Judit ZÃ¡dor

List of Publications by Year in descending order

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63	2,983	159358	168136
papers	citations	30 h-index	53 g-index

69	69	69	2322
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A theoretical investigation of the hydrolysis of uranium hexafluoride: the initiation mechanism and vibrational spectroscopy. Physical Chemistry Chemical Physics, 2022, 24, 9634-9647.	1.3	4
2	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. Progress in Energy and Combustion Science, 2021, 83, 100886.	15.8	89
3	Quantitative Detection of Products and Radical Intermediates in Low-Temperature Oxidation of Cyclopentane. Journal of Physical Chemistry A, 2021, 125, 4467-4479.	1.1	19
4	Geometry optimization speedup through a geodesic approach to internal coordinates. Journal of Chemical Physics, 2021, 155, 094105.	1.2	5
5	A New Pathway for Intersystem Crossing: Unexpected Products in the O(³P) + Cyclopentene Reaction. Journal of Physical Chemistry A, 2021, 125, 9785-9801.	1.1	7
6	KinBot: Automated stationary point search on potential energy surfaces. Computer Physics Communications, 2020, 248, 106947.	3.0	80
7	Simulated production of OH, HO2, CH2O, and CO2 during dilute fuel oxidation can predict 1st-stage ignition delays. Combustion and Flame, 2020, 216, 472-484.	2.8	12
8	A Filon-like integration strategy for calculating exact exchange in periodic boundary conditions: a plane-wave DFT implementation. Materials Theory, 2020, 4, .	2.2	5
9	Accelerated Saddle Point Refinement through Full Exploitation of Partial Hessian Diagonalization. Journal of Chemical Theory and Computation, 2019, 15, 6536-6549.	2.3	18
10	Comment on â€œInfluence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicalsâ€• Journal of Physical Chemistry A, 2019, 123, 1129-1130.	1.1	1
11	Direct measurement of Ë™OH and HO₂Ë™ formation in Ë™R + O₂ reactions of cyclohexane and tetrahydropyran. Physical Chemistry Chemical Physics, 2018, 20, 10815-10825.	1.3	13
12	Unimolecular Reaction Pathways of a Î³-Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. Journal of the American Chemical Society, 2018, 140, 1035-1048.	6.6	82
13	Decomposition and isomerization of 1-pentanol radicals and the pyrolysis of 1-pentanol. Combustion and Flame, 2018, 196, 500-514.	2.8	23
14	Thermochemistry of the smallest QOOH radical from the roaming fragmentation of energy selected methyl hydroperoxide ions. Physical Chemistry Chemical Physics, 2018, 20, 21085-21094.	1.3	6
15	Influence of oxygenation in cyclic hydrocarbons on chain-termination reactions from R + O2: tetrahydropyran and cyclohexane. Proceedings of the Combustion Institute, 2017, 36, 597-606.	2.4	33
16	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	2.4	42
17	Initiation Reactions in Acetylene Pyrolysis. Journal of Physical Chemistry A, 2017, 121, 4203-4217.	1.1	22
18	Photoionization Efficiencies of Five Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2017, 121, 4447-4454.	1.1	8

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19	Critical Assessment of Photoionization Efficiency Measurements for Characterization of Soot-Precursor Species. Journal of Physical Chemistry A, 2017, 121, 4475-4485.	1.1	18
20	Elucidating reactivity regimes in cyclopentane oxidation: Jet stirred reactor experiments, computational chemistry, and kinetic modeling. Proceedings of the Combustion Institute, 2017, 36, 469-477.	2.4	34
21	Pressure-Dependent Competition among Reaction Pathways from First- and Second-O₂ Additions in the Low-Temperature Oxidation of Tetrahydrofuran. Journal of Physical Chemistry A, 2016, 120, 6582-6595.	1.1	40
22	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	1.1	30
23	Direct observation and kinetics of a hydroperoxyalkyl radical (QOOH). Science, 2015, 347, 643-646.	6.0	130
24	A Combined Experimental and Theoretical Study of the Reaction OH + 2-Butene in the 400â€“800 K Temperature Range. Journal of Physical Chemistry A, 2015, 119, 7742-7752.	1.1	21
25	Multiscale Informatics for Low-Temperature Propane Oxidation: Further Complexities in Studies of Complex Reactions. Journal of Physical Chemistry A, 2015, 119, 7095-7115.	1.1	37
26	Threshold photoelectron spectrum of the benzyl radical. Molecular Physics, 2015, 113, 2217-2227.	0.8	32
27	Adventures on the C3H5O potential energy surface: OH + propyne, OH + allene and related reactions. Proceedings of the Combustion Institute, 2015, 35, 181-188.	2.4	42
28	Probing the low-temperature chain-branching mechanism of n -butane autoignition chemistry via time-resolved measurements of ketohydroperoxide formation in photolytically initiated n- C 4 H 10 oxidation. Proceedings of the Combustion Institute, 2015, 35, 291-298.	2.4	48
29	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.	1.1	19
30	Low-temperature combustion chemistry of novel biofuels: resonance-stabilized QOOH in the oxidation of diethyl ketone. Physical Chemistry Chemical Physics, 2014, 16, 13027-13040.	1.3	25
31	First principles study of photo-oxidation degradation mechanisms in P3HT for organic solar cells. Physical Chemistry Chemical Physics, 2014, 16, 8092-8099.	1.3	70
32	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	2.1	38
33	Low-Temperature Combustion Chemistry of n-Butanol: Principal Oxidation Pathways of Hydroxybutyl Radicals. Journal of Physical Chemistry A, 2013, 117, 11983-12001.	1.1	40
34	Directly measuring reaction kinetics of Ë™QOOH â€“ a crucial but elusive intermediate in hydrocarbon autoignition. Physical Chemistry Chemical Physics, 2013, 15, 10753.	1.3	58
35	Uncertainty quantification in the ab initio rate-coefficient calculation for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mtext>+</mml:mtext><mml:msub><mml:mrow><mml:mtext>O</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> reaction. Proceedings of the Combustion Institute, 2013, 34, 583-590.	2.4	36
36	Unimolecular dissociation of hydroxypropyl and propoxy radicals. Proceedings of the Combustion Institute, 2013, 34, 519-526.	2.4	21

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37	Low-temperature combustion chemistry of biofuels: pathways in the initial low-temperature (550) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	88
38	Pressure-Dependent OH Yields in Alkene + HO₂ Reactions: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10218-10225.	1.1	56
39	Competing Channels in the Propene + OH Reaction: Experiment and Validated Modeling over a Broad Temperature and Pressure Range. Zeitschrift Fur Physikalische Chemie, 2011, 225, 1271-1291.	1.4	14
40	New experiments and validated master-equation modeling for OH production in propyl+O2 reactions. Proceedings of the Combustion Institute, 2011, 33, 293-299.	2.4	35
41	Kinetics of elementary reactions in low-temperature autoignition chemistry. Progress in Energy and Combustion Science, 2011, 37, 371-421.	15.8	586
42	OH yields for C2H5CO+O2 at low pressure: Experiment and theory. Chemical Physics Letters, 2010, 495, 179-181.	1.2	4
43	High-Temperature Measurements and a Theoretical Study of the Reaction of OH with 1,3-Butadiene. Journal of Physical Chemistry A, 2010, 114, 8312-8318.	1.1	24
44	The reaction of hydroxyethyl radicals with O2: A theoretical analysis and experimental product study. Proceedings of the Combustion Institute, 2009, 32, 271-277.	2.4	90
45	Temperature-Dependent Kinetics of the Vinyl Radical (C₂H₃) Self-Reaction. Journal of Physical Chemistry A, 2009, 113, 1278-1286.	1.1	27
46	The reaction between propene and hydroxyl. Physical Chemistry Chemical Physics, 2009, 11, 11040.	1.3	147
47	Formally direct pathways and low-temperature chain branching in hydrocarbon autoignition: the cyclohexyl + O2 reaction at high pressure. Physical Chemistry Chemical Physics, 2009, 11, 1320.	1.3	76
48	Rate constant for the reaction of bromine atoms with ethane: Kinetic and thermochemical implications. Reaction Kinetics and Catalysis Letters, 2008, 95, 355-363.	0.6	2
49	Analysis of a budding yeast cell cycle model using the shapes of local sensitivity functions. International Journal of Chemical Kinetics, 2008, 40, 710-720.	1.0	17
50	Uncertainty analysis of NO production during methane combustion. International Journal of Chemical Kinetics, 2008, 40, 754-768.	1.0	55
51	Kinetics and mechanism of the reactions of CH3CO and CH3C(O)CH2 radicals with O2. Low-pressure discharge flow experiments and quantum chemical computations. Physical Chemistry Chemical Physics, 2007, 9, 4142.	1.3	26
52	Local and global uncertainty analysis of complex chemical kinetic systems. Reliability Engineering and System Safety, 2006, 91, 1232-1240.	5.1	81
53	Measurement and investigation of chamber radical sources in the European Photoreactor (EUPHORE). Journal of Atmospheric Chemistry, 2006, 55, 147-166.	1.4	38
54	Time scale and dimension analysis of a budding yeast cell cycle model. BMC Bioinformatics, 2006, 7, 494.	1.2	34

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55	Quantitative assessment of uncertainties for a model of tropospheric ethene oxidation using the European Photoreactor (EUPHORE). Atmospheric Environment, 2005, 39, 2805-2817.	1.9	29
56	Uncertainty analysis of updated hydrogen and carbon monoxide oxidation mechanisms. Proceedings of the Combustion Institute, 2005, 30, 1273-1281.	2.4	97
57	On the similarity of the sensitivity functions of methane combustion models. Combustion Theory and Modelling, 2005, 9, 721-738.	1.0	16
58	Local and Global Uncertainty Analyses of a Methane Flame Model. Journal of Physical Chemistry A, 2005, 109, 9795-9807.	1.1	90
59	Investigation of the correlation of sensitivity vectors of hydrogen combustion models. International Journal of Chemical Kinetics, 2004, 36, 238-252.	1.0	10
60	OH and HO₂ chemistry in clean marine air during SOAPEX-2. Atmospheric Chemistry and Physics, 2004, 4, 839-856.	1.9	92
61	Similarity of Sensitivity Functions of Reaction Kinetic Models. Journal of Physical Chemistry A, 2003, 107, 2216-2238.	1.1	26
62	Unimolecular isomerisation of 1,5-hexadiyne observed by threshold photoelectron photoion coincidence spectroscopy. Faraday Discussions, 0, 238, 645-664.	1.6	6
63	Stereoisomer-dependent unimolecular kinetics of 2,4-dimethyloxetanyl peroxy radicals. Faraday Discussions, 0, 238, 295-319.	1.6	9