Ze-Rong Li

List of Publications by Year
in descending order

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39	453	687363 13	794594 19
papers	citations	h-index	g-index

39	39	39	492
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Kinetic Study of Thermal Decomposition of Cyclohexane. Energy & Fuels, 2012, 26, 2811-2820.	5.1	44
2	Low- and intermediate-temperature oxidation of ethylcyclohexane: A theoretical study. Combustion and Flame, 2015, 162, 4167-4182.	5.2	39
3	Identification of small molecule aggregators from large compound libraries by support vector machines. Journal of Computational Chemistry, 2010, 31, 752-763.	3.3	26
4	Pressure-Dependent Kinetics of Initial Reactions in Iso-octane Pyrolysis. Journal of Physical Chemistry A, 2015, 119, 4093-4107.	2.5	25
5	Prediction of the acute toxicity of chemical compounds to the fathead minnow by machine learning approaches. Chemometrics and Intelligent Laboratory Systems, 2010, 100, 66-73.	3.5	24
6	Pressure-dependent rate rules for intramolecular H-migration reactions of normal-alkyl cyclohexylperoxy radicals. Combustion and Flame, 2019, 204, 176-188.	5.2	24
7	Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature. Journal of Physical Chemistry A, 2017, 121, 3001-3018.	2.5	20
8	Mechanism construction and simulation for high-temperature combustion of n-propylcyclohexane. Chemical Research in Chinese Universities, 2014, 30, 480-488.	2.6	19
9	Prediction of antifungal activity by support vector machine approach. Computational and Theoretical Chemistry, 2005, 731, 73-81.	1.5	16
10	Interpretation and Application of Reaction Class Transition State Theory for Accurate Calculation of Thermokinetic Parameters Using Isodesmic Reaction Method. Journal of Physical Chemistry A, 2013, 117, 3279-3291.	2.5	15
11	Reaction of ketenyl radical with hydroxyl radical over C2H2O2 potential energy surface: A theoretical study. Combustion and Flame, 2014, 161, 885-897.	5.2	14
12	Temperature and Pressure Dependent Rate Coefficients for the Reaction of C₂H₄ + HO₂ on the C₂H₄O₂H Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 3161-3170.	2.5	14
13	Pressure-dependent rate rules for cycloaddition, intramolecular H-shift, and concerted elimination reactions of alkenyl peroxy radicals at low temperature. Physical Chemistry Chemical Physics, 2019, 21, 10693-10705.	2.8	14
14	Theoretical Study of Radicalâ€“Molecule Reactions with Negative Activation Energies in Combustion: Hydroxyl Radical Addition to Alkenes. ACS Omega, 2020, 5, 12777-12788.	3.5	14
15	Kinetic study of the formation of triphenylene from the condensation of C12H10+C6H5. Computational and Theoretical Chemistry, 2012, 985, 1-7.	2.5	13
16	Theoretical and kinetic study of reaction C2HÂ+ÂC3H6 on the C5H7 potential energy surface. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	12
17	Progress in Combustion Kinetics. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2016, 32, 131-153.	4.9	10
18	Reactions of Î²-hydroxypropyl radicals with O2 on the HOC3H6OOâ€¢ potential energy surfaces: A theoretical study. Combustion and Flame, 2020, 211, 202-217.	5.2	10

#	Article	IF	Citations
19	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO2 Elimination Reaction Class and Î²-Scission Reaction Class. Journal of Physical Chemistry A, 2021, 125, 8942-8958.	2.5	9
20	In silico identification of human pregnane X receptor activators from molecular descriptors by machine learning approaches. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 271-279.	3.5	8
21	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
22	Automatic construction of transition states and on-the-fly accurate kinetic calculations for reaction classes in automated mechanism generators. Computational and Theoretical Chemistry, 2020, 1184, 112852.	2.5	7
23	Accurate prediction of thermodynamic properties of alkyl peroxides by combining density functional theory calculation with leastâ€square calibration. Journal of Computational Chemistry, 2009, 30, 1007-1015.	3.3	6
24	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
25	Potential Energy Surface for Large Barrierless Reaction Systems: Application to the Kinetic Calculations of the Dissociation of Alkanes and the Reverse Recombination Reactions. Journal of Physical Chemistry A, 2018, 122, 4869-4881.	2.5	6
26	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
27	Rate rules for hydrogen abstraction reaction kinetics of polycyclic aromatic hydrocarbons and vinyl radical. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
28	Prediction of HIVâ€1 Protease Inhibitors Using Machine Learning Approaches. QSAR and Combinatorial Science, 2009, 28, 1346-1357.	1.4	5
29	Identification of DNA adduct formation of small molecules by molecular descriptors and machine learning methods. Molecular Simulation, 2012, 38, 259-273.	2.0	5
30	Accurate Calculation of the Energy Barriers and Rate Constants of the Large-size Molecular Reaction System for Abstraction from Alkyl Hydroperoxides. Acta Chimica Sinica, 2018, 76, 311.	1.4	5
31	Rate rules for hydrogen abstraction reaction kinetics of alkenes from allylic sites by HO2 radical. Computational and Theoretical Chemistry, 2020, 1179, 112795.	2.5	4
32	Influence of pin-fin height and diameter on flow and cooling characteristics of three-layer porous laminates: An experimental study. Experimental Heat Transfer, 0, , 1-16.	3.2	4
33	Prediction of human major histocompatibility complex class II binding peptides by continuous kernel discrimination method. Artificial Intelligence in Medicine, 2012, 55, 107-115.	6.5	3
34	Accurate Calculation of the Energy Barriers and Rate Constants of Hydrogen Abstraction from Alkanes by Hydroperoxyl Radical. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2017, 33, 763-768.	4.9	3
35	Kinetic Analysis for Reaction of Cyclopentadiene with Hydroperoxyl Radical under Low- and Medium-Temperature Combustion. Journal of Physical Chemistry A, 2020, 124, 8280-8291.	2.5	3
36	Accurate prediction of enthalpies of formation for a large set of organic compounds. Journal of Computational Chemistry, 2010, 31, 2585-2592.	3.3	2

#	Article	IF	Citations
37	Development of a detailed pyrolysis mechanism for C 1 â€“C 4 hydrocarbons under a wide range of temperature and pressure. International Journal of Chemical Kinetics, 2020, 52, 796-821.	1.6	2
38	High-Pressure-Limit Rate Coefficients for HO₂ Elimination Reactions of Hydroperoxyalkenylperoxy Radicals based on the Reaction Class Transition State Theory. ACS Omega, 2022, 7, 20020-20031.	3.5	2
39	High-pressure limit rate rules for intramolecular H-migration reactions of Î±,Î²-hydroxyalkylperoxy radicals. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0