Stephen J Klippenstein

List of Publications by Year
in descending order

308	24,000	5434	10107
papers	citations	84 h-index	142 g-index

318	318	318	11069
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An experimental, theoretical, and kinetic modeling study of post-flame oxidation of ammonia. Combustion and Flame, 2024, 261, 113325.	5.3	2
2	Tribute to Marsha I. Lester. Journal of Physical Chemistry A, 2024, 128, 501-502.	2.6	0
3	Observational evidence for Criegee intermediate oligomerization reactions relevant to aerosol formation in the troposphere. Nature Geoscience, 2024, 17, 219-226.	11.9	2
4	Isomer-resolved unimolecular dynamics of the hydroperoxyalkyl intermediate (â€¢QOOH) in cyclohexane oxidation. Proceedings of the National Academy of Sciences of the United States of America, 2024, 121, .	7.6	1
5	The role of stereochemistry in combustion processes. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2024, 14, .	16.9	1
6	Quasi-Classical Trajectory Calculation of Rate Constants Using an Ab Initio Trained Machine Learning Model (aML-MD) with Multifidelity Data. Journal of Physical Chemistry A, 2024, 128, 3449-3457.	2.6	0
7	Radical Stereochemistry: Accounting for Diastereomers in Kinetic Mechanism Development. Journal of Physical Chemistry A, 2024, 128, 3711-3725.	2.6	0
8	High-pressure oxidation of hydrogen diluted in N2 with added H2O or CO2 at 100 atm in a supercritical-pressure jet-stirred reactor. Combustion and Flame, 2024, 266, 113543.	5.3	0
9	Resolving discrepancies between theory and experiment for the NCN + H reaction. Proceedings of the Combustion Institute, 2024, 40, 105403.	4.5	0
10	Infrared signature of the hydroperoxyalkyl intermediate (Â·QOOH) in cyclohexane oxidation: An isomer-resolved spectroscopic study. Journal of Chemical Physics, 2024, 161, .	3.1	0
11	High pressure ammonia/methanol oxidation up to 100 atm. Proceedings of the Combustion Institute, 2024, 40, 105489.	4.5	0
12	Systematic exploration of the thermochemistry for a set of peroxy hydroperoxy-alkyl radicals. Proceedings of the Combustion Institute, 2024, 40, 105618.	4.5	0
13	On the prediction of pressure effects for the combination kinetics of two alkyl radicals with the geometric mean rule. Proceedings of the Combustion Institute, 2024, 40, 105380.	4.5	0
14	Competing radical and molecular channels in the unimolecular dissociation of methylformate. Proceedings of the Combustion Institute, 2024, 40, 105684.	4.5	0
15	The influence of thermochemistry on the reactivity of propane, the pentane isomers and n-heptane in the low temperature regime. Proceedings of the Combustion Institute, 2023, 39, 653-662.	4.5	3
16	Automated identification and calculation of prompt effects in kinetic mechanisms using statistical models. Combustion and Flame, 2023, 257, 112422.	5.3	4
17	Group additivity values for the heat of formation of C2â€“C8 alkanes, alkyl hydroperoxides, and their radicals. Combustion and Flame, 2023, 257, 112492.	5.3	9
18	A wide range experimental study and further development of a kinetic model describing propane oxidation. Combustion and Flame, 2023, 248, 112562.	5.3	17

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19	The role of energy transfer and competing bimolecular reactions in characterizing the unimolecular dissociations of allylic radicals. Combustion and Flame, 2023, 257, 112502.	5.3	3
20	Bimolecular Peroxy Radical (RO₂) Reactions and Their Relevance in Radical Initiated Oxidation of Hydrocarbons. Journal of Physical Chemistry A, 2023, 127, 300-315.	2.6	1
21	Systematically derived thermodynamic properties for alkane oxidation. Combustion and Flame, 2023, 257, 112487.	5.3	8
22	High-Accuracy Heats of Formation for Alkane Oxidation: From Small to Large via the Automated CBH-ANL Method. Journal of Physical Chemistry A, 2023, 127, 1512-1531.	2.6	16
23	Radicalâ€“Radical Reactions in Molecular Weight Growth: The Phenyl + Propargyl Reaction. Journal of Physical Chemistry A, 2023, 127, 2577-2590.	2.6	4
24	Group additivity values for entropy and heat capacities of C2â€“C8 alkanes, alkyl hydroperoxides, and their radicals. Combustion and Flame, 2023, 257, 112706.	5.3	2
25	Combustion in a Sustainable World: From Molecules to Processes. Journal of Physical Chemistry A, 2023, 127, 3737-3742.	2.6	0
26	OH Roaming and Beyond in the Unimolecular Decay of the Methyl-Ethyl-Substituted Criegee Intermediate: Observations and Predictions. Journal of the American Chemical Society, 2023, 145, 19405-19420.	14.6	8
27	Dedication to James A. Miller. Combustion and Flame, 2023, 257, 113013.	5.3	0
28	Theoretical Kinetics Predictions for Reactions on the NH₂O Potential Energy Surface. Journal of Physical Chemistry A, 2023, 127, 8650-8662.	2.6	6
29	Uncovering novel liquid organic hydrogen carriers: a systematic exploration of chemical compound space using cheminformatics and quantum chemical methods. Digital Discovery, 2023, 2, 1813-1830.	5.7	2
30	Bimolecular Reaction of Methyl-Ethyl-Substituted Criegee Intermediate with SO₂. Journal of Physical Chemistry A, 2023, 127, 8994-9002.	2.6	3
31	Modelingâ€“Experimentâ€“Theory Analysis of Reactions Initiated from Cl + Methyl Formate. Journal of Physical Chemistry A, 2023, 127, 9804-9819.	2.6	0
32	Quantum and anharmonic effects in non-adiabatic transition state theory. Journal of Chemical Physics, 2023, 159, .	3.1	2
33	OH Roaming during the Ozonolysis of Î±-Pinene: A New Route to Highly Oxygenated Molecules?. Journal of Physical Chemistry A, 2023, 127, 10647-10662.	2.6	1
34	Theoretical kinetics predictions for NH2Â+ÂHO2. Combustion and Flame, 2022, 236, 111787.	5.3	45
35	HÈ®2Â+ÂHÈ®2: High level theory and the role of singlet channels. Combustion and Flame, 2022, 243, 111975.	5.3	32
36	Infrared spectroscopic signature of a hydroperoxyalkyl radical (â€¢QOOH). Journal of Chemical Physics, 2022, 156, 014301.	3.1	13

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37	Low- and intermediate-temperature oxidation of dimethyl ether up to 100 atm in a supercritical pressure jet-stirred reactor. Combustion and Flame, 2022, 243, 112059.	5.3	21
38	Rapid Allylic 1,6 H-Atom Transfer in an Unsaturated Criegee Intermediate. Journal of the American Chemical Society, 2022, 144, 5945-5955.	14.6	9
39	Dramatic Conformer-Dependent Reactivity of the Acetaldehyde Oxide Criegee Intermediate with Dimethylamine Via a 1,2-Insertion Mechanism. Journal of Physical Chemistry A, 2022, 126, 710-719.	2.6	6
40	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. Proceedings of the Combustion Institute, 2021, 38, 375-384.	4.5	34
41	Termolecular chemistry facilitated by radical-radical recombinations and its impact on flame speed predictions. Proceedings of the Combustion Institute, 2021, 38, 515-522.	4.5	15
42	Low-temperature oxidation of diethyl ether: Reactions of hot radicals across coupled potential energy surfaces. Proceedings of the Combustion Institute, 2021, 38, 671-679.	4.5	16
43	Substitution Reactions in the Pyrolysis of Acetone Revealed through a Modeling, Experiment, Theory Paradigm. Journal of the American Chemical Society, 2021, 143, 3124-3142.	14.6	33
44	Functionalized Hydroperoxide Formation from the Reaction of Methacrolein-Oxide, an Isoprene-Derived Criegee Intermediate, with Formic Acid: Experiment and Theory. Molecules, 2021, 26, 3058.	3.9	16
45	Entanglement Effect and Angular Momentum Conservation in a Nonseparable Tunneling Treatment. Journal of Chemical Theory and Computation, 2021, 17, 3863-3885.	5.6	5
46	Watching a hydroperoxyalkyl radical (â€¢QOOH) dissociate. Science, 2021, 373, 679-682.	20.9	38
47	Diastereomers and Low-Temperature Oxidation. Journal of Physical Chemistry A, 2021, 125, 8064-8073.	2.6	13
48	Non-Boltzmann Effects in Chain Branching and Pathway Branching for Diethyl Ether Oxidation. Energy & Fuels, 2021, 35, 17890-17908.	5.2	16
49	Photodissociation transition states characterized by chirped pulse millimeter wave spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 146-151.	7.6	11
50	Formic acid catalyzed isomerization and adduct formation of an isoprene-derived Criegee intermediate: experiment and theory. Physical Chemistry Chemical Physics, 2020, 22, 26796-26805.	2.9	13
51	Experimental and theoretical studies of the doubly substituted methyl-ethyl Criegee intermediate: Infrared action spectroscopy and unimolecular decay to OH radical products. Journal of Chemical Physics, 2020, 152, 094301.	3.1	18
52	Reaction Profiles and Kinetics for Radicalâ€“Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 1511-1525.	5.6	9
53	Direct kinetic measurements and theoretical predictions of an isoprene-derived Criegee intermediate. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 9733-9740.	7.6	70
54	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. Proceedings of the Combustion Institute, 2019, 37, 363-371.	4.5	70

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55	Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate. Proceedings of the Combustion Institute, 2019, 37, 419-428.	4.5	48
56	High-pressure oxidation of propane. Proceedings of the Combustion Institute, 2019, 37, 461-468.	4.5	50
57	Kinetics of 1-butyl and 2-butyl radical reactions with molecular oxygen: Experiment and theory. Proceedings of the Combustion Institute, 2019, 37, 291-298.	4.5	16
58	Propane clusters in Titanâ€™s lower atmosphere: insights from a combined theory/laboratory study. Monthly Notices of the Royal Astronomical Society, 2019, 488, 676-684.	4.6	2
59	Synthesis, Electronic Spectroscopy, and Photochemistry of Methacrolein Oxide: A Four-Carbon Unsaturated Criegee Intermediate from Isoprene Ozonolysis. Journal of the American Chemical Society, 2019, 141, 15058-15069.	14.6	55
60	Ab initio kinetics for pyrolysis and combustion systems. Computer Aided Chemical Engineering, 2019, , 115-167.	0.1	29
61	Nonthermal rate constants for CH4* + X â†' CH3 + HX, X = H, O, OH, and O2. Journal of Chemical Physics, 2019, 150, 114112.	3.1	22
62	Simulating the density of organic species in the atmosphere of Titan with a coupled ion-neutral photochemical model. Icarus, 2019, 324, 120-197.	2.5	139
63	EStokTP: Electronic Structure to Temperature- and Pressure-Dependent Rate Constantsâ€"A Code for Automatically Predicting the Thermal Kinetics of Reactions. Journal of Chemical Theory and Computation, 2019, 15, 1122-1145.	5.6	95
64	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	32.4	1,151
65	Unimolecular Decay of Criegee Intermediates to OH Radical Products: Prompt and Thermal Decay Processes. Accounts of Chemical Research, 2018, 51, 978-985.	16.6	105
66	H-Abstraction reactions by OH, HO₂, O, O₂ and benzyl radical addition to O₂ and their implications for kinetic modelling of toluene oxidation. Physical Chemistry Chemical Physics, 2018, 20, 10607-10627.	2.9	93
67	Anharmonic Rovibrational Partition Functions for Fluxional Species at High Temperatures via Monte Carlo Phase Space Integrals. Journal of Physical Chemistry A, 2018, 122, 1727-1740.	2.6	15
68	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	3.1	38
69	Theory and modeling of relevance to prompt-NO formation at high pressure. Combustion and Flame, 2018, 195, 3-17.	5.3	60
70	Four-Carbon Criegee Intermediate from Isoprene Ozonolysis: Methyl Vinyl Ketone Oxide Synthesis, Infrared Spectrum, and OH Production. Journal of the American Chemical Society, 2018, 140, 10866-10880.	14.6	116
71	Recombination of aromatic radicals with molecular oxygen. Proceedings of the Combustion Institute, 2017, 36, 169-177.	4.5	21
72	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	4.5	48

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73	First-Principles Chemical Kinetic Modeling of Methyl trans-3-Hexenoate Epoxidation by HO₂. Journal of Physical Chemistry A, 2017, 121, 1909-1915.	2.6	7
74	High-pressure oxidation of ethane. Combustion and Flame, 2017, 182, 150-166.	5.3	77
75	Accurate Anharmonic Zero-Point Energies for Some Combustion-Related Species from Diffusion Monte Carlo. Journal of Physical Chemistry A, 2017, 121, 4334-4340.	2.6	22
76	Tunneling effects in the unimolecular decay of (CH3)2COO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2017, 146, 134307.	3.1	35
77	Theoretical Kinetics Analysis for á¸¢ Atom Addition to 1,3-Butadiene and Related Reactions on the ÄŠ₄H₇ Potential Energy Surface. Journal of Physical Chemistry A, 2017, 121, 7433-7445.	2.6	61
78	Ab Initio Computations and Active Thermochemical Tables Hand in Hand: Heats of Formation of Core Combustion Species. Journal of Physical Chemistry A, 2017, 121, 6580-6602.	2.6	151
79	Ephemeral collision complexes mediate chemically termolecular transformations that affect system chemistry. Nature Chemistry, 2017, 9, 1078-1082.	14.3	93
80	Time-Resolved Kinetic Chirped-Pulse Rotational Spectroscopy in a Room-Temperature Flow Reactor. Journal of Physical Chemistry Letters, 2017, 8, 6180-6188.	4.9	19
81	Selective deuteration illuminates the importance of tunneling in the unimolecular decay of Criegee intermediates to hydroxyl radical products. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12372-12377.	7.6	35
82	From theoretical reaction dynamics to chemical modeling of combustion. Proceedings of the Combustion Institute, 2017, 36, 77-111.	4.5	215
83	Ramifications of including non-equilibrium effects for HCO in flame chemistry. Proceedings of the Combustion Institute, 2017, 36, 525-532.	4.5	38
84	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. Proceedings of the Combustion Institute, 2017, 36, 919-926.	4.5	126
85	Theoretical investigation of intersystem crossing in the cyanonitrene molecule, 1NCN â†'â€ˆ3NCN. Journal of Chemical Physics, 2017, 147, 084310.	3.1	6
86	Communication: Real time observation of unimolecular decay of Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 144, 061102.	3.1	104
87	Deep tunneling in the unimolecular decay of CH3CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 234308.	3.1	61
88	Direct observation of unimolecular decay of CH3CH2CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 044312.	3.1	50
89	Pressure dependent low temperature kinetics for CN + CH₃CN: competition between chemical reaction and van der Waals complex formation. Physical Chemistry Chemical Physics, 2016, 18, 15118-15132.	2.9	21
90	High-pressure oxidation of methane. Combustion and Flame, 2016, 172, 349-364.	5.3	168

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91	Low Temperature Kinetics of the First Steps of Water Cluster Formation. Physical Review Letters, 2016, 116, 113401.	8.0	27
92	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. Faraday Discussions, 2016, 195, 637-670.	3.7	81
93	Weakly Bound Free Radicals in Combustion: â€œPromptâ€•Dissociation of Formyl Radicals and Its Effect on Laminar Flame Speeds. Journal of Physical Chemistry Letters, 2016, 7, 85-89.	4.9	69
94	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	2.6	32
95	Dimethylamine Addition to Formaldehyde Catalyzed by a Single Water Molecule: A Facile Route for Atmospheric Carbinolamine Formation and Potential Promoter of Aerosol Growth. Journal of Physical Chemistry A, 2016, 120, 1358-1368.	2.6	41
96	Ab initio Variational Transition State Theory and Master Equation Study of the Reaction (OH)₃SiOCH₂â€+â€CH₃â€â‡Œâ€(OH)₃SiOC₂H₅. Zeitschrift Fur Physikalische Chemie, 2015, 229, 691-708.	2.6	8
97	Comment on â€œA novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition statesâ€•[J. Chem. Phys. 142, 124312 (2015)]. Journal of Chemical Physics, 2015, 143, 167101.	3.1	3
98	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	2.6	89
99	Towards a quantitative understanding of the role of non-Boltzmann reactant distributions in low temperature oxidation. Proceedings of the Combustion Institute, 2015, 35, 205-213.	4.5	48
100	The role of radical + fuel-radical well-skipping reactions in ethanol and methylformate low-pressure flames. Proceedings of the Combustion Institute, 2015, 35, 447-455.	4.5	30
101	Hydrolysis of Ketene Catalyzed by Formic Acid: Modification of Reaction Mechanism, Energetics, and Kinetics with Organic Acid Catalysis. Journal of Physical Chemistry A, 2015, 119, 4347-4357.	2.6	48
102	Effects of New Ab Initio Rate Coefficients on Predictions of Species Formed duringn-Butanol Ignition and Pyrolysis. Journal of Physical Chemistry A, 2015, 119, 543-551.	2.6	7
103	Pressure-dependent branching in the reaction of 1 CH 2 with C 2 H 4 and other reactions on the C 3 H 6 potential energy surface. Proceedings of the Combustion Institute, 2015, 35, 223-230.	4.5	32
104	A Tribute to Lawrence B. Harding, Joe V. Michael, and Albert F. Wagner for Their 100 Years of Combustion Kinetics Studies at Argonne. Journal of Physical Chemistry A, 2015, 119, 7075-7077.	2.6	2
105	Multiscale Informatics for Low-Temperature Propane Oxidation: Further Complexities in Studies of Complex Reactions. Journal of Physical Chemistry A, 2015, 119, 7095-7115.	2.6	39
106	Global uncertainty analysis for RRKM/master equation based kinetic predictions: A case study of ethanol decomposition. Combustion and Flame, 2015, 162, 3427-3436.	5.3	34
107	New Insights into Low-Temperature Oxidation of Propane from Synchrotron Photoionization Mass Spectrometry and Multiscale Informatics Modeling. Journal of Physical Chemistry A, 2015, 119, 7116-7129.	2.6	37
108	Kinetics of Propargyl Radical Dissociation. Journal of Physical Chemistry A, 2015, 119, 7780-7791.	2.6	36

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109	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.6	61
110	Resolving Some Paradoxes in the Thermal Decomposition Mechanism of Acetaldehyde. Journal of Physical Chemistry A, 2015, 119, 7724-7733.	2.6	33
111	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	5.3	128
112	THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY. Astrophysical Journal, Supplement Series, 2015, 217, 20.	8.1	304
113	Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. Proceedings of the Combustion Institute, 2015, 35, 283-290.	4.5	58
114	Secondary channels in the thermal decomposition of monomethylhydrazine (CH₃NHNH₂). RSC Advances, 2014, 4, 62951-62964.	3.7	3
115	First-principles binary diffusion coefficients for H, H2, and four normal alkanes + N2. Journal of Chemical Physics, 2014, 141, 124313.	3.1	45
116	Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Ââ†'ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.5	22
117	Chemical Kinetics and Mechanisms of Complex Systems: AÂPerspective on Recent Theoretical Advances. Journal of the American Chemical Society, 2014, 136, 528-546.	14.6	223
118	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	4.9	39
119	Collision Efficiency of Water in the Unimolecular Reaction CH₄ (+H₂O) â‡† CH₃ + H (+H₂O): One-Dimensional and Two-Dimensional Solutions of the Low-Pressure-Limit Master Equation. Journal of Physical Chemistry A, 2013, 117, 12243-12255.	2.6	66
120	Uncertainty propagation in the derivation of phenomenological rate coefficients from theory: A case study of n-propyl radical oxidation. Proceedings of the Combustion Institute, 2013, 34, 177-185.	4.5	66
121	Theoretical kinetics for the decomposition of iso-butanol and related <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si14.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">)</mml:mo></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mi mathvariant="normal">H</mml:mi><mml:mi mathvariant="normal">O</mml:mi><mml:mi mathvariant="normal">H</mml:mi></mml:mrow></mml:math> isomers. Proceedings of the Combustion Institute, 2013, 34, 547-555.	4.5	17
122	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 12146-12154.	2.6	499
123	A quantitative explanation for the apparent anomalous temperature dependence of OH + HO2= H2O + O2 through multi-scale modeling. Proceedings of the Combustion Institute, 2013, 34, 547-555.	4.5	75
124	Determining phenomenological rate coefficients from a time-dependent, multiple-well master equation: â€œspecies reductionâ€•at high temperatures. Physical Chemistry Chemical Physics, 2013, 15, 4744.	2.9	76
125	Low Temperature Rate Coefficients for the Reaction CN + HC₃N. Journal of Physical Chemistry A, 2013, 117, 12155-12164.	2.6	20
126	Dissociation of Propyl Radicals and Other Reactions on a C₃H₇ Potential. Journal of Physical Chemistry A, 2013, 117, 2718-2727.	2.6	77

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127	Ab Initio Kinetics for the Decomposition of Hydroxybutyl and Butoxy Radicals ofn-Butanol. Journal of Physical Chemistry A, 2013, 117, 1890-1906.	2.6	59
128	Propargyl + O₂ Reaction in Helium Droplets: Entrance Channel Barrier or Not?. Journal of Physical Chemistry A, 2013, 117, 13626-13635.	2.6	41
129	Rate Constant and Branching Fraction for the NH₂ + NO₂ Reaction. Journal of Physical Chemistry A, 2013, 117, 9011-9022.	2.6	43
130	Predictive Theory for the Addition and Insertion Kinetics of ¹CH₂ Reacting with Unsaturated Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 12677-12692.	2.6	22
131	A KINETIC DATABASE FOR ASTROCHEMISTRY (KIDA). Astrophysical Journal, Supplement Series, 2012, 199, 21.	8.1	449
132	RAPID ASSOCIATION REACTIONS AT LOW PRESSURE: IMPACT ON THE FORMATION OF HYDROCARBONS ON TITAN. Astrophysical Journal, 2012, 744, 11.	4.7	56
133	Shock Tube Explorations of Roaming Radical Mechanisms: The Decompositions of Isobutane and Neopentane. Journal of Physical Chemistry A, 2012, 116, 5981-5989.	2.6	34
134	Role of O₂ + QOOH in Low-Temperature Ignition of Propane. 1. Temperature and Pressure Dependent Rate Coefficients. Journal of Physical Chemistry A, 2012, 116, 3325-3346.	2.6	237
135	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	2.6	49
136	Exploring formation pathways of aromatic compounds in laboratory-based model flames of aliphatic fuels. Combustion, Explosion and Shock Waves, 2012, 48, 508-515.	0.8	69
137	Comment on â€œAutomatic estimation of pressure-dependent rate coefficientsâ€•(J. W. Allen, C. F.) Tj ETQq1 1 0.784314 rgBT /Over Physics, 2012, 14, 8431.	2.9	8
138	Comprehensive H₂/O₂ kinetic model for highâ€pressure combustion. International Journal of Chemical Kinetics, 2012, 44, 444-474.	1.7	733
139	Pressure-Dependent OH Yields in Alkene + HO₂ Reactions: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10218-10225.	2.6	56
140	Statistical Theory for the Kinetics and Dynamics of Roaming Reactions. Journal of Physical Chemistry A, 2011, 115, 14370-14381.	2.6	77
141	Shock Tube and Theoretical Studies on the Thermal Decomposition of Propane: Evidence for a Roaming Radical Channel. Journal of Physical Chemistry A, 2011, 115, 3366-3379.	2.6	60
142	Combustion Chemistry: Important Features of the C₃H₅ Potential Energy Surface, Including Allyl Radical, Propargyl + H₂, Allene + H, and Eight Transition States. Journal of Physical Chemistry A, 2011, 115, 14209-14214.	2.6	26
143	Long-Range Interaction Potential of Open Shell Atoms with Neutral Molecules : Application to the Calculation of the Rate Constant for the C2H(2Î£+)+O(3P) Reaction. Proceedings of the International Astronomical Union, 2011, 7, 372-382.	0.0	2
144	Insights into the role of polycyclic aromatic hydrocarbon condensation in haze formation in Jupiterâ€™s atmosphere. Astronomy and Astrophysics, 2011, 532, A40.	5.3	10

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145	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	14.3	62
146	Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory. Combustion and Flame, 2011, 158, 618-632.	5.3	92
147	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	4.5	77
148	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	5.3	329
149	Ab initio kinetics for the decomposition of monomethylhydrazine (CH3NHNH2). Proceedings of the Combustion Institute, 2011, 33, 425-432.	4.5	21
150	Uncertainty driven theoretical kinetics studies for CH3OH ignition: HO2+CH3OH and O2+CH3OH. Proceedings of the Combustion Institute, 2011, 33, 351-357.	4.5	153
151	DISEQUILIBRIUM CARBON, OXYGEN, AND NITROGEN CHEMISTRY IN THE ATMOSPHERES OF HD 189733b AND HD 209458b. Astrophysical Journal, 2011, 737, 15.	4.7	389
152	Insights into the condensation of PAHsin the envelope of IRC +10216. EAS Publications Series, 2011, 46, 191-199.	0.3	1
153	The Effect of Spinâ^'Orbit Splitting on the Association Kinetics of Barrierless Halogen Atomâ^'Hydrocarbon Radical Reactions. Journal of Physical Chemistry A, 2010, 114, 5759-5768.	2.6	40
154	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	2.6	67
155	Exploring the Role of PAHs in the Formation of Soot: Pyrene Dimerization. Journal of Physical Chemistry Letters, 2010, 1, 2962-2967.	4.9	161
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