Jingjing Zheng

List of Publications by Year
in descending order

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58	6,347	101496	143943
papers	citations	36 h-index	57 g-index

58	58	58	5723
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. Journal of Chemical Theory and Computation, 2010, 6, 2872-2887.	2.3	1,183
2	Minimally augmented Karlsruhe basis sets. Theoretical Chemistry Accounts, 2011, 128, 295-305.	0.5	638
3	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. Journal of Chemical Theory and Computation, 2011, 7, 3027-3034.	2.3	566
4	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.	2.3	462
5	Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. Journal of Chemical Theory and Computation, 2009, 5, 1197-1202.	2.3	236
6	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.	2.3	207
7	Tests of the RPBE, revPBE, Ï„-HCTHhyb, Ï‰B97X-D, and MOHLYP density functional approximations and 29 others against representative databases for diverse bond energies and barrier heights in catalysis. Journal of Chemical Physics, 2010, 132, 164117.	1.2	206
8	Practical methods for including torsional anharmonicity in thermochemical calculations on complex molecules: The internal-coordinate multi-structural approximation. Physical Chemistry Chemical Physics, 2011, 13, 10885.	1.3	196
9	Kinetics of hydrogen-transfer isomerizations of butoxyl radicals. Physical Chemistry Chemical Physics, 2010, 12, 7782.	1.3	151
10	Quantum Thermochemistry: Multistructural Method with Torsional Anharmonicity Based on a Coupled Torsional Potential. Journal of Chemical Theory and Computation, 2013, 9, 1356-1367.	2.3	144
11	Multi-structural variational transition state theory. Kinetics of the 1,4-hydrogen shift isomerization of the pentyl radical with torsional anharmonicity. Chemical Science, 2011, 2, 2199.	3.7	140
12	Multireference Model Chemistries for Thermochemical Kinetics. Journal of Chemical Theory and Computation, 2008, 4, 1208-1219.	2.3	131
13	Multi-path variational transition state theory for chemical reaction rates of complex polyatomic species: ethanol + OH reactions. Faraday Discussions, 2012, 157, 59.	1.6	125
14	MSTor: A program for calculating partition functions, free energies, enthalpies, entropies, and heat capacities of complex molecules including torsional anharmonicity. Computer Physics Communications, 2012, 183, 1803-1812.	3.0	115
15	QM/MM Study of Mechanisms for Compound I Formation in the Catalytic Cycle of Cytochrome P450cam. Journal of the American Chemical Society, 2006, 128, 13204-13215.	6.6	105
16	MSTor version 2013: A new version of the computer code for the multi-structural torsional anharmonicity, now with a coupled torsional potential. Computer Physics Communications, 2013, 184, 2032-2033.	3.0	103
17	Photodissociation Dynamics of Phenol: Multistate Trajectory Simulations including Tunneling. Journal of the American Chemical Society, 2014, 136, 16378-16386.	6.6	102
18	Density functional approximations for charge transfer excitations with intermediate spatial overlap. Physical Chemistry Chemical Physics, 2010, 12, 12697.	1.3	101

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19	Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. Journal of the American Chemical Society, 2018, 140, 2906-2918.	6.6	100
20	Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. Chemical Science, 2014, 5, 4661-4680.	3.7	90
21	Kinetics of Hydrogen Radical Reactions with Toluene Including Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory. Journal of the American Chemical Society, 2016, 138, 2690-2704.	6.6	72
22	Multipath Variational Transition State Theory: Rate Constant of the 1,4-Hydrogen Shift Isomerization of the 2-Cyclohexylethyl Radical. Journal of Physical Chemistry A, 2012, 116, 297-308.	1.1	71
23	Prediction of Experimentally Unavailable Product Branching Ratios for Biofuel Combustion: The Role of Anharmonicity in the Reaction of Isobutanol with OH. Journal of the American Chemical Society, 2014, 136, 5150-5160.	6.6	69
24	Potential-energy surface for the electronic ground state of NH3 up to 20000cmâ^'1 above equilibrium. Journal of Chemical Physics, 2005, 123, 134308.	1.2	68
25	Thermochemical Kinetics of Hydrogen-Atom Transfers between Methyl, Methane, Ethynyl, Ethyne, and Hydrogen. Journal of Physical Chemistry A, 2007, 111, 4632-4642.	1.1	59
26	Rotationâ€“vibration motion of pyramidal XY3molecules described in the Eckart frame: Theory and application to NH3. Molecular Physics, 2005, 103, 359-378.	0.8	55
27	New Features in the Catalytic Cycle of Cytochrome P450 during the Formation of Compound I from Compound 0. Journal of Physical Chemistry B, 2005, 109, 19946-19951.	1.2	52
28	Common system setup for the entire catalytic cycle of cytochrome P450cam in quantum mechanical/molecular mechanical studies. Journal of Computational Chemistry, 2007, 28, 2147-2158.	1.5	46
29	Reactions of Hydrogen Atom with Hydrogen Peroxide. Journal of Physical Chemistry A, 2007, 111, 13554-13566.	1.1	44
30	Dipole moment and rovibrational intensities in the electronic ground state of NH3: Bridging the gap betweenab initiotheory and spectroscopic experiment. Journal of Chemical Physics, 2005, 122, 104317.	1.2	43
31	Phase Space Prediction of Product Branching Ratios: Canonical Competitive Nonstatistical Model. Journal of the American Chemical Society, 2009, 131, 15754-15760.	6.6	43
32	Role of conformational structures and torsional anharmonicity in controlling chemical reaction rates and relative yields: butanal + HO₂reactions. Chemical Science, 2013, 4, 200-212.	3.7	40
33	Direct Dynamics Study of Hydrogen-Transfer Isomerization of 1-Pentyl and 1-Hexyl Radicals. Journal of Physical Chemistry A, 2009, 113, 11919-11925.	1.1	39
34	Global Analytical Potential Energy Surface for the Electronic Ground State of NH₃ from High Level ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 7502-7522.	1.1	39
35	Chloroform as a Hydrogen Atom Donor in Barton Reductive Decarboxylation Reactions. Journal of Organic Chemistry, 2013, 78, 6677-6687.	1.7	39
36	Efficient Geometry Minimization and Transition Structure Optimization Using Interpolated Potential Energy Surfaces and Iteratively Updated Hessians. Journal of Chemical Theory and Computation, 2017, 13, 6424-6432.	2.3	38

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37	On the Study of Resonance Interactions and Splittings in the PH3 Molecule: Î½1, Î½3, Î½2+Î½4, and 2Î½4 Bands. Journal of Molecular Spectroscopy, 2002, 215, 295-308.	0.4	35
38	Quantum and Molecular Mechanical Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450cam and Its Mutant D251N. Journal of Physical Chemistry B, 2008, 112, 5126-5138.	1.2	35
39	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. Journal of Physical Chemistry A, 2012, 116, 12206-12213.	1.1	35
40	Density Functional Study of Methyl Radical Association Kinetics. Journal of Physical Chemistry A, 2008, 112, 11509-11513.	1.1	33
41	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. Physical Chemistry Chemical Physics, 2012, 14, 4204.	1.3	33
42	Multi-structural thermodynamics of Câ€“H bond dissociation in hexane and isohexane yielding seven isomeric hexyl radicals. Physical Chemistry Chemical Physics, 2011, 13, 19318.	1.3	29
43	Kinetics of the Hydrogen Abstraction Reaction From 2-Butanol by OH Radical. Journal of Physical Chemistry A, 2015, 119, 12182-12192.	1.1	28
44	Statistical thermodynamics of the isomerization reaction between n-heptane and isoheptane. Physical Chemistry Chemical Physics, 2012, 14, 482-494.	1.3	24
45	Army ants tunneling for classical simulations. Chemical Science, 2014, 5, 2091-2099.	3.7	24
46	A product branching ratio controlled by vibrational adiabaticity and variational effects: Kinetics of the H + trans-N2H2 reactions. Journal of Chemical Physics, 2012, 136, 184310.	1.2	23
47	Including Torsional Anharmonicity in Canonical and Microcanonical Reaction Path Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2875-2881.	2.3	23
48	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. Journal of Chemical Physics, 2008, 128, 044108.	1.2	20
49	Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. Journal of the American Chemical Society, 2015, 137, 8026-8029.	6.6	18
50	Including Tunneling in Non-Bornâ€“Oppenheimer Simulations. Journal of Physical Chemistry Letters, 2014, 5, 2039-2043.	2.1	17
51	A new cylindrical photoacoustic cell with improved performance. Review of Scientific Instruments, 2002, 73, 404-410.	0.6	16
52	High-resolution spectrum of the , and Î½3+Î½4(A2) bands of the PH3 molecule: assignments and preliminary analysis. Journal of Quantitative Spectroscopy and Radiative Transfer, 2004, 83, 599-618.	1.1	11
53	Entropic Effects on the Free Energies of Clusters in Silane Plasmas. Journal of Physical Chemistry C, 2015, 119, 10085-10101.	1.5	11
54	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4â€²-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. Journal of Chemical Theory and Computation, 2009, 5, 59-67.	2.3	8

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55	Study of the stretching vibrational band intensities of XH4 molecules employing four-dimensionalab initio(X=C and Sn) andeffective(X=C and Si) dipole moment surfaces. Journal of Chemical Physics, 2002, 117, 10073-10080.	1.2	3
56	Anab initioanharmonic force field of SiHCl3. Molecular Physics, 2003, 101, 1165-1170.	0.8	1
57	Re-integration with anchor points algorithm for ab initio molecular dynamics. Journal of Chemical Physics, 2021, 155, 074106.	1.2	1
58	Theoretical Quantitative Spectroscopy: Computer Simulation of Molecular Spectra. , 2006, , 171-183.		1