Yulei Guan

List of Publications by Year
in descending order

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25	224	1163117	996975
papers	citations	8	15
		h-index	g-index

25	25	25	160
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Salting-Out-Assisted Liquidâ€“Liquid Extraction for Nicotine from Its Aqueous Solutions. Journal of Chemical & Engineering Data, 2022, 67, 453-462.	1.9	1
2	High-temperature thermal decomposition of iso-octane based on reactive molecular dynamics simulations. Journal of Molecular Modeling, 2022, 28, 124.	1.8	1
3	Theoretical mechanistic study on the reaction of the methoxymethyl radical with nitrogen dioxide. Journal of Molecular Modeling, 2021, 27, 18.	1.8	0
4	Initial Thermal Decomposition Mechanism of (NH₂)₂Câ•C(NO₂)(ONO) Revealed by Double-Hybrid Density Functional Calculations. ACS Omega, 2021, 6, 15292-15299.	3.5	3
5	Mechanism investigation on the reaction of methylmethoxy radical with nitrogen monoxide. Structural Chemistry, 2021, 32, 1563-1570.	2.0	0
6	Reactive molecular dynamics simulation on thermal decomposition of n-heptane and methylcyclohexane initiated by nitroethane. Fuel, 2020, 261, 116447.	6.4	22
7	Computational investigation on the reaction of dimethyl ether with nitric dioxide. II. Detailed chemical kinetic modeling. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	25
8	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
9	Investigation on the Thermal Dissociation of Vinyl Nitrite with a Saddle Point Involved. ACS Omega, 2019, 4, 16052-16061.	3.5	2
10	Computational Study of the Reaction of Dimethyl Ether with Nitric Oxide. Mechanism and Kinetic Modeling. Journal of Physical Chemistry A, 2019, 123, 26-36.	2.5	6
11	Crystal Structure, Thermal Behavior and Detonation Characterization of Bis(3,3â€dinitroazetidinâ€1â€yl)methane. Propellants, Explosives, Pyrotechnics, 2018, 43, 69-74.	1.6	2
12	Kinetic modeling for unimolecular Î²-scission of the methoxymethyl radical from quantum chemical and RRKM analyses. Combustion and Flame, 2018, 197, 243-253.	5.2	8
13	Thermodynamic Properties of the Methylmethoxy Radical with Intricate Treatment of Two-Dimensional Hindered Internal Rotations. Journal of Chemical & Engineering Data, 2018, 63, 3640-3649.	1.9	3
14	Variational Effect and Anharmonic Torsion on Kinetic Modeling for Initiation Reaction of Dimethyl Ether Combustion. Journal of Physical Chemistry A, 2017, 121, 1121-1132.	2.5	12
15	Hydrogen transfer between dimethyl ether and the methoxy radical: Understanding and kinetic modeling with anharmonic torsions. Computational and Theoretical Chemistry, 2016, 1089, 43-53.	2.5	6
16	Nonlinear parametric predictive control for the temperature control of bench-scale batch reactor. Applied Thermal Engineering, 2016, 102, 134-143.	6.0	5
17	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
18	Kinetic study of the catalytic hydrogenation of the methylcyclopentadiene dimer over Pd/C catalyst. Reaction Kinetics, Mechanisms and Catalysis, 2015, 115, 311-319.	1.7	1

#	Article	IF	Citations
19	Synergistic actions between tebuconazole ligand and Cu(<scp>ii</scp>) cation: reasons for the enhanced antifungal activity of four Cu(<scp>ii</scp>) complexes based on the fungicide tebuconazole. New Journal of Chemistry, 2015, 39, 9550-9556.	2.8	15
20	Understanding the Initial Decomposition Pathways of the nâ€Alkane/Nitroalkane Binary Mixture. Chinese Journal of Chemistry, 2013, 31, 1087-1094.	4.9	12
21	Kinetic modeling for hydrogen-abstraction reaction of methylcyclohexane with the CH3 radical. Chemical Engineering Science, 2012, 79, 200-209.	3.8	5
22	Kinetics for the hydrogenâ€abstraction of CH₄ with NO₂. Journal of Computational Chemistry, 2012, 33, 1870-1879.	3.3	2
23	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
24	Synthesis, Crystal Structure, Theoretical Calculation and Thermal Behavior of DNAZÂ·NTO. Chinese Journal of Chemistry, 2009, 27, 2284-2290.	4.9	5
25	Preparation, non-isothermal decomposition kinetics, heat capacity and adiabatic time-to-explosion of NTOÂ·DNAZ. Journal of Hazardous Materials, 2009, 169, 1068-1073.	12.4	63