

Jingjing Zheng

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58
papers

5,066
citations

35
h-index

58
g-index

58
ext. papers

5,720
ext. citations

5.7
avg, IF

5.85
L-index

#	Paper	IF	Citations
58	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2872-87	6.4	892
57	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 808-21	6.4	410
56	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3027-34	6.4	393
55	Minimally augmented Karlsruhe basis sets. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 295-305	1.9	388
54	Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1197-202	6.4	206
53	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 569-82	6.4	193
52	Tests of the RPBE, revPBE, tau-HCTHhyb, omegaB97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. <i>Journal of Chemical Physics</i> , 2010 , 132, 164117	3.9	178
51	Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: the internal-coordinate multi-structural approximation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 10885-907	3.6	166
50	Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7782-93	3.6	135
49	Multi-structural variational transition state theory. Kinetics of the 1,4-hydrogen shift isomerization of the pentyl radical with torsional anharmonicity. <i>Chemical Science</i> , 2011 , 2, 2199	9.4	111
48	Quantum Thermochemistry: Multistructural Method with Torsional Anharmonicity Based on a Coupled Torsional Potential. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1356-67	6.4	110
47	Multireference Model Chemistries for Thermochemical Kinetics. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1208-19	6.4	107
46	Multi-path variational transition state theory for chemical reaction rates of complex polyatomic species: ethanol + OH reactions. <i>Faraday Discussions</i> , 2012 , 157, 59-88; discussion 113-40	3.6	106
45	QM/MM study of mechanisms for compound I formation in the catalytic cycle of cytochrome P450cam. <i>Journal of the American Chemical Society</i> , 2006 , 128, 13204-15	16.4	98
44	Photodissociation dynamics of phenol: multistate trajectory simulations including tunneling. <i>Journal of the American Chemical Society</i> , 2014 , 136, 16378-86	16.4	88
43	Density functional approximations for charge transfer excitations with intermediate spatial overlap. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 12697-701	3.6	86
42	MSTor: A program for calculating partition functions, free energies, enthalpies, entropies, and heat capacities of complex molecules including torsional anharmonicity. <i>Computer Physics Communications</i> , 2012 , 183, 1803-1812	4.2	84

41	Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. <i>Chemical Science</i> , 2014 , 5, 4661-4680	9.4	80
40	MSTor version 2013: A new version of the computer code for the multi-structural torsional anharmonicity, now with a coupled torsional potential. <i>Computer Physics Communications</i> , 2013 , 184, 2032-2033	4.2	75
39	Potential-energy surface for the electronic ground state of NH ₃ up to 20,000 cm ⁻¹ above equilibrium. <i>Journal of Chemical Physics</i> , 2005 , 123, 134308	3.9	66
38	Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. <i>Journal of the American Chemical Society</i> , 2018 , 140, 2906-2918	16.4	61
37	Multipath variational transition state theory: rate constant of the 1,4-hydrogen shift isomerization of the 2-cyclohexylethyl radical. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 297-308	2.8	61
36	Thermochemical kinetics of hydrogen-atom transfers between methyl, methane, ethynyl, ethyne, and hydrogen. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 4632-42	2.8	54
35	Rotation-vibration motion of pyramidal XY ₃ molecules described in the Eckart frame: Theory and application to NH ₃ . <i>Molecular Physics</i> , 2005 , 103, 359-378	1.7	52
34	Prediction of experimentally unavailable product branching ratios for biofuel combustion: the role of anharmonicity in the reaction of isobutanol with OH. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5150-60	16.4	51
33	Kinetics of Hydrogen Radical Reactions with Toluene Including Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2690-704	16.4	50
32	New features in the catalytic cycle of cytochrome P450 during the formation of compound I from compound O. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19946-51	3.4	50
31	Common system setup for the entire catalytic cycle of cytochrome P450(cam) in quantum mechanical/molecular mechanical studies. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2147-58	3.5	46
30	Dipole moment and rovibrational intensities in the electronic ground state of NH ₃ : bridging the gap between ab initio theory and spectroscopic experiment. <i>Journal of Chemical Physics</i> , 2005 , 122, 10431-7	3.9	41
29	Phase space prediction of product branching ratios: canonical competitive nonstatistical model. <i>Journal of the American Chemical Society</i> , 2009 , 131, 15754-60	16.4	39
28	Reactions of hydrogen atom with hydrogen peroxide. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 13554-668		39
27	Direct dynamics study of hydrogen-transfer isomerization of 1-pentyl and 1-hexyl radicals. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 11919-25	2.8	38
26	Role of conformational structures and torsional anharmonicity in controlling chemical reaction rates and relative yields: butanal + HO ₂ reactions. <i>Chemical Science</i> , 2013 , 4, 200-212	9.4	37
25	Global analytical potential energy surface for the electronic ground state of NH ₃ from high level ab initio calculations. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 7502-22	2.8	35
24	Quantum and molecular mechanical study of the first proton transfer in the catalytic cycle of cytochrome P450cam and its mutant D251N. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 5126-38	3.4	35

23	Biofuel combustion. Energetics and kinetics of hydrogen abstraction from carbon-1 in n-butanol by the hydroperoxyl radical calculated by coupled cluster and density functional theories and multistructural variational transition-state theory with multidimensional tunneling. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 12206-13	2.8	33
22	On the Study of Resonance Interactions and Splittings in the PH ₃ Molecule: $\bar{1}$, $\bar{2}$, $\bar{2}+\bar{4}$, and $2\bar{4}$ Bands. <i>Journal of Molecular Spectroscopy</i> , 2002 , 215, 295-308	1.3	33
21	Multi-structural variational transition state theory: kinetics of the 1,5-hydrogen shift isomerization of the 1-butoxyl radical including all structures and torsional anharmonicity. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4204-16	3.6	31
20	Chloroform as a hydrogen atom donor in Barton reductive decarboxylation reactions. <i>Journal of Organic Chemistry</i> , 2013 , 78, 6677-87	4.2	31
19	Efficient Geometry Minimization and Transition Structure Optimization Using Interpolated Potential Energy Surfaces and Iteratively Updated Hessians. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6424-6432	6.4	28
18	Multi-structural thermodynamics of C-H bond dissociation in hexane and isohexane yielding seven isomeric hexyl radicals. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 19318-24	3.6	26
17	Statistical thermodynamics of the isomerization reaction between n-heptane and isoheptane. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 482-94	3.6	23
16	Including Torsional Anharmonicity in Canonical and Microcanonical Reaction Path Calculations. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2875-81	6.4	23
15	Density functional study of methyl radical association kinetics. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 11509-13	2.8	23
14	Army ants tunneling for classical simulations. <i>Chemical Science</i> , 2014 , 5, 2091-2099	9.4	22
13	A comparative assessment of the perturbative and renormalized coupled cluster theories with a noniterative treatment of triple excitations for thermochemical kinetics, including a study of basis set and core correlation effects. <i>Journal of Chemical Physics</i> , 2008 , 128, 044108	3.9	20
12	A product branching ratio controlled by vibrational adiabaticity and variational effects: kinetics of the H + trans-N ₂ H ₂ reactions. <i>Journal of Chemical Physics</i> , 2012 , 136, 184310	3.9	19
11	Kinetics of the Hydrogen Abstraction Reaction From 2-Butanol by OH Radical. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 12182-92	2.8	17
10	Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. <i>Journal of the American Chemical Society</i> , 2015 , 137, 8026-9	16.4	15
9	Including Tunneling in Non-Born-Oppenheimer Simulations. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2039-43	6.4	15
8	A new cylindrical photoacoustic cell with improved performance. <i>Review of Scientific Instruments</i> , 2002 , 73, 404-410	1.7	14
7	Entropic Effects on the Free Energies of Clusters in Silane Plasmas. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 10085-10101	3.8	9
6	High-resolution spectrum of the $\bar{1}$, and $\bar{2}+\bar{4}$ (A ₂) bands of the PH ₃ molecule: assignments and preliminary analysis. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2004 , 83, 599-618	2.1	9

5	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4Rnitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 59-67	6.4	8
4	Study of the stretching vibrational band intensities of XH ₄ molecules employing four-dimensional ab initio (X=C and Sn) and effective (X=C and Si) dipole moment surfaces. <i>Journal of Chemical Physics</i> , 2002 , 117, 10073-10080	3.9	3
3	An ab initio anharmonic force field of SiHCl ₃ . <i>Molecular Physics</i> , 2003 , 101, 1165-1170	1.7	1
2	Re-integration with anchor points algorithm for ab initio molecular dynamics. <i>Journal of Chemical Physics</i> , 2021 , 155, 074106	3.9	1
1	Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra 2006 , 171-183		1