemistry, 2021, 45, 16978-16988.	2.8	2
2046	Improving the Stability of Trinitramide by Chemical Substitution: N(NF ₂) ₃ has Higher Stability and Excellent Propulsion Performance. Propellants, Explosives, Pyrotechnics, 2021, 46, 245-252.	1.6	4
2047	How stable can the pentanitrogen cation be in kinetics?. Chemical Communications, 2021, 57, 4432-4435.	4.1	2
2048	<i>Ab initio</i> rate coefficients for reactions of 2,5-dimethylhexyl isomers with O ₂ : temperature- and pressure-dependent branching ratios. Physical Chemistry Chemical Physics, 2021, 23, 6225-6240.	2.8	3
2049	Isomerization and Fragmentation Reactions on the [C ₂ SH ₄] Potential Energy Surface: The Metastable Thione <i>S</i> -Methylide Isomer. Journal of Organic Chemistry, 2021, 86, 2941-2956.	3.2	11
2050	Benchmark calculations for bond dissociation energies and enthalpy of formation of chlorinated and brominated polycyclic aromatic hydrocarbons. RSC Advances, 2021, 11, 29690-29701.	3.6	5
2051	Elementary gas-phase reactions of radical species during chemical vapor deposition of silicon carbide using CH ₃ SiCl ₃ . International Journal of Chemical Kinetics, 2021, 53, 638-645.	1.6	5
2052	Thermal and evolved gas analyses on Michael addition oligomers of acrylic acid. Journal of Thermal Analysis and Calorimetry, 0, , 1.	3.6	3
2053	Temperature-dependence of radical-trapping activity of phenoxazine, phenothiazine and their aza-analogues clarifies the way forward for new antioxidant design. Chemical Science, 2021, 12, 11065-11079.	7.4	7
2054	Theoretical and experimental study on the O(3P) + 2,5-dimethylfuran reaction in the gas phase. Physical Chemistry Chemical Physics, 2021, 23, 19424-19434.	2.8	0
2055	Using computational chemistry to design pump-probe schemes for measuring nitrobenzene radical cation dynamics. Physical Chemistry Chemical Physics, 2021, 23, 13338-13348.	2.8	6
2056	Mechanism insight into the formation of H ₂ S from thiophene pyrolysis: A theoretical study. Frontiers of Environmental Science and Engineering, 2021, 15, 1.	6.0	12
2057	Prediction Models on <i>pKa</i> and Base-Catalyzed Hydrolysis Kinetics of Parabens: Experimental and Quantum Chemical Studies. Environmental Science & Technology, 2021, 55, 6022-6031.	10.0	31
2058	A Theoretical Study on the Degenerate Cope Rearrangement of Hypostrophene Using the RRKM Theory and Topological Approaches. ChemistrySelect, 2021, 6, 1607-1615.	1.5	1
2059	Prototypical π - π dimers re-examined by means of high-level CCSDT(Q) composite <i>ab initio</i> methods. Journal of Chemical Physics, 2021, 154, 124117.	3.0	9
2060	Choosing a solvation model for simulating reactions in KOH(KOBu ^t)/DMSO superbasic media. Journal of Physics: Conference Series, 2021, 1847, 012054.	0.4	4

#	ARTICLE	IF	CITATIONS
2061	VUV photoprocessing of oxygen-containing polycyclic aromatic hydrocarbons: Threshold photoelectron spectra. <i>Journal of Molecular Spectroscopy</i> , 2021, 377, 111446.	1.2	6
2062	Atmospheric Chemistry of Allylic Radicals from Isoprene: A Successive Cyclization-Driven Autoxidation Mechanism. <i>Environmental Science & Technology</i> , 2021, 55, 4399-4409.	10.0	20
2063	Systematic Convergence of the Numerical Taylor Series to the Best Standard and Its Potential Implication for the Development of Composite Methods. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2231-2243.	5.3	1
2064	Net Electronic Charge as an Effective Electronic Descriptor for Oxygen Release and Transport Properties of SrFeO ₃ -Based Oxygen Sorbents. <i>Chemistry of Materials</i> , 2021, 33, 2446-2456.	6.7	22
2065	Theoretical modeling study of the reaction H + CF ₄ → HF + CF ₃ . <i>International Journal of Chemical Kinetics</i> , 2021, 53, 939-945.	1.6	0
2066	Pyrolysis and Combustion Chemistry of Pyrrole, a Reference Component for Bio-oil Surrogates: Jet-Stirred Reactor Experiments and Kinetic Modeling. <i>Energy & Fuels</i> , 2021, 35, 7265-7284.	5.1	26
2067	Sequential C–F bond functionalizations of trifluoroacetamides and acetates via spin-center shifts. <i>Science</i> , 2021, 371, 1232-1240.	12.6	166
2068	Temperature-Dependent Effects of Alkyl Substitution on Diarylamine Antioxidant Reactivity. <i>Journal of Organic Chemistry</i> , 2021, 86, 6538-6550.	3.2	9
2069	Unimolecular Pyrolysis Mechanism of Thiophene and Furan: An Ab Initio Comparative Study. <i>Energy & Fuels</i> , 2021, 35, 7819-7832.	5.1	5
2070	Thermo-kinetic theoretical studies on pyrolysis of dimethoxymethane fuel additive. <i>Fuel</i> , 2021, 290, 119970.	6.4	22
2071	Focal Point Evaluation of Energies for Tautomers and Isomers for 3-hydroxy-2-butenamide: Evaluation of Competing Internal Hydrogen Bonds of Types -OH⋯O=, -OH⋯N, -NH⋯O=, and CH⋯X (X=O and N). <i>Molecules</i> , 2021, 26, 2623.	3.8	3
2072	Thermal isomerism and pyrolysis mechanism of α -pinene and β -pinene in a solvent-free solution and ethanol based on density functional theory. <i>Chemical Physics</i> , 2021, 544, 111103.	1.9	0
2073	CaI ₄ MgO: Global Minima with a Planar Tetracoordinate Carbon Atom. <i>Atoms</i> , 2021, 9, 24.	1.6	18
2074	Theoretical investigation of solvent effect on the keto–enol tautomerization of pentane-2,4-dione and a comparison between experimental data and theoretical calculations. <i>Canadian Journal of Chemistry</i> , 2021, 99, 411-424.	1.1	5
2075	Benchmark calculations of proton affinity and gas-phase basicity using multilevel (<sc>G4</sc> and) Tj ETQq0 0 0 rgBT /Overlock 1 benzaldehyde compounds. <i>Journal of Computational Chemistry</i> , 2021, 42, 1106-1117.	3.3	8
2077	Six Low-Lying Isomers of C ₁₁ H ₈ Are Unidentified in the Laboratory—A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4352-4364.	2.5	8
2078	A reduced mechanism with optimal rate-kinetics parameters for liquid-phase decomposition of bis(triaminoguanidinium) 5,5'-azotetrazolate (TAGzT): Quantum chemical calculations, thermolysis experiments and kinetic modeling. <i>Thermochimica Acta</i> , 2021, 699, 178895.	2.7	1
2079	Electronic structure and reactivity of tirapazamine as a radiosensitizer. <i>Journal of Molecular Modeling</i> , 2021, 27, 177.	1.8	2

#	ARTICLE	IF	CITATIONS
2080	Exploring reactions of amines-model compounds with NH ₂ : In relevance to nitrogen conversion chemistry in biomass. <i>Fuel</i> , 2021, 291, 120076.	6.4	12
2081	Computational molecular spectroscopy. <i>Nature Reviews Methods Primers</i> , 2021, 1, .	21.2	73
2082	SVECV â€”12: Benchmark of a composite scheme for accurate and cost effective evaluation of reaction barriers. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26745.	2.0	18
2083	NITROGEN ASTRALENS: THEORETICAL INVESTIGATION OF THE STRUCTURE OF NOVEL HIGH-ENERGY NITROGEN ALLOTROPES. <i>Journal of Structural Chemistry</i> , 2021, 62, 661-670.	1.0	2
2084	Exploring the chemical kinetics on oxygen addition reactions of o-xylyl radical at the low temperature. <i>Combustion and Flame</i> , 2021, 227, 95-105.	5.2	5
2085	Molecular design of long intraâ€”annular nitrogen chains: 3Hâ€”tetrazolo[1,5â€”d]tetrazoleâ€”based highâ€”energyâ€”density materials. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26743.	2.0	3
2086	The Formation of C ₃ O ₃ H ₆ Structural Isomers in the Gas Phase through Barrierless Pathways: Formation and Spectroscopic Characterization of Methoxy Acetic Acid. <i>Astrophysical Journal</i> , 2021, 913, 21.	4.5	3
2087	The C5â€”substituent effects on the formic acidâ€”assisted tautomerization of protonated cytosine: A lower isomerization barrier and potential biological importance. <i>Journal of Physical Organic Chemistry</i> , 2021, 34, e4220.	1.9	0
2089	Fluorinated interphase enables reversible aqueous zinc battery chemistries. <i>Nature Nanotechnology</i> , 2021, 16, 902-910.	31.5	560
2090	Theoretical study of the kinetics of F-atom abstraction reactions from F ₂ , CF ₂ (OF) ₂ , CF ₃ OF and SF ₅ OF by CO. <i>Molecular Physics</i> , 0, , e1939899.	1.7	0
2091	Development of a Detailed Kinetic Model for the Oxidation of <i>n</i> -Butane in the Liquid Phase. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6955-6967.	2.6	8
2092	Can Cytosine, Uracil, and Thymine Be Formed from HC ₃ N and H ₂ NCO ⁺ in Interstellar Space?. <i>Astrophysical Journal</i> , 2021, 914, 136.	4.5	11
2093	A Spectroscopic Validation of the Improved Lennardâ€”Jones Model. <i>Molecules</i> , 2021, 26, 3906.	3.8	6
2095	Fate of Protonated Formates in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5096-5102.	2.5	4
2096	A Divergent Strategy for Siteâ€”Selective Radical Disulfuration of Carboxylic Acids with Trisulfideâ€”1,1â€”Dioxides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15598-15605.	13.8	38
2097	Learning Molecular Representations for Thermochemistry Prediction of Cyclic Hydrocarbons and Oxygenates. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5166-5179.	2.5	10
2098	Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. <i>Journal of Computational Chemistry</i> , 2021, 42, 1590-1601.	3.3	44
2099	A Divergent Strategy for Siteâ€”Selective Radical Disulfuration of Carboxylic Acids with Trisulfideâ€”1,1â€”Dioxides. <i>Angewandte Chemie</i> , 2021, 133, 15726-15733.	2.0	6

#	ARTICLE	IF	CITATIONS
2100	Kinetic Analysis of Unimolecular Reactions Following the Addition of the Hydroxyl Radical to 1,1,2-Trifluoroethene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5375-5384.	2.5	3
2101	Accurate binding energies of ammonia clusters and benchmarking of hybrid DFT functionals. <i>Computational and Theoretical Chemistry</i> , 2021, 1200, 113236.	2.5	10
2102	Updated yields of nitrogenated species in flames of ammonia/benzene via introducing an aniline sub-mechanism. <i>Combustion and Flame</i> , 2021, 228, 433-442.	5.2	7
2103	Primary Thermal Decomposition Pathways of Hydroxycinnamaldehydes. <i>Energy & Fuels</i> , 2021, 35, 12216-12226.	5.1	8
2104	First-principle kinetic studies of unimolecular pyrolysis of isopropyl esters as biodiesel surrogates. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	8
2105	Combustion chemistry of methoxymethanol. Part I: Chemical kinetics of hydrogen-abstraction reactions and the unimolecular reactions of the product [C ₂ H ₅ O ₂] radicals. <i>Combustion and Flame</i> , 2021, 229, 111396.	5.2	10
2106	Study of the Synchrotron Photoionization Oxidation of Alpha-Angelica Lactone (AAL) Initiated by O(3P) at 298, 550, and 700 K. <i>Molecules</i> , 2021, 26, 4070.	3.8	0
2107	Kinetic Modeling of API Oxidation: (1) The AIBN/H ₂ O/CH ₃ OH Radical "Soup" Molecular Pharmaceutics, 2021, 18, 3037-3049.	4.6	12
2108	VUV-Induced Photodissociation of the Chloroacetone Molecule Studied by Photoelectron-Photoion Coincidence Spectroscopy. <i>Journal of the American Society for Mass Spectrometry</i> , 2021, 32, 2186-2195.	2.8	1
2109	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4872-4890.	5.3	22
2110	HCl elimination in the photolysis of chlorobenzene at 266 nm: An FT-IR spectroscopy and quantum chemical study. <i>Chemical Physics Letters</i> , 2021, 774, 138601.	2.6	4
2111	A detailed mechanism for the initial hypergolic reaction in liquid hydrazine/nitrogen tetroxide mixtures based on quantum chemistry calculations. <i>Combustion and Flame</i> , 2021, 229, 111389.	5.2	5
2112	Methane Adsorption on Heteroatom-Modified Maquettes of Porous Carbon Surfaces. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6042-6058.	2.5	5
2113	Revisiting the conformational analysis of unsaturated organic compounds using the bent bond / antiperiplanar hypothesis. <i>Tetrahedron</i> , 2021, 92, 132249.	1.9	2
2114	Quantum-chemical study on the relative stability of sildenafil tautomers. <i>Structural Chemistry</i> , 2021, 32, 1733-1743.	2.0	2
2115	BEP-Like Correction of Nonequilibrium Thermodynamic Parameters of the Solvent-Assisted Reactions: The DFT and Ab Initio Study of Hydration, Peroxidation, and Enolization of Acetone and 1,1,1-Trifluoroacetone in Aqueous Solutions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7369-7381.	2.5	1
2116	Product Detection of the CH(X ²) Radical Reaction with Cyclopentadiene: A Novel Route to Benzene. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6927-6939.	2.5	6
2117	A comprehensive study on low-temperature oxidation chemistry of cyclohexane. I. Conformational analysis and theoretical study of first and second oxygen addition. <i>Combustion and Flame</i> , 2022, 235, 111658.	5.2	6

#	ARTICLE	IF	CITATIONS
2118	Mechanistic Investigations into the Catalytic Levulinic Acid Hydrogenation, Insight in H/D Exchange Pathways, and a Synthetic Route to d ₈ - ¹³ -Valerolactone. ACS Catalysis, 2021, 11, 10467-10477.	11.2	15
2119	A Fragmentation-Based Graph Embedding Framework for QM/ML. Journal of Physical Chemistry A, 2021, 125, 6872-6880.	2.5	9
2120	Mechanical insight into the formation of H ₂ S from thiophene pyrolysis: The influence of H ₂ O. Chemosphere, 2021, 279, 130628.	8.2	9
2121	Thermodynamic and Physical Property Estimation of Compounds Derived from the Fast Pyrolysis of Lignocellulosic Materials. Energy & Fuels, 2021, 35, 17114-17137.	5.1	15
2122	Unraveling the low-temperature oxidation mechanism between methyl crotonate radicals and O ₂ . Combustion and Flame, 2021, 231, 111473.	5.2	9
2123	Absolute Photoionization Cross Section of the Simplest Enol, Vinyl Alcohol. Journal of Physical Chemistry A, 2021, 125, 7920-7928.	2.5	8
2124	Initial Steps and Thermochemistry of Unimolecular Decomposition of Oxadiazole Energetic Materials: Quantum Chemistry Modeling. Journal of Physical Chemistry A, 2021, 125, 7929-7939.	2.5	2
2125	The Reaction of CO ₂ with a Borylnitrene: Formation of an β -Oxaziridinone. Angewandte Chemie - International Edition, 2021, 60, 23112-23116.	13.8	7
2126	Reactions of NO ₃ with aromatic aldehydes: gas-phase kinetics and insights into the mechanism of the reaction. Atmospheric Chemistry and Physics, 2021, 21, 13537-13551.	4.9	7
2127	Phosphorus Chemistry in the Earth's Upper Atmosphere. Journal of Geophysical Research: Space Physics, 2021, 126, e2021JA029881.	2.4	6
2128	Synthesis and Tetraphenylethylene-Based Aggregation-Induced Emission Probe for Rapid Detection of Nitroaromatic Compounds in Aqueous Media. ACS Omega, 2021, 6, 25447-25460.	3.5	42
2129	Kinetics of the Reactions of CH ₂ OO with Acetone, β -Diketones, and γ -Diketones. Journal of Physical Chemistry A, 2021, 125, 8557-8571.	2.5	8
2130	Influence of functional groups on low-temperature combustion chemistry of biofuels. Progress in Energy and Combustion Science, 2021, 86, 100925.	31.2	58
2131	Theoretical spectroscopic study of acetyl (CH ₃ CO), vinoxy (CH ₂ CHO), and 1-methylvinoxy (CH ₃ COCH ₂) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	1
2132	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO ₂ Elimination Reaction Class and γ -Scission Reaction Class. Journal of Physical Chemistry A, 2021, 125, 8942-8958.	2.5	9
2133	A theoretical study of γ -hydroxybutenyl with O ₂ on the HOC ₄ H ₆ OO \dot{A} potential energy surface. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
2134	Hidden Reactivity of Barbituric and Meldrum TM s Acids: Atom-Efficient Free Radical C=O Coupling with N-Hydroxy Compounds. Synthesis, 0, 54, .	2.3	6
2135	The Reaction of CO ₂ with a Borylnitrene: Formation of an β -Oxaziridinone. Angewandte Chemie, 2021, 133, 23296.	2.0	0

#	ARTICLE	IF	CITATIONS
2136	Reaction of the N Atom with Electronically Excited O ₂ Revisited: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 8294-8312.	2.5	2
2137	Interactions of Cellulose Model Compound D-Cellulobiose with Selected Metal Chlorides in Water: Identification of Chelating Oxygen Atoms. European Journal of Organic Chemistry, 2021, 2021, 4968-4973.	2.4	2
2138	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal-Alkyl Cyclohexane Combustion. 2. Cyclization Reaction Class. Journal of Physical Chemistry A, 2021, 125, 8959-8977.	2.5	8
2139	Shapeshifting radicals. Chemical Physics, 2022, 552, 111373.	1.9	1
2140	Chemical kinetics modeling for combustion of Al in CO ₂ . Combustion and Flame, 2021, 233, 111613.	5.2	3
2141	An experimental and modeling study of oxidation of real RP-3 aviation kerosene. Fuel, 2021, 305, 121476.	6.4	5
2142	Experimental and kinetic modeling investigation on 2,5-hexanedione oxidation in a jet-stirred reactor. Combustion and Flame, 2021, 234, 111648.	5.2	2
2143	A comprehensive theoretical analysis of Curtius rearrangement of syn-syn and syn-anti conformers of oxalyl diazide. Journal of Molecular Graphics and Modelling, 2021, 109, 108012.	2.4	1
2144	Kinetic fall-off behavior for the Cl + Furan-2,5-dione (C ₄ H ₂ O ₃), Tj ETQq0 0 0 rgBT /Overlock 10 T	2.8	1
2145	High energy density aqueous zinc-benzoquinone batteries enabled by carbon cloth with multiple anchoring effects. Journal of Materials Chemistry A, 2021, 9, 6131-6138.	10.3	22
2146	Arylpentazoles with surprisingly high kinetic stability. Chemical Communications, 2021, 57, 5310-5313.	4.1	7
2147	Basis Sets for Correlated Methods. Lecture Notes in Quantum Chemistry II, 2021, , 129-155.	0.3	0
2148	Understanding extreme fast charge limitations in carbonate mixtures. Journal of Materials Chemistry A, 2021, 9, 4858-4869.	10.3	21
2149	Mechanism and kinetics for the reaction of methyl peroxy radical with O ₂ . Physical Chemistry Chemical Physics, 2021, 23, 23508-23516.	2.8	0
2150	Theoretical study on adiabatic electron affinity of fatty acids. New Journal of Chemistry, 2021, 45, 16892-16905.	2.8	4
2152	Theoretical Thermochemistry of Radicals. , 2001, , 161-197.		1
2153	Density Functional Calculations. , 2016, , 483-563.		1
2154	Three-Body Dispersion Corrections to the Spherical Atom Model: The PFD-3B Density Functional. Journal of Physical Chemistry A, 2020, 124, 10296-10311.	2.5	4

#	ARTICLE	IF	CITATIONS
2155	On the Accuracy of the Direct Method to Calculate p_K^a from Electronic Structure Calculations. Journal of Physical Chemistry A, 2021, 125, 65-73.	2.5	39
2156	The simplest Diels-Alder reactions are not <i>endo</i> -selective. Chemical Science, 2020, 11, 11915-11926.	7.4	28
2157	Unexpected chemistry from the homogeneous thermal decomposition of acetylene: An ab initio study. Chinese Journal of Chemical Physics, 2018, 31, 761-766.	1.3	4
2159	Decomposition Pathways for Aqueous Hydroxylammonium Nitrate Solutions: a DFT Study. Central European Journal of Energetic Materials, 2017, 14, 888-916.	0.4	7
2164	PAH growth assisted by five-membered ring: pyrene formation from acenaphthylene. Combustion Theory and Modelling, 0, , 1-19.	1.9	2
2165	Antiaromaticity-Promoted Radical Stability in β -Methyl Heterocyclics. Journal of Organic Chemistry, 2021, 86, 15558-15567.	3.2	6
2166	$\text{Ga}(\text{CN})_2\text{SnO}_2$ electrocatalysts for active and selective ozone production. AIChE Journal, 2021, 67, e17486.	3.6	8
2167	High-level thermochemistry for the octasulfur ring: A converged coupled cluster perspective for a challenging second-row system. Chemical Physics Impact, 2021, 3, 100047.	3.5	4
2168	Computational Chemistry. , 2008, , 140-164.		0
2169	Chemical accuracy in ab initio thermochemistry and spectroscopy: current strategies and future challenges. , 2012, , 161-180.		0
2170	Density functional and chemical model study of the competition between methyl and hydrogen scission of propane and $\dot{\text{I}}^2$ -scission of the propyl radical. Highlights in Theoretical Chemistry, 2014, , 63-80.	0.0	0
2172	XYG3 Results for Some Selected Applications. Springer Briefs in Molecular Science, 2014, , 79-101.	0.1	0
2176	Calculation of Gas-Phase Gibbs free Energy Changes of Some Small Molecules with Monte Carlo, DFT (MPW1PW91), Composite (CBS-QB3), Gaussian-n (G1, G2) and Gaussian Modified (G2MP2) Methods. Oriental Journal of Chemistry, 2019, 35, 947-957.	0.3	1
2177	$\text{BAI4Mg}^{+/0}$: Global Minima with a Planar Tetracoordinate or Hypercoordinate Boron Atom. Atoms, 2021, 9, 89.	1.6	7
2178	Computer Design of Structure of Molecules of High-Energy Tetrazines. Calculation of Thermochemical Properties. Supercomputing Frontiers and Innovations, 2020, 7, .	0.4	2
2179	Experimental and kinetic modeling studies of 2-acetylfuran pyrolysis at atmospheric pressure. Combustion and Flame, 2022, 236, 111824.	5.2	6
2180	Estimation of Heat of Formation for Chemical Systems using the Lasso Regression-Based Approach. , 2020, , .		0
2181	Radical-Trapping Antioxidant Activity of Copper and Nickel Bis(Thiosemicarbazone) Complexes Underlies Their Potency as Inhibitors of Ferroptotic Cell Death. Journal of the American Chemical Society, 2021, 143, 19043-19057.	13.7	28

#	ARTICLE	IF	CITATIONS
2182	Conformation-Dependent Antioxidant Properties of Î ² -Carotene. Organic and Biomolecular Chemistry, 2021, , .	2.8	7
2183	Three decades of unveiling the complex chemistry of <i>C</i>-nitroso species with computational chemistry. Organic Chemistry Frontiers, 2021, 9, 223-264.	4.5	11
2184	The Effect of Dicarboxylic Acid Catalyst Structure on Hydrolysis of Cellulose Model Compound D-Cellobiose in Water. Current Organocatalysis, 2022, 9, 163-171.	0.5	1
2185	Computational study of the gas-phase reactions of sulfuric acid with OH(2Î), O(3PJ), Cl(2PJ) and O(1D2) radicals. Chemical Physics Letters, 2022, 787, 139203.	2.6	1
2186	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. Scientific Data, 2021, 8, 300.	5.3	9
2187	A review of quantum chemical methods for treating energetic molecules. Energetic Materials Frontiers, 2021, 2, 292-305.	3.2	21
2188	Jet-Stirred Reactor Study of Low-Temperature Neopentane Oxidation: A Combined Theoretical, Chromatographic, Mass Spectrometric, and PEPICO Analysis. Energy & Fuels, 2021, 35, 19689-19704.	5.1	12
2189	Benchmark calculations and error cancelations for bond dissociation enthalpies of Xâ€“NO ₂ . Defence Technology, 2023, 22, 144-155.	4.2	6
2190	Ab initio composite methodologies: Their significance for the chemistry community. Annual Reports in Computational Chemistry, 2021, 17, 113-161.	1.7	4
2191	Thermodynamic Properties: Enthalpy, Entropy, Heat Capacity, and Bond Energies of Fluorinated Carboxylic Acids. Journal of Physical Chemistry A, 2022, 126, 3-15.	2.5	5
2192	Lactic acid photochemistry following excitation of S 0 to S 1 at 220 to 250â€“nm. Journal of Physical Organic Chemistry, 0, , e4316.	1.9	3
2193	Kinetics and molecular mechanism of the Schonberg rearrangement. Computational and Theoretical Chemistry, 2022, 1208, 113585.	2.5	1
2194	Comparative investigation of the reactivity of the ignored radical HO ₂ * with that of HO* in the case of guanine/cytosine complex. Computational and Theoretical Chemistry, 2022, 1208, 113561.	2.5	0
2195	Toward Accurate Formation Routes of Complex Organic Molecules in the Interstellar Medium: The Paradigmatic Cases of Acrylonitrile and Cyanomethanimine. Frontiers in Astronomy and Space Sciences, 2022, 8, .	2.8	7
2196	Identifying the mechanism of formation of chlorinated silane polymer byâ€“products during chemical vapor infiltration of SiC from CH ₃ SiCl ₃ /H ₂ . International Journal of Chemical Kinetics, 2022, 54, 300-308.	1.6	2
2197	Detailed Kinetic Modeling for the Pyrolysis of a Jet A Surrogate. Energy & Fuels, 2022, 36, 1304-1315.	5.1	11
2198	Conformation-dependent low-temperature oxidation chemistry of methylcyclohexane: First oxygen addition and chain-branching. Combustion and Flame, 2022, 243, 111963.	5.2	8
2199	Thermodynamics and Reaction Mechanisms for Decomposition of a Simple Protonated Tripeptide, H ⁺ GGA: From H ⁺ GGG to H ⁺ GAG to H ⁺ GGA. Journal of the American Society for Mass Spectrometry, 2022, 33, 355-368.	2.8	3

#	ARTICLE	IF	CITATIONS
2200	CH ₂ + O ₂ : reaction mechanism, biradical and zwitterionic character, and formation of CH ₂ OO, the simplest Criegee intermediate. Physical Chemistry Chemical Physics, 2022, 24, 914-927.	2.8	4
2201	Quantum-chemical calculations of physicochemical properties of high enthalpy 1,2,3,4- and 1,2,4,5-tetrazines annelated with polynitroderivatives of pyrrole and pyrazole. Comparison of different calculation methods. Computational and Theoretical Chemistry, 2022, 1209, 113608.	2.5	0
2202	Antiaromaticity-promoted radical anion stability in $\hat{1}\pm$ -vinyl heterocyclics. Organic Chemistry Frontiers, 0, , .	4.5	3
2203	Theoretical structural and thermochemical characterization of partially fluorinated alcohols. Computational and Theoretical Chemistry, 2022, 1209, 113600.	2.5	0
2204	Combustion chemistry of alkenes and alkadienes. Progress in Energy and Combustion Science, 2022, 90, 100983.	31.2	28
2205	Ab initio kinetics of OH-initiated oxidation of cyclopentadiene. Fuel, 2022, 317, 123305.	6.4	5
2206	Mechanistic Understanding of Superoxide Radical-Mediated Degradation of Perfluorocarboxylic Acids. Environmental Science & Technology, 2022, 56, 624-633.	10.0	45
2207	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
2208	The unimolecular decomposition of dimethoxymethane: channel switching as a function of temperature and pressure. Faraday Discussions, 0, , .	3.2	2
2209	Master equation modelling of non-equilibrium chemistry in stellar outflows. Faraday Discussions, 0, 238, 461-474.	3.2	4
2210	The reactions of propanal/acetone with hydroperoxyl radicals: A theoretical and modeling study. Combustion and Flame, 2022, , 112018.	5.2	0
2211	Autoxidation of Formaldehyde with Oxygen – A Comparison of Reaction Channels. ACS Omega, 2022, 7, 6778-6786.	3.5	0
2212	Theoretical spectroscopic study of acetyl (CH ₃ CO), vinoxy (CH ₂ CHO), and 1-methylvinoxy (CH ₃ COCH ₂) radicals. Barrierless formation processes of acetone in the gas phase. Open Research Europe, 0, 1, 116.	2.0	0
2213	Thermodynamic Modeling of Solubility of Corundum in Water at Supercritical Conditions. ACS Earth and Space Chemistry, 2022, 6, 656-671.	2.7	0
2214	Theoretical investigations on the unimolecular decomposition mechanisms of isopropyl acetate. Journal of Molecular Structure, 2022, 1262, 133006.	3.6	6
2215	Superalkalis for the Activation of Carbon Dioxide: A Review. Frontiers in Physics, 2022, 10, .	2.1	3
2216	Ab Initio Kinetics of Initial Thermal Pyrolysis of Isopropyl Propionate: A Revisited Study. ACS Omega, 2022, 7, 661-668.	3.5	0
2217	<i>Ab Initio</i> Composite Approaches for Heavy Element Energetics: Ionization Potentials for the Actinide Series of Elements. Journal of Physical Chemistry A, 2022, 126, 3027-3042.	2.5	3

#	ARTICLE	IF	CITATIONS
2218	Toward Chemical Accuracy in Predicting Enthalpies of Formation with General-Purpose Data-Driven Methods. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3479-3491.	4.6	22
2219	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4252.	4.1	12
2223	Improved Computational Modeling of the Kinetics of the Acetylperoxy + HO ₂ Reaction. <i>Faraday Discussions</i> , 0, , .	3.2	0
2224	Temperature-dependent kinetics of the atmospheric reaction between CH ₂ OO and acetone. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13066-13073.	2.8	14
2225	A quantum chemistry study on C-H homolytic bond dissociation enthalpies of five-membered and six-membered heterocyclic compounds. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100527.	2.8	1
2226	Detailed Kinetic Model for the Thermal Decomposition of Hydrazine Nitrate in Nitric Acid Solution Based on Quantum Chemistry Calculations Combined with the Polarizable Continuum Model. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2998-3005.	2.5	0
2227	Spectroscopic Detection of Cyano-Cyclopentadiene Ions as Dissociation Products upon Ionization of Aniline. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2989-2997.	2.5	5
2228	Potassium Binding Interactions with Aliphatic Amino Acids: Thermodynamic and Entropic Effects Analyzed via a Guided Ion Beam and Computational Study. <i>Journal of the American Society for Mass Spectrometry</i> , 2022, 33, 1427-1442.	2.8	3
2229	Arsenite oxidation and (thio)arsenates formation in arsenite- and sulfide-containing solution under air atmosphere. <i>Applied Geochemistry</i> , 2022, 142, 105344.	3.0	3
2230	Toward size-dependent thermodynamics of nanoparticles from quantum chemical calculations of small atomic clusters: a case study of (B ₂ O ₃) _n . <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	1
2231	Advances in the molecular simulation and numerical calculations of the green high-energy oxidant ADN. <i>Materials Today Communications</i> , 2022, 31, 103699.	1.9	12
2232	VUV photoprocessing of oxygen-containing polycyclic aromatic hydrocarbons: iPEPICO study of the unimolecular dissociation of ionized benzofuran. <i>Canadian Journal of Chemistry</i> , 2022, 100, 729-736.	1.1	4
2233	Multichannel Gas-Phase Unimolecular Decomposition Reaction of C5-Perfluorinated Ketone, C5-PFK: Theoretical Kinetics Studies. <i>Plasma Chemistry and Plasma Processing</i> , 2022, 42, 973-987.	2.4	2
2234	Zinc-Based Cyclens Containing Pyridine and Cross-Bridges: X-Ray and DFT Structures, Lewis Acidity, Gas-Phase Acidity, and pKa Values. <i>Polyhedron</i> , 2022, , 115941.	2.2	1
2236	Spiers Memorial Lecture: Theory of unimolecular reactions. <i>Faraday Discussions</i> , 0, 238, 11-67.	3.2	6
2237	Dipolar 1,3-cycloaddition of thioformaldehyde S-methylide (CH ₂ SCH) Tj ETQq1 1 0.784314 rgBT /Overl ₃ /sc> , <sc> SO ₂ /sc> , <sc>. <i>Journal of Computational Chemistry</i> , 2022, 43, 1420-1433.	3.3	6
2238	Comprehensive Quantum Chemical Characterization of the Astrochemically Relevant HC_nH Chain Family: An Attempt to Aid Astronomical Observations. <i>Advanced Theory and Simulations</i> , 2022, 5, , .	2.8	8
2239	Pyrolysis study of iso-propylamine with SVUV-photoionization molecular-beam mass spectrometry. <i>Combustion and Flame</i> , 2022, 244, 112232.	5.2	6

#	ARTICLE	IF	CITATIONS
2240	Photolytic insertion of carbon monoxide into nitrosyl chloride: formation of nitrosoformyl chloride. <i>Physical Chemistry Chemical Physics</i> , 0, , .	2.8	1
2241	Why Are MgC_3H Isomers Missing in the Interstellar Medium?. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4465-4475.	2.5	1
2242	Improving the Accuracy of Composite Methods: A G4MP2 Method with G4-like Accuracy and Implications for Machine Learning. <i>Journal of Physical Chemistry A</i> , 2022, 126, 4528-4536.	2.5	3
2243	<i>Ab initio</i> composite strategies and multireference approaches for lanthanide sulfides and selenides. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	6
2244	The secondary chemistry of synthetic fuel oxymethylene ethers unraveled: Theoretical and kinetic modeling of methoxymethyl formate and formic anhydride decomposition. <i>Journal of the Energy Institute</i> , 2022, 104, 46-54.	5.3	3
2245	Mechanism of Visible Light-Mediated Alkene Aminoarylation with Arylsulfonylacetamides. <i>ACS Catalysis</i> , 2022, 12, 8511-8526.	11.2	21
2246	Dielectric Failure of Hydrofluoroolefine HFO-1234ze in the Presence of Water Impurity. , 2022, , .		0
2247	Sensing the ortho Positions in C_6Cl_6 and $\text{C}_6\text{H}_4\text{Cl}_2$ from $\text{Cl}_2^{\bullet -}$ Formation upon Molecular Reduction. <i>Molecules</i> , 2022, 27, 4820.	3.8	0
2248	Stability of Terpenoid-Derived Secondary Ozonides in Aqueous Organic Media. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5386-5397.	2.5	6
2249	Simultaneously remove organic pollutants and improve pyrolysis gas quality during the co-pyrolysis of soybean straw and oil shale. <i>Journal of Analytical and Applied Pyrolysis</i> , 2022, 167, 105665.	5.5	5
2250	Non-physical Species in Chemical Kinetic Models: A Case Study of Diazenyl Hydroxy and Diazenyl Peroxide. <i>ChemPhysChem</i> , 0, , .	2.1	2
2251	Product Identification in the Low-Temperature Oxidation of Cyclohexane Using a Jet-Stirred Reactor in Combination with SVUV-PEPICO Analysis and Theoretical Quantum Calculations. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5784-5799.	2.5	6
2252	Understanding the Kinetics and Topological Events Within the Thione- \rightarrow -Thiol Rearrangement of Xanthates. <i>ChemistrySelect</i> , 2022, 7, .	1.5	1
2253	Density functional theory model of Li^+S^- electrochemical system with explicit solvation of lithium polysulfides by sulfolane. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	2.0	2
2254	Chemical kinetics of cyclic ethers in combustion. <i>Progress in Energy and Combustion Science</i> , 2022, 92, 101019.	31.2	15
2255	Exploring the kinetics and thermochemistry effects on C2-C6 alkene combustion chemistry by $\dot{\text{E}}\text{H}$ radical; Implications for Combustion Modeling and Simulation. <i>Combustion and Flame</i> , 2022, 245, 112302.	5.2	6
2256	The kinetic model of ethylcyclohexane combustion over a wide temperature range and its comprehensive validation. <i>Combustion and Flame</i> , 2022, 245, 112307.	5.2	2
2257	Theoretical Study of the Thermal Decomposition of Urea Derivatives. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6264-6277.	2.5	2

#	ARTICLE	IF	CITATIONS
2258	Acid-triggered polyether sulfone - Polyvinyl pyrrolidone blend anion exchange membranes for the recovery of titania waste acid via diffusion dialysis. <i>Journal of Membrane Science</i> , 2022, 662, 120980.	8.2	6
2259	Dinitriles and nitriles are common intermediates of pyrrole pyrolysis. <i>Combustion and Flame</i> , 2022, 245, 112358.	5.2	3
2260	High-temperature pyrolysis experiments and chemical kinetics of diisopropyl methylphosphonate (DIMP), a simulant for Sarin. <i>Combustion and Flame</i> , 2022, 245, 112345.	5.2	5
2261	An experimental and kinetic modeling investigation on low-temperature oxidation chemistry of 1,3,5-trimethylcyclohexane in a jet-stirred reactor. <i>Combustion and Flame</i> , 2022, 245, 112365.	5.2	1
2262	Unraveling the carbene chemistry of oxymethylene ethers: Experimental investigation and kinetic modeling of the high-temperature pyrolysis of OME-2. <i>Proceedings of the Combustion Institute</i> , 2022, , .	3.9	3
2263	Correcting the Experimental Enthalpies of Formation of Some Members of the Biologically Significant Sulfenic Acids Family. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6091-6109.	2.5	4
2264	Energy- and atom-efficient chemical synthesis with endergonic photocatalysis. <i>Nature Reviews Chemistry</i> , 2022, 6, 745-755.	30.2	27
2265	Atmospheric oxidation mechanism and kinetics of indole initiated by $\cdot\text{OH}$ and $\cdot\text{Cl}$: a computational study. <i>Atmospheric Chemistry and Physics</i> , 2022, 22, 11543-11555.	4.9	7
2266	Rapid Gas-Phase Autoxidation of Nicotine in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2022, 126, 6495-6501.	2.5	6
2267	Metal-Catalyzed Formation of Organic Pollutants Intermediated by Organic Free Radicals. <i>Environmental Science & Technology</i> , 2022, 56, 14550-14561.	10.0	4
2268	Impact of the size and degree of branching of alkanes on the rate rules approach: The case of isomerizations. <i>Proceedings of the Combustion Institute</i> , 2022, , .	3.9	0
2269	Experimental and Theoretical Study of Oxolan-3-one Thermal Decomposition. <i>Journal of Physical Chemistry A</i> , 2022, 126, 7084-7093.	2.5	4
2270	Mechanism of Prebiotic Uracil Synthesis from Urea and HC_3O^+ in Space. <i>Astrobiology</i> , 2022, 22, 1363-1369.	3.0	1
2271	Quantum mechanical thermochemical predictions 100 years after the Schrödinger equation. <i>Annual Reports in Computational Chemistry</i> , 2022, , 123-166.	1.7	21
2272	Oxidative C=O Coupling: Radical and Ionic Pathways of Reaction in $\text{Bu}_4\text{NI}/t\text{-BuOOH}$ System. <i>Doklady Chemistry</i> , 2022, 504, 67-73.	0.9	2
2273	Chemical bonding in representative astrophysically relevant neutral, cation, and anion HC_n chains. <i>Chinese Physics B</i> , 2022, 31, 123101.	1.4	2
2274	Experimental and theoretical insights on the thermal oxidation of epoxy-amine networks. <i>Polymer Degradation and Stability</i> , 2022, 206, 110188.	5.8	3
2275	Computational studies on thermo-kinetics aspects of pyrolysis of isopropyl acetate and its methyl, bromide and hydroxyl derivatives. <i>Heliyon</i> , 2022, 8, e11274.	3.2	3

#	ARTICLE	IF	CITATIONS
2276	Evaluating the role of hydroxyl keto-hydroperoxide in the low temperature oxidation of alkenes. Combustion and Flame, 2022, 246, 112414.	5.2	2
2277	Does boron or nitrogen substitution affect hydrogen physisorption on open carbon surfaces?. Physical Chemistry Chemical Physics, 2022, 24, 28121-28126.	2.8	3
2278	Free and Complexed Fluoropentazoles: Anomalous Ring Charge and Appreciable Kinetic Stability. Journal of Physical Chemistry Letters, 2022, 13, 10567-10574.	4.6	4
2279	Application of Multiconfiguration Pair-Density Functional Theory to the Diels-Alder Reaction. Journal of Physical Chemistry A, 2022, 126, 8834-8843.	2.5	1
2280	Exploring the Origin of the Anomeric Effects in 2,3-Dihalo-1,4-Diphosphinane-1,4-Diium. Russian Journal of Physical Chemistry A, 2022, 96, 2459-2465.	0.6	0
2281	Exploration on laminar flame propagation of 3,3-dimethyl-1-butene, 2,3-dimethyl-1-butene and 2,3-dimethyl-2-butene. Proceedings of the Combustion Institute, 2022, , .	3.9	0
2282	Breaking and Formation of Intramolecular Hydrogen Bonds in Dihydroxybenzaldehydes through UV-Induced Conformational Changes in a Low-Temperature Matrix. Journal of Physical Chemistry A, 2022, 126, 8645-8657.	2.5	3
2283	From electronic structure to model application of key reactions for gasoline/alcohol combustion: Hydrogen-atom abstraction by CH ₃ OE [®] radicals. Proceedings of the Combustion Institute, 2023, 39, 415-423.	3.9	5
2284	Atmospheric breakdown chemistry of the new "green" solvent 2,2,5,5-tetramethyloxolane via gas-phase reactions with OH and Cl radicals. Atmospheric Chemistry and Physics, 2022, 22, 14589-14602.	4.9	1
2285	Exploring fuel molecular structure effects on the pyrolysis chemistry of branched hexenes. Proceedings of the Combustion Institute, 2022, , .	3.9	0
2286	Atmospheric chemistry of CF ₃ CH ₂ : Kinetics, products, mechanism of gas-phase reaction with OH radicals, and atmospheric implications-an effort for novel "class" of refrigerant. Atmospheric Environment, 2022, , 119467.	4.1	1
2287	Theoretical exploration to the significance of n(S)/n(O) at f* (C-COOMe) stereoelectronic interactions. New Journal of Chemistry, 2022, 47, 384-391.	2.8	0
2288	A comprehensive benchmark investigation of quantum chemical methods for carbocations. Physical Chemistry Chemical Physics, 2023, 25, 1903-1922.	2.8	3
2289	Direct bond fission and hydrogen migration as the trigger forces in the pyrolysis of n-pentyl nitrate at low pressure. Combustion and Flame, 2023, 248, 112576.	5.2	1
2290	An experimental and kinetic modeling study on pyrolysis of chlorobenzene. Combustion and Flame, 2023, 248, 112548.	5.2	0
2291	Effect of Symmetry State and Electron Delocalization on the Conformational and Structural Properties of S ₂ X ₂ (S ₂ F ₂ /S ₂ Cl ₂ /S ₂ Br ₂). Russian Journal of Physical Chemistry B, 2022, 16, 809-819.	1.3	0
2292	The Fate of Protonated Guaiacol and Its Derivatives in the Gas Phase. Journal of Physical Chemistry A, 2022, 126, 9051-9058.	2.5	0
2293	Threshold Photoelectron Spectrum of the Phenoxy Radical. Journal of Physical Chemistry A, 2022, 126, 9022-9030.	2.5	5

#	ARTICLE	IF	CITATIONS
2294	Physical Chemistry Research in the Shields Lab by Goldwater Scholars: Including Lessons Learned. ACS Symposium Series, 0, , 1-30.	0.5	0
2295	Nonempirical Prediction of the Relative Electrospray Ionization Efficiencies of Nitroanilines by Combined CBS-QB3 and SCC-DFTB Calculations. Journal of Physical Chemistry A, 2022, 126, 8939-8944.	2.5	0
2296	Halogen Doping to Control the Band Gap of Ascorbic Acid: A Theoretical Study. ACS Omega, 2022, 7, 44390-44397.	3.5	6
2297	Temperatureâ€dependent kinetics of the reactions of CH ₂ OO with acetone, biacetyl, and acetylacetone. International Journal of Chemical Kinetics, 2023, 55, 154-166.	1.6	1
2298	<scp>SVECV</scp>â€12: A composite scheme for accurate and costâ€effective evaluation of reaction barriers. <scp>ll</scp>. Benchmarking using Karton's <scp>BH28</scp> barrier heights database. International Journal of Quantum Chemistry, 2023, 123, .	2.0	3
2299	Active Thermochemical Tables: Enthalpies of Formation of Bromo- and Iodo-Methanes, Ethenes and Ethynes. Journal of Physical Chemistry A, 2023, 127, 704-723.	2.5	2
2300	Complex Reactive Acids from Methanol and Carbon Dioxide Ice: Glycolic Acid (HOCH ₂ COOH) and Carbonic Acid Monomethyl Ester (CH ₃ OCOOH). Astrophysical Journal, 2023, 942, 43.	4.5	4
2301	An Imbalance in the Force: The Need for Standardized Benchmarks for Molecular Simulation. Journal of Chemical Information and Modeling, 2023, 63, 412-431.	5.4	4
2302	Kinetic Modeling of a Poly(<i>N</i>-vinylcaprolactam-<i>co</i>-glycidyl methacrylate) Microgel Synthesis: A Hybrid In Silico and Experimental Approach. Industrial & Engineering Chemistry Research, 2023, 62, 893-902.	3.7	5
2303	A theoretical and modeling study about the low-temperature reaction mechanism between diethoxymethane radicals and O2. Combustion and Flame, 2023, 249, 112616.	5.2	4
2304	Cool flame product characterization from the low-temperature oxidation of n-dodecane. Combustion and Flame, 2023, 249, 112601.	5.2	2
2305	Ab Initio Group Additive Values for Thermodynamic Carbenium Ion Property Prediction. Industrial & Engineering Chemistry Research, 2023, 62, 223-237.	3.7	2
2306	Benchmark of general-purpose machine learning-based quantum mechanical method AIQM1 on reaction barrier heights. Journal of Chemical Physics, 2023, 158, .	3.0	4
2307	A Reaction Kinetics Study on Benzene Oxidation in the Claus Process by Sulfur Monoxide. Journal of Physical Chemistry A, 2023, 127, 1013-1025.	2.5	1
2308	Tautomeric Equilibrium in 1-Benzamidoisoquinoline Derivatives. Molecules, 2023, 28, 1101.	3.8	0
2309	Understanding the Monomer Deuteration Effect on the Transition Temperature of poly(<i>N</i>-isopropylacrylamide) Microgels in H ₂ O. Polymer Chemistry, 0, , .	3.9	1
2310	Benchmarking composite methods for thermodynamic properties of nitro, nitrite, and nitrate species relevant to energetic materials. Chemical Physics Letters, 2023, 815, 140360.	2.6	0
2311	Isopropylcyclohexane pyrolysis at high pressure and temperature: PartÂ2. Experiment and simulation. Combustion and Flame, 2023, 256, 112773.	5.2	1

#	ARTICLE	IF	CITATIONS
2312	Reaction mechanism and kinetics of H and Cl atom abstraction in Dichloromethane with OH radical. Computational and Theoretical Chemistry, 2023, 1223, 114082.	2.5	1
2313	Revisiting the hydrogen atom transfer reactions through a simple and accurate theoretical model: Role of hydrogen bond energy in polyphenolic antioxidants. Computational and Theoretical Chemistry, 2023, 1223, 114097.	2.5	2
2314	A wide range experimental and kinetic modeling study of the oxidation of 2,3-dimethyl-2-butene: Part 1. Combustion and Flame, 2023, 251, 112731.	5.2	0
2315	Characterization of cool flame products during the low temperature oxidation of n-pentylbenzene. Fuel, 2023, 346, 128285.	6.4	2
2316	Pyrolytic elimination of ethylene from ethoxyquinolines and ethoxyisoquinolines: a computational study. Scientific Reports, 2023, 13, .	3.3	3
2317	Dissociative electron attachment to c-C4F8 molecules and clusters. European Physical Journal D, 2023, 77, .	1.3	3
2318	Projected Hybrid Density Functionals: Method and Application to Core Electron Ionization. Journal of Chemical Theory and Computation, 2023, 19, 837-847.	5.3	3
2319	Tautomerism unveils a self-inhibition mechanism of crystallization. Nature Communications, 2023, 14, .	12.8	13
2320	New Insights into the Formation of CH ₃ OCH ₃ and CH ₃ SCH ₃ without and with the Assistance of Na ⁺ Ions and Some Implications for Interstellar Chemistry: An <i>In Silico</i> Approach. ACS Earth and Space Chemistry, 2023, 7, 388-403.	2.7	0
2321	Theoretical simulations on metal nanocluster systems. , 2023, , 201-231.		0
2322	Metal ion-decorated hexasilaprismane and its derivative as a molecular container for the separation of CO ₂ from flue gas molecules: a computational study. Dalton Transactions, 2023, 52, 4336-4348.	3.3	0
2323	From electronic structure to model application for alkyl cyclohexane combustion chemistry: H-atom abstraction reactions by HĖ ₂ radical. Physical Chemistry Chemical Physics, 2023, 25, 10795-10810.	2.8	3
2324	Oxidation of norbornadiene: Theoretical investigation on H-atom abstraction and related radical decomposition reactions. Propulsion and Power Research, 2023, 12, 104-113.	4.3	1
2325	Is DFT Accurate Enough to Calculate Regioselectivity? The Case of 1,3-â€Dipolar Cycloaddition of Azide to Alkynes and Alkenes. ChemPhysChem, 2023, 24, .	2.1	2
2326	Theoretical study on the kinetics of hydrogen cyanide and hydrogen isocyanide reactions with the methyl radical. Physical Chemistry Chemical Physics, 2023, 25, 10121-10128.	2.8	0
2327	Polymorph Screening of the Antitumor Drug Ripretinibâ€™Selective Preference of Dimer Synthons. Crystal Growth and Design, 2023, 23, 2470-2484.	3.0	4
2328	Abstraction and addition reactions of four Î³-â€Lactones with Hâ€atoms and methyl radicals. International Journal of Chemical Kinetics, 2023, 55, 324-332.	1.6	0
2329	Butyl Acetate Pyrolysis and Combustion Chemistry: Mechanism Generation and Shock Tube Experiments. Journal of Physical Chemistry A, 2023, 127, 3231-3245.	2.5	3

#	ARTICLE	IF	CITATIONS
2330	Aromaticity of Cope and Claisen rearrangements. Theoretical Chemistry Accounts, 2023, 142, .	1.4	3
2331	A comprehensive kinetic framework for solid carbon deposition and hydrogen production from the pyrolysis of light hydrocarbons streams. Carbon Trends, 2023, 11, 100263.	3.0	4
2332	The gas-phase pyrolysis of cyclopropylamine. A computational study on the kinetics and reaction mechanism. Combustion and Flame, 2023, 253, 112774.	5.2	0
2333	An Ab Initio RRKM-Based Master Equation Study for Kinetics of OH-Initiated Oxidation of 2-Methyltetrahydrofuran and Its Implications in Kinetic Modeling. Energies, 2023, 16, 3730.	3.1	2
2334	Investigation of Potential Energy Surfaces of Reaction Systems Containing Ethylene, Hydrogen, and Oxygen Atoms by Quantum Chemical Calculations. Russian Journal of Physical Chemistry B, 2023, 17, 336-345.	1.3	2
2335	A Shortâ€Cut to Substituted Fused Pyrrolo[2,1â€c<i>c</i>][1,4]oxazines: A Hybrid Theoretical and Experimental Study. Asian Journal of Organic Chemistry, 2023, 12, .	2.7	2
2336	The<i>meta</i> and<i>para</i> OH Substitution Effect on<i>C</i>-Phenylâ€Nitrilimine Bondâ€Shift Isomers. European Journal of Organic Chemistry, 2023, 26, .	2.4	1
2337	Mechanistic and Kinetic Approach on the Propargyl Radical (C₃H₃) with the Criegee Intermediate (CH₂OO). ACS Omega, 2023, 8, 16859-16868.	3.5	0
2338	An experimental and kinetic modeling study on the low-temperature oxidation of oxymethylene ether-2 (OME-2) by means of stabilized cool flames. Combustion and Flame, 2023, 253, 112792.	5.2	1
2339	Mechanisms of glycine formation from aminoacetonitrile in space. Physical Chemistry Chemical Physics, 2023, 25, 16001-16008.	2.8	0
2340	Theoretical study of H-abstraction reactions of di-n-propyl ether oxidation by H, CH3, HO2 and OH radicals. Fuel, 2023, 350, 128785.	6.4	2
2341	Investigating the Effect of Emtricitabine Cocrystals with Aromatic Carboxylic Acids on Solubility and Diffusion Permeability. Crystal Growth and Design, 2023, 23, 5289-5300.	3.0	3
2342	Unveiling the low-temperature oxidation mechanism of a carbon-neutral fuel â€“ Monoglyme via theoretical study. Fuel Processing Technology, 2023, 250, 107875.	7.2	5
2343	Substituent Effects on Torsional Strain in Cyclopentene Derivatives: A Computational Study. Journal of Physical Chemistry A, 2023, 127, 5005-5017.	2.5	2
2344	Exploring pyrolysis of the aromatics in shale oil by experimental study and kinetic modelling. Energy, 2023, 279, 127998.	8.8	3
2345	Hydroxy sulfonic acid catalyzed hydrolysis of cellulose. Biofuels, 0, , 1-7.	2.4	1
2346	Comprehensive study on selective dehydrochlorination of 2-chloro-3,3,3-trifluoropropene over carbon-based catalysts and catalyst deactivation. Molecular Catalysis, 2023, 547, 113314.	2.0	0
2347	Temperature -and pressure-dependent branching ratios for 2,6-dimethylheptyl radicals (C9H19)Â+ÂO2 reaction: An ab initio and RRKM/ME approach on a key component of bisabolane biofuel. Fuel, 2023, 351, 128969.	6.4	0

#	ARTICLE	IF	CITATIONS
2348	Approaching Coupled Cluster Accuracy with Density Functional Theory Using the Generalized Connectivity-Based Hierarchy. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3763-3778.	5.3	2
2349	Quantum chemical mechanism on the depletion of C3O by oxygen atoms: barrierless to produce CO. <i>Monthly Notices of the Royal Astronomical Society: Letters</i> , 0, , .	3.3	0
2350	Ab initio calculations on structure and stability of BN/CC isosterism in azulene. <i>Scientific Reports</i> , 2023, 13, .	3.3	0
2351	Isopropylcyclohexane pyrolysis at high pressure and temperature: Part 1- theoretical study. <i>Combustion and Flame</i> , 2023, , 112776.	5.2	0
2353	Comprehensive Theoretical Study on Four Typical Intramolecular Hydrogen Shift Reactions of Peroxy Radicals: Multireference Character, Recommended Model Chemistry, and Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 3284-3302.	5.3	3
2354	Coupled Cluster Accuracy at DFT Cost: Generalized Isodesmic Schemes in Quantum Chemistry and Illustrative Applications. , 2024, , 94-110.		0
2355	Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113.		1
2356	Quantum investigation of the reaction between triplet oxygen O(3P) atom and butadiene. <i>Turkish Computational and Theoretical Chemistry</i> , 2023, 7, 1-11.	0.5	0
2357	Trimorphic forms of 5-fluorocytosineâ€“gentisic acid with enhanced hydration stability. <i>CrystEngComm</i> , 2023, 25, 4199-4212.	2.6	0
2358	Bond dissociation energies of ethyl valerate and tripropionin. <i>Journal of Molecular Modeling</i> , 2023, 29, .	1.8	0
2359	Benchmark Accuracy in Thermochemistry, Kinetics, and Noncovalent Interactions. , 2024, , 47-68.		0
2360	Combined DFT and Machine Learning Study of the Dissociation and Migration of H in Pyrrole Derivatives. <i>Journal of Physical Chemistry A</i> , 0, , .	2.5	0
2361	Intramolecular H-Atom Transfers in Alkoxy Radical Intermediates Underlie the Apparent Oxidation of Lipid Hydroperoxides by Fe(II). <i>ACS Chemical Biology</i> , 2023, 18, 2073-2081.	3.4	1
2362	Accurate ab initio thermochemistry of the Groups 10â€“12 difluorides, dichlorides, oxides and sulfides. <i>Journal of Chemical Thermodynamics</i> , 2023, 187, 107151.	2.0	1
2363	Detailed Multiphase Chemical Kinetic Model for Polymer Fouling in a Distillation Column. <i>Industrial & Engineering Chemistry Research</i> , 2023, 62, 14266-14285.	3.7	1
2364	Mechanism of Interaction between Ammonium Perchlorate and Aluminum. <i>Journal of Physical Chemistry A</i> , 2023, 127, 6532-6540.	2.5	2
2365	Mechanosynthesis of Stable Salt Hydrates of Allopurinol with Enhanced Dissolution, Diffusion, and Pharmacokinetics. <i>ACS Omega</i> , 2023, 8, 34120-34133.	3.5	1
2366	Local reactivity descriptors to decipher the electrochemical hydrogenation of unsaturated carboxylic acids. <i>Green Chemistry</i> , 2023, 25, 10387-10397.	9.0	1

#	ARTICLE	IF	CITATIONS
2367	Mechanistic insights into trisulfur radical generation in lithium–sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2023, 11, 18922-18932.	10.3	2
2368	Substitution effect on the adiabatic ionization potential, vertical ionization potential, electrophilicity, and nucleophilicity of some hydantoin drug derivatives: Computational study. <i>Journal of Physical Organic Chemistry</i> , 2023, 36, .	1.9	1
2369	Self-Consistent Implementation of a Solvation Free Energy Framework to Predict the Salt Solubilities of Six Alkali Halides. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 5586-5601.	5.3	0
2370	Quantum Algorithms for the Study of Electronic Structure and Molecular Dynamics: Novel Computational Protocols. , 2024, , 228-251.		0
2371	Isosterism in pyrrole via azaboroles substitution, a theoretical investigation for electronic structural, stability and aromaticity. <i>Heliyon</i> , 2023, 9, e20542.	3.2	1
2372	Theoretical prediction for redox potentials of oxygen-centered organic anions in aprotic solvents. <i>Theoretical Chemistry Accounts</i> , 2023, 142, .	1.4	0
2373	A combined theoretical and experimental study of the pyrolysis of pyrrolidine. <i>Combustion and Flame</i> , 2023, 258, 113063.	5.2	1
2374	Accurate Prediction of Adiabatic Ionization Energies for PAHs and Substituted Analogues. <i>Journal of Physical Chemistry A</i> , 2023, 127, 8447-8458.	2.5	0
2375	Data Quality, Data Sampling and Data Fitting: A Tutorial Guide for Constructing Full-Dimensional Accurate Potential Energy Surfaces (PESs) of Molecules and Reactions. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2023, , 161-201.	0.6	0
2376	A Theoretical Kinetic Study on Concerted Elimination Reaction Class of Peroxyl-hydroperoxyl-alkyl Radicals (ROOQOOH) in Normal-alkyl Cyclohexanes. <i>Molecules</i> , 2023, 28, 6612.	3.8	1
2377	Theoretical calculation of the adiabatic electron affinity and vertical electron affinity of some hydantoin drugs. <i>Journal of Saudi Chemical Society</i> , 2023, 27, 101725.	5.2	0
2378	Mechanistic study on levoglucosan condensation and decomposition in the condensed phase during cellulose pyrolysis. <i>Fuel</i> , 2024, 358, 130109.	6.4	1
2379	Can G4-like composite $\langle i \rangle \text{Ab Initio} \langle /i \rangle$ methods accurately predict vibrational harmonic frequencies?. <i>Molecular Physics</i> , 0, , .	1.7	2
2381	Detailed kinetic mechanism of polyoxymethylene dimethyl ether 3 (PODE3). Part I: Ab initio thermochemistry and kinetic predictions for key reactions. <i>Combustion and Flame</i> , 2023, 256, 112990.	5.2	3
2382	Experimental, Kinetic Modeling and Theoretical Methods. <i>Springer Theses</i> , 2023, , 23-40.	0.1	0
2383	Does the dissociation of guaiacol family radical cations mimic their thermal decomposition?. <i>Computational and Theoretical Chemistry</i> , 2023, 1229, 114323.	2.5	0
2384	Refining the chain-branching process in the low-temperature oxidation of 1-hexene with synchrotron-based PEPICO spectroscopy. <i>Combustion and Flame</i> , 2023, 258, 113065.	5.2	0
2385	Thermal Decomposition of 2- and 4-Iodobenzyl Iodide Yields Fulvenallene and Ethynylcyclopentadienes: A Joint Threshold Photoelectron and Matrix Isolation Spectroscopic Study. <i>Journal of Physical Chemistry A</i> , 2023, 127, 8574-8583.	2.5	1

#	ARTICLE	IF	CITATION
2386	Fragment-based models for dissociation of strong acids in water: Electrostatic embedding minimizes the dependence on the fragmentation schemes. Journal of Chemical Physics, 2023, 159, .	3.0	0
2387	Chemical bonding in potential PFAS products from the thermal degradation of energetic devices, a DFT analysis. Chemosphere, 2023, 345, 140363.	8.2	1
2388	Enthalpy of Formation of Carbocycles: A Precise Theoretical Determination of Experimentally Imprecise Measurements.. Chemical Thermodynamics and Thermal Analysis, 2023, 12, 100121.	1.5	0
2389	Threshold photoelectron spectroscopy and dissociative photoionization of benzonitrile. Physical Chemistry Chemical Physics, 2023, 25, 29070-29079.	2.8	2
2390	Oxidation of <i>n</i> -Nonane: Measurements of Low-Temperature Products in Jet-Stirred Reactors. Energy & Fuels, 0, , .	5.1	0
2391	Photocatalytic C=S Bond Formation Using <i>N</i> -Thiophthalimide and <i>N</i> -Perthiophthalimide Derivatives. ACS Catalysis, 0, , 13912-13919.	11.2	0
2392	Theoretical investigation on the mechanism and kinetics of the OH-initiated atmospheric degradation of p-chloroaniline: Addition of  $\text{C}_6\text{H}_4\text{Cl}$ and OH radical. Journal of Molecular Graphics and Modelling, 2024, 126, 108651.	2.4	0
2393	Expansion of Bond Dissociation Prediction with Machine Learning to Medicinally and Environmentally Relevant Chemical Space. , 0, , .		0
2394	DFT Model of Elemental Sulfur in Sulfolane Solutions. Journal of Physical Chemistry A, 0, , .	2.5	0
2395	Graph- <i>Q</i> $\hat{A}^{\dagger} \hat{C}$: A Quantum Algorithm with Reduced Quantum Circuit Depth for Electronic Structure. Journal of Physical Chemistry A, 2023, 127, 9334-9345.	2.5	2
2396	Accuracy of enthalpies of formation of hydrocarbons using the SVECV-f12 protocol and comparison to other composite methods. Journal of Chemical Thermodynamics, 2024, 189, 107197.	2.0	0
2397	Multiple-well master equation study on the propargyl+indenyl recombination and subsequent reactions. Combustion and Flame, 2024, 259, 113143.	5.2	2
2398	Photoelectron spectroscopic study of 2-naphthyl nitrene and its thermal rearrangement to cyanoindenes. Physical Chemistry Chemical Physics, 2023, 25, 31146-31152.	2.8	1
2399	Mechanism-based structure-activity relationship investigation on hydrolysis kinetics of atmospheric organic nitrates. Npj Climate and Atmospheric Science, 2023, 6, .	6.8	0
2400	Investigating the kinetics of the intramolecular H-migration reaction class of methyl-ester peroxy radicals in low-temperature oxidation mechanisms of biodiesel. Physical Chemistry Chemical Physics, 2023, 25, 32078-32092.	2.8	0
2401	High-throughput design of energetic molecules. Journal of Materials Chemistry A, 2023, 11, 25031-25044.	10.3	2
2402	Theoretical study on the P=N bond dissociation enthalpy in phosphamide and phosphoramidate flame retardants. Journal of the Indian Chemical Society, 2024, 101, 101114.	2.8	0
2403	Capturing Weak Interactions in Surface Adsorbate Systems at Coupled Cluster Accuracy: A Graph-Theoretic Molecular Fragmentation Approach Improved through Machine Learning. Journal of Chemical Theory and Computation, 2023, 19, 8541-8556.	5.3	1

#	ARTICLE	IF	CITATIONS
2404	Probing the Thermochemistry Properties and Rate Kinetics of Trimethyl Phosphate (TMP): An H-Atom Abstraction (HAA) Reactions Perspective. ACS Omega, 2023, 8, 47134-47145.	3.5	1
2406	Simple Composite Approach to Efficiently Estimate Basis Set Limit CCSD(T) Harmonic Frequencies and Reaction Thermochemistry. Journal of Physical Chemistry A, 2023, 127, 10026-10031.	2.5	0
2407	Activation mechanisms of recombination processes in irradiated poly(arylenephthalides). Journal of Photochemistry and Photobiology A: Chemistry, 2024, 448, 115347.	3.9	0
2408	Unraveling the Unimolecular Ion Chemistry of Protonated Isoprene and Prenol. Journal of the American Society for Mass Spectrometry, 0, , .	2.8	0
2409	Experimental and kinetic study on 2-methoxyethanol part I: Molecular chemistry and pyrolysis investigation. Combustion and Flame, 2024, 260, 113238.	5.2	0
2411	Oxidation of the 1-phenyl radical C ₁₀ H ₇ with oxygen: Thermochemistry, kinetics, and possible reaction pathways. International Journal of Chemical Kinetics, 2024, 56, 210-232.	1.6	0
2412	Tailoring the optical and spectroscopic properties of ascorbic acid via solvation with DMSO: A theoretical study using different quantum models. Chemical Physics Impact, 2024, 8, 100429.	3.5	0
2413	Ab initio prediction of metallic nature of sp ³ -hybridized germanium structures. Computational and Theoretical Chemistry, 2024, 1231, 114441.	2.5	0
2414	On the Development of Descriptor-Based Machine Learning Models for Thermodynamic Properties: Part 2—Applicability Domain and Outliers. Algorithms, 2023, 16, 573.	2.1	0
2415	Experimental and theoretical study of cyclopropanated fuel exo,exo-Tetracyclo[3.3.1.0 ^{2,4} .0 ^{6,8}]nonane pyrolysis in a jet-stirred reactor. Fuel, 2024, 361, 130702.	6.4	0
2416	Calculation of the Formation Enthalpy and the Ionic Equilibrium Constant of Organic Substances by Quantum Chemistry Methods. Russian Journal of General Chemistry, 2023, 93, 2785-2797.	0.8	0
2417	An experimental and kinetic modeling study of the auto-ignition delay times of trimethyl phosphate-in-air mixtures. Applications in Energy and Combustion Science, 2024, 17, 100237.	1.5	0
2418	Atomic Charge Dependency of Spiropyran/Merocyanine Adsorption as a Precursor to Surface Isomerization Reactions. ACS Omega, 0, , .	3.5	0
2420	Interrupted Homolytic Substitution Enables Organoboron Compounds to Inhibit Radical Chain Reactions Rather than Initiate Them. Journal of the American Chemical Society, 0, , .	13.7	0
2421	Ab initio kinetics of OH-initiated oxidation of naphthalene: A comprehensive revisited study. Atmospheric Environment, 2024, 322, 120342.	4.1	0
2422	On the sensitivity of computed partial charges toward basis set and (exchange-)correlation treatment. Journal of Computational Chemistry, 2024, 45, 1017-1032.	3.3	0
2423	Reformulation of All ONIOM-Type Molecular Fragmentation Approaches and Many-Body Theories Using Graph-Theory-Based Projection Operators: Applications to Dynamics, Molecular Potential Surfaces, Machine Learning, and Quantum Computing. Journal of Physical Chemistry A, 2024, 128, 466-478.	2.5	0
2424	Bromine-Substituted Indolo[3,2- <i>bc</i>]carbazole-Based Small Organic Molecules as Dopant-Free Hole-Transporting Layers for Inverted Perovskite Solar Cells. Energy & Fuels, 2024, 38, 2351-2357.	5.1	0

#	ARTICLE	IF	CITATIONS
2426	A theoretical assessment of Curtius rearrangement of malonyl azide: Molecular mechanism insight and solvent effects. Journal of Molecular Liquids, 2024, 396, 124078.	4.9	0
2427	Achieving Accuracy and Economy for Calculating Vertical Detachment Energies of Molecular Anions: A Model Chemistry Composite Methods. ChemPhysChem, 2024, 25, .	2.1	0
2428	Oxygen Chemistry in Polymer Fouling: Insights from Multiphase Detailed Kinetic Modeling. Industrial & Engineering Chemistry Research, 2024, 63, 1013-1028.	3.7	0
2429	Global potential energy surface survey of pentanitrogen cation. Molecular Physics, 0, , .	1.7	0
2430	Thermochemical Studies of Small Carbohydrates. Journal of Organic Chemistry, 2024, 89, 1769-1776.	3.2	0
2431	Nature or number of species in a transition state: the key role of catalytically active molecules in hydrogen transfer stages in atmospheric aldehyde reactions. Physical Chemistry Chemical Physics, 2024, 26, 5693-5703.	2.8	0
2432	Application of thermodynamics at different scales to describe the behaviour of fast reacting binary mixtures in vapour-liquid equilibrium. Chemical Engineering Journal, 2024, 483, 148961.	12.7	1
2433	High-Pressure Limit and Pressure-Dependent Rate Rules for $\hat{\text{I}}^2$ -Scission Reaction Class of Hydroperoxyl Alkyl Hydroperoxyl Radicals ($\hat{\text{A}}\text{P}(\text{OOH})_2$) in Normal-Alkyl Cyclohexanes Combustion. Molecules, 2024, 29, 544.	3.8	0
2434	Estimate of the $\text{C}\hat{\text{a}}^{\sim}\text{Cl}$ photoionization cross section and absolute photoionization cross sections of chlorinated organic compounds. ChemPhysChem, 2024, 25, .	2.1	0
2435	Exploring the unimolecular chemistry of protonated limonene and $\hat{\text{I}}\pm$ -terpineol. International Journal of Mass Spectrometry, 2024, 498, 117204.	1.5	0
2436	Elucidating the low temperature chemistry of o-xylene enhanced by the reaction pool of dimethyl ether. Fuel, 2024, 364, 131075.	6.4	0
2437	Formation of negative ions from cobalt tricarbonyl nitrosyl $\text{Co}(\text{CO})_3\text{NO}$ clusters. Physical Chemistry Chemical Physics, 2024, 26, 7522-7533.	2.8	0
2438	Predicting the Decomposition Mechanism of the Serine $\hat{\text{I}}\pm$ -Amino Acid in the Gas Phase and Condensed Media. ACS Omega, 0, , .	3.5	0
2439	Tracing Photoinduced Hydrogen Migration in Alcohol Dications from Time-Resolved Molecular-Frame Photoelectron Angular Distributions. Journal of Physical Chemistry A, 2024, 128, 1241-1249.	2.5	0
2440	Thermochemistry of Species in Gas-Phase Thermal Oxidation of C_{20} to C_{28} Perfluorinated Carboxylic Acids. Journal of Physical Chemistry A, 2024, 128, 1313-1326.	2.5	0
2441	Ring Growth Mechanism in the Reaction between Fulvenallenyl and Cyclopentadienyl Radicals. Journal of Physical Chemistry A, 2024, 128, 1327-1338.	2.5	0
2442	Kinetic study of H-abstraction and preliminary pyrolysis of n-decane in post-injection fuels. Combustion and Flame, 2024, 262, 113367.	5.2	1
2443	Computational study of the solvation effect of supercritical water on o-phthalic acid decarboxylation by varying the solvent dielectric constant. Journal of Supercritical Fluids, 2024, 208, 106214.	3.2	0

#	ARTICLE	IF	CITATIONS
2444	What a difference a chlorine makes: The remarkable unimolecular ion chemistry of phenyl formate and phenyl chloroformate. Journal of Mass Spectrometry, 2024, 59, .	1.6	0
2445	Atmospheric reaction of chlorine radical and cyclic amide: A theoretical approach. Computational and Theoretical Chemistry, 2024, 1234, 114527.	2.5	0
2446	Temperature-Dependent Kinetics of the Reactions of the Criegee Intermediate CH_2OO with Hydroxyketones. Journal of Physical Chemistry A, 2024, 128, 1880-1891.	2.5	0
2447	Benchmarking model chemistry composite calculations for vertical ionization potential of molecular systems. Chinese Chemical Letters, 2024, , 109721.	9.0	0
2448	Self-assembled organic molecules with a fused aromatic ring as hole-transport layers for inverted perovskite solar cells: the effect of linkers on performance. New Journal of Chemistry, 2024, 48, 6833-6841.	2.8	0
2449	Modeling Hexaazacyclododeca Metal Complexes as a Radical Trapping Antioxidant: Prospects as a Potential Drug. ChemistrySelect, 2024, 9, .	1.5	0
2450	A new chapter in the never ending story of cycloadditions: The puzzling case of SO_2 and acetylene. Journal of Computational Chemistry, 0, , .	3.3	0
2451	Theoretical and kinetic study of the hydrogen abstraction reactions of ethyl propionate. Fuel, 2024, 367, 131492.	6.4	0