Stephen J Klippenstein

List of Publications by Year
in descending order

276	22,853	5574 82	10445 139
papers	citations	h-index	g-index

281	281	281	9018
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical kinetics predictions for NH2Â+ÂHO2. Combustion and Flame, 2022, 236, 111787.	5.2	41
2	HÈ®2Â+ÂHÈ®2: High level theory and the role of singlet channels. Combustion and Flame, 2022, 243, 111975.	5.2	23
3	Infrared spectroscopic signature of a hydroperoxyalkyl radical (â€¢QOOH). Journal of Chemical Physics, 2022, 156, 014301.	3.0	8
4	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.	5.2	16
5	Rapid Allylic 1,6 H-Atom Transfer in an Unsaturated Criegee Intermediate. Journal of the American Chemical Society, 2022, 144, 5945-5955.	13.7	5
6	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.	2.5	4
7	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. Proceedings of the Combustion Institute, 2021, 38, 375-384.	3.9	28
8	Termolecular chemistry facilitated by radical-radical recombinations and its impact on flame speed predictions. Proceedings of the Combustion Institute, 2021, 38, 515-522.	3.9	15
9	Low-temperature oxidation of diethyl ether: Reactions of hot radicals across coupled potential energy surfaces. Proceedings of the Combustion Institute, 2021, 38, 671-679.	3.9	16
10	Substitution Reactions in the Pyrolysis of Acetone Revealed through a Modeling, Experiment, Theory Paradigm. Journal of the American Chemical Society, 2021, 143, 3124-3142.	13.7	28
11	Functionalized Hydroperoxide Formation from the Reaction of Methacrolein-Oxide, an Isoprene-Derived Criegee Intermediate, with Formic Acid: Experiment and Theory. Molecules, 2021, 26, 3058.	3.8	16
12	Entanglement Effect and Angular Momentum Conservation in a Nonseparable Tunneling Treatment. Journal of Chemical Theory and Computation, 2021, 17, 3863-3885.	5.3	4
13	Watching a hydroperoxyalkyl radical (â€¢QOOH) dissociate. Science, 2021, 373, 679-682.	12.6	31
14	Diastereomers and Low-Temperature Oxidation. Journal of Physical Chemistry A, 2021, 125, 8064-8073.	2.5	11
15	Non-Boltzmann Effects in Chain Branching and Pathway Branching for Diethyl Ether Oxidation. Energy & Fuels, 2021, 35, 17890-17908.	5.1	16
16	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.	7.1	11
17	Formic acid catalyzed isomerization and adduct formation of an isoprene-derived Criegee intermediate: experiment and theory. Physical Chemistry Chemical Physics, 2020, 22, 26796-26805.	2.8	13
18	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.	3.0	17

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19	Reaction Profiles and Kinetics for Radicalâ€“Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 1511-1525.	5.3	8
20	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.	7.1	63
21	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. Proceedings of the Combustion Institute, 2019, 37, 363-371.	3.9	62
22	Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate. Proceedings of the Combustion Institute, 2019, 37, 419-428.	3.9	45
23	High-pressure oxidation of propane. Proceedings of the Combustion Institute, 2019, 37, 461-468.	3.9	48
24	Kinetics of 1-butyl and 2-butyl radical reactions with molecular oxygen: Experiment and theory. Proceedings of the Combustion Institute, 2019, 37, 291-298.	3.9	15
25	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.	4.4	2
26	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.	13.7	52
27	Ab initio kinetics for pyrolysis and combustion systems. Computer Aided Chemical Engineering, 2019, , 115-167.	0.5	27
28	Nonthermal rate constants for CH4* + X â†' CH3 + HX, X = H, O, OH, and O2. Journal of Chemical Physics, 2019, 150, 114112.	3.0	21
29	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	125
30	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.	5.3	80
31	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	31.2	980
32	Unimolecular Decay of Criegee Intermediates to OH Radical Products: Prompt and Thermal Decay Processes. Accounts of Chemical Research, 2018, 51, 978-985.	15.6	101
33	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.	2.8	80
34	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.	2.5	15
35	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	3.0	36
36	Theory and modeling of relevance to prompt-NO formation at high pressure. Combustion and Flame, 2018, 195, 3-17.	5.2	57

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37	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.	13.7	109
38	Recombination of aromatic radicals with molecular oxygen. Proceedings of the Combustion Institute, 2017, 36, 169-177.	3.9	20
39	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	3.9	42
40	First-Principles Chemical Kinetic Modeling of Methyl trans-3-Hexenoate Epoxidation by HO₂. Journal of Physical Chemistry A, 2017, 121, 1909-1915.	2.5	6
41	High-pressure oxidation of ethane. Combustion and Flame, 2017, 182, 150-166.	5.2	76
42	Accurate Anharmonic Zero-Point Energies for Some Combustion-Related Species from Diffusion Monte Carlo. Journal of Physical Chemistry A, 2017, 121, 4334-4340.	2.5	22
43	Tunneling effects in the unimolecular decay of (CH3)2COO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2017, 146, 134307.	3.0	34
44	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.	2.5	55
45	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.	2.5	144
46	Ephemeral collision complexes mediate chemically termolecular transformations that affect system chemistry. Nature Chemistry, 2017, 9, 1078-1082.	13.6	85
47	Time-Resolved Kinetic Chirped-Pulse Rotational Spectroscopy in a Room-Temperature Flow Reactor. Journal of Physical Chemistry Letters, 2017, 8, 6180-6188.	4.6	18
48	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.	7.1	32
49	From theoretical reaction dynamics to chemical modeling of combustion. Proceedings of the Combustion Institute, 2017, 36, 77-111.	3.9	199
50	Ramifications of including non-equilibrium effects for HCO in flame chemistry. Proceedings of the Combustion Institute, 2017, 36, 525-532.	3.9	36
51	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. Proceedings of the Combustion Institute, 2017, 36, 919-926.	3.9	115
52	Theoretical investigation of intersystem crossing in the cyanonitrene molecule, 1NCN â†'â€ˆ3NCN. Journal of Chemical Physics, 2017, 147, 084310.	3.0	6
53	Communication: Real time observation of unimolecular decay of Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 144, 061102.	3.0	99
54	Deep tunneling in the unimolecular decay of CH3CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 234308.	3.0	56

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55	Direct observation of unimolecular decay of CH3CH2CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 044312.	3.0	49
56	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.	2.8	21
57	High-pressure oxidation of methane. Combustion and Flame, 2016, 172, 349-364.	5.2	157
58	Low Temperature Kinetics of the First Steps of Water Cluster Formation. Physical Review Letters, 2016, 116, 113401.	7.8	26
59	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. Faraday Discussions, 2016, 195, 637-670.	3.2	76
60	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.	4.6	63
61	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	2.5	30
62	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.	2.5	41
63	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.	2.8	8
64	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.	3.0	3
65	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	2.5	88
66	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.	3.9	48
67	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.	3.9	30
68	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.	2.5	48
69	Effects of New Ab Initio Rate Coefficients on Predictions of Species Formed during n-Butanol Ignition and Pyrolysis. Journal of Physical Chemistry A, 2015, 119, 543-551.	2.5	7
70	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.	3.9	28
71	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.	2.5	2
72	Multiscale Informatics for Low-Temperature Propane Oxidation: Further Complexities in Studies of Complex Reactions. Journal of Physical Chemistry A, 2015, 119, 7095-7115.	2.5	37

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73	Global uncertainty analysis for RRKM/master equation based kinetic predictions: A case study of ethanol decomposition. Combustion and Flame, 2015, 162, 3427-3436.	5.2	32
74	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.	2.5	32
75	Kinetics of Propargyl Radical Dissociation. Journal of Physical Chemistry A, 2015, 119, 7780-7791.	2.5	35
76	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.5	59
77	Resolving Some Paradoxes in the Thermal Decomposition Mechanism of Acetaldehyde. Journal of Physical Chemistry A, 2015, 119, 7724-7733.	2.5	33
78	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	5.2	122
79	THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY. Astrophysical Journal, Supplement Series, 2015, 217, 20.	7.7	291
80	Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. Proceedings of the Combustion Institute, 2015, 35, 283-290.	3.9	58
81	Secondary channels in the thermal decomposition of monomethylhydrazine (CH3NHNH2). RSC Advances, 2014, 4, 62951-62964.	3.6	3
82	Predictive a priori pressure-dependent kinetics. Science, 2014, 346, 1212-1215.	12.6	142
83	First-principles binary diffusion coefficients for H, H2, and four normal alkanes + N2. Journal of Chemical Physics, 2014, 141, 124313.	3.0	42
84	Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Ââ†'ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	21
85	Chemical Kinetics and Mechanisms of Complex Systems: AÂPerspective on Recent Theoretical Advances. Journal of the American Chemical Society, 2014, 136, 528-546.	13.7	212
86	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	4.6	38
87	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.	2.5	65
88	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.	3.9	64
89	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:mrow></mml:math> radicals. Proceedings of the Combustion Institute, 2013, 34, 187-194.	3.9	16
90	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 12146-12154.	2.5	461

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91	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.	3.9	73
92	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.	2.8	73
93	Low Temperature Rate Coefficients for the Reaction CN + HC₃N. Journal of Physical Chemistry A, 2013, 117, 12155-12164.	2.5	20
94	Dissociation of Propyl Radicals and Other Reactions on a C₃H₇ Potential. Journal of Physical Chemistry A, 2013, 117, 2718-2727.	2.5	74
95	Ab Initio Kinetics for the Decomposition of Hydroxybutyl and Butoxy Radicals of n-Butanol. Journal of Physical Chemistry A, 2013, 117, 1890-1906.	2.5	52
96	Propargyl + O₂ Reaction in Helium Droplets: Entrance Channel Barrier or Not?. Journal of Physical Chemistry A, 2013, 117, 13626-13635.	2.5	39
97	Rate Constant and Branching Fraction for the NH₂ + NO₂ Reaction. Journal of Physical Chemistry A, 2013, 117, 9011-9022.	2.5	37
98	Predictive Theory for the Addition and Insertion Kinetics of ¹CH₂ Reacting with Unsaturated Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 12677-12692.	2.5	21
99	A KINETIC DATABASE FOR ASTROCHEMISTRY (KIDA). Astrophysical Journal, Supplement Series, 2012, 199, 21.	7.7	436
100	RAPID ASSOCIATION REACTIONS AT LOW PRESSURE: IMPACT ON THE FORMATION OF HYDROCARBONS ON TITAN. Astrophysical Journal, 2012, 744, 11.	4.5	54
101	Shock Tube Explorations of Roaming Radical Mechanisms: The Decompositions of Isobutane and Neopentane. Journal of Physical Chemistry A, 2012, 116, 5981-5989.	2.5	34
102	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.	2.5	223
103	Interception of Excited Vibrational Quantum States by O ₂ in Atmospheric Association Reactions. Science, 2012, 337, 1066-1069.	12.6	90
104	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	2.5	48
105	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	68
106	Comment on â€œAutomatic estimation of pressure-dependent rate coefficientsâ€•(J. W. Allen, C. F.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Physics, 2012, 14, 8431.	2.8	8
107	Comprehensive H₂/O₂ kinetic model for highâ€pressure combustion. International Journal of Chemical Kinetics, 2012, 44, 444-474.	1.6	682
108	Pressure-Dependent OH Yields in Alkene + HO₂ Reactions: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10218-10225.	2.5	56

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109	Statistical Theory for the Kinetics and Dynamics of Roaming Reactions. Journal of Physical Chemistry A, 2011, 115, 14370-14381.	2.5	76
110	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.	2.5	57
111	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.	2.5	25
112	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
113	Insights into the role of polycyclic aromatic hydrocarbon condensation in haze formation in Jupiterâ€™s atmosphere. Astronomy and Astrophysics, 2011, 532, A40.	5.1	10
114	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	13.6	60
115	Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory. Combustion and Flame, 2011, 158, 618-632.	5.2	92
116	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	3.9	75
117	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	5.2	304
118	Ab initio kinetics for the decomposition of monomethylhydrazine (CH3NHNH2). Proceedings of the Combustion Institute, 2011, 33, 425-432.	3.9	18
119	Uncertainty driven theoretical kinetics studies for CH3OH ignition: HO2+CH3OH and O2+CH3OH. Proceedings of the Combustion Institute, 2011, 33, 351-357.	3.9	149
120	DISEQUILIBRIUM CARBON, OXYGEN, AND NITROGEN CHEMISTRY IN THE ATMOSPHERES OF HD 189733b AND HD 209458b. Astrophysical Journal, 2011, 737, 15.	4.5	374
121	Insights into the condensation of PAHsin the envelope of IRC +10216. EAS Publications Series, 2011, 46, 191-199.	0.3	1
122	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.	2.5	40
123	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	2.5	66
124	Exploring the Role of PAHs in the Formation of Soot: Pyrene Dimerization. Journal of Physical Chemistry Letters, 2010, 1, 2962-2967.	4.6	152
125	Rate Constants for the Thermal Decomposition of Ethanol and Its Bimolecular Reactions with OH and D: Reflected Shock Tube and Theoretical Studies. Journal of Physical Chemistry A, 2010, 114, 9425-9439.	2.5	139
126	Temperature Dependence of Two Key Interstellar Reactions of H₃⁺: O(³P) + H₃⁺ and CO + H₃⁺. Journal of Physical Chemistry A, 2010, 114, 278-290.	2.5	44

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127	D-Atom Products in Predissociation of CD₂CD₂OH from the 202â˜215 nm Photodissociation of 2-Bromoethanol. Journal of Physical Chemistry A, 2010, 114, 5453-5461.	2.5	10
128	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	2.5	84
129	Roaming Radical Pathways for the Decomposition of Alkanes. Journal of Physical Chemistry Letters, 2010, 1, 3016-3020.	4.6	73
130	Roaming Radical Kinetics in the Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 765-777.	2.5	125
131	Experimental and Theoretical Investigation of the Self-Reaction of Phenyl Radicals. Journal of Physical Chemistry A, 2010, 114, 8240-8261.	2.5	63
132	Direct Observation of Roaming Radicals in the Thermal Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 755-764.	2.5	112
133	Formation of NH3 and CH2NH in Titan's upper atmosphere. Faraday Discussions, 2010, 147, 31.	3.2	66
134	A shock-tube and theory study of the dissociation of acetone and subsequent recombination of methyl radicals. Proceedings of the Combustion Institute, 2009, 32, 123-130.	3.9	38
135	Theoretical rate coefficients for the reaction of methyl radical with hydroperoxyl radical and for methylhydroperoxide decomposition. Proceedings of the Combustion Institute, 2009, 32, 279-286.	3.9	87
136	Kinetics of the H+NCO reaction. Proceedings of the Combustion Institute, 2009, 32, 149-155.	3.9	17
137	Thermal Decomposition of NH₂OH and Subsequent Reactions: Ab Initio Transition State Theory and Reflected Shock Tube Experiments. Journal of Physical Chemistry A, 2009, 113, 10241-10259.	2.5	86
138	Shock Tube and Theory Investigation of Cyclohexane and 1-Hexene Decomposition. Journal of Physical Chemistry A, 2009, 113, 13570-13583.	2.5	88
139	Detailed balance in multiple-well chemical reactions. Physical Chemistry Chemical Physics, 2009, 11, 1128.	2.8	43
140	A CROSSED MOLECULAR BEAMS STUDY ON THE FORMATION OF THE EXOTIC CYANOETHYNYL RADICAL IN TITAN'S ATMOSPHERE. Astrophysical Journal, 2009, 701, 1797-1803.	4.5	18
141	Kinetics of CH + N₂ Revisited with Multireference Methods. Journal of Physical Chemistry A, 2008, 112, 522-532.	2.5	62
142	Reactions over Multiple, Interconnected Potential Wells: Unimolecular and Bimolecular Reactions on a C3H5 Potential. Journal of Physical Chemistry A, 2008, 112, 9429-9438.	2.5	73
143	A combined ab initio and photoionization mass spectrometric study of polyynes in fuel-rich flames. Physical Chemistry Chemical Physics, 2008, 10, 366-374.	2.8	68
144	Thermal Decomposition of CF3and the Reaction of CF2+ OH â†' CF2O + H. Journal of Physical Chemistry A, 2008, 112, 31-37.	2.5	30

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145	Kinetics and Product Branching Ratios of the Reaction of ¹CH₂ with H₂ and D₂. Journal of Physical Chemistry A, 2008, 112, 9575-9583.	2.5	23
146	An experimental and theoretical high temperature kinetic study of the thermal unimolecular dissociation of fluoroethane. Physical Chemistry Chemical Physics, 2008, 10, 6266.	2.8	13
147	Theory of Low Temperature Gas-Phase Reactions. , 2008, , 175-229.		6
148	Direct Measurement and Theoretical Calculation of the Rate Coefficient for Cl + CH3in the Range fromT= 202â^'298 K. Journal of Physical Chemistry A, 2007, 111, 1015-1023.	2.5	15
149	Understanding Reactivity at Very Low Temperatures: The Reactions of Oxygen Atoms with Alkenes. Science, 2007, 317, 102-105.	12.6	131
150	Ab initio methods for reactive potential surfaces. Physical Chemistry Chemical Physics, 2007, 9, 4055.	2.8	158
151	Tribute to James A. Miller. Journal of Physical Chemistry A, 2007, 111, 3673-3675.	2.5	0
152	Reaction Kinetics of CO + HO2â†' Products:Â Ab Initio Transition State Theory Study with Master Equation Modelingâ€. Journal of Physical Chemistry A, 2007, 111, 4031-4042.	2.5	92
153	A Two Transition State Model for Radicalâ^'Molecule Reactions:Â Applications to Isomeric Branching in the OHâ^'Isoprene Reaction. Journal of Physical Chemistry A, 2007, 111, 5582-5592.	2.5	71
154	Association rate constants for reactions between resonance-stabilized radicals: C3H3 + C3H3, C3H3 + C3H5, and C3H5 + C3H5. Physical Chemistry Chemical Physics, 2007, 9, 4259.	2.8	141
155	Theory, measurements, and modeling of OH and HO2 formation in the reaction of cyclohexyl radicals with O2. Physical Chemistry Chemical Physics, 2007, 9, 4315.	2.8	92
156	Reflected Shock Tube and Theoretical Studies of High-Temperature Rate Constants for OH + CF3H â‡† CF3+ H2O and CF3+ OH â†' Productsâ€. Journal of Physical Chemistry A, 2007, 111, 6822-6831.	2.5	18
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