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	Current Status of Transition-State Theory. The Journal of Physical Chemistry, 1996, 100, 12771-12800.	2.9	1,862
2	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	32.4	1,151
3	Comprehensive H₂/O₂ kinetic model for highâ€pressure combustion. International Journal of Chemical Kinetics, 2012, 44, 444-474.	1.7	733
4	Modeling the Kinetics of Bimolecular Reactions. Chemical Reviews, 2006, 106, 4518-4584.	51.4	551
5	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 12146-12154.	2.6	499
6	A KINETIC DATABASE FOR ASTROCHEMISTRY (KIDA). Astrophysical Journal, Supplement Series, 2012, 199, 21.	8.1	449
7	Master Equation Methods in Gas Phase Chemical Kinetics. Journal of Physical Chemistry A, 2006, 110, 10528-10544.	2.6	397
8	DISEQUILIBRIUM CARBON, OXYGEN, AND NITROGEN CHEMISTRY IN THE ATMOSPHERES OF HD 189733b AND HD 209458b. Astrophysical Journal, 2011, 737, 15.	4.7	389
9	The Recombination of Propargyl Radicals and Other Reactions on a C6H6Potential. Journal of Physical Chemistry A, 2003, 107, 7783-7799.	2.6	374
10	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	5.3	329
11	Enols Are Common Intermediates in Hydrocarbon Oxidation. Science, 2005, 308, 1887-1889.	20.9	310
12	THE 2014 KIDA NETWORK FOR INTERSTELLAR CHEMISTRY. Astrophysical Journal, Supplement Series, 2015, 217, 20.	8.1	304
13	Variational optimizations in the Riceâ€“Ramspergerâ€“Kasselâ€“Marcus theory calculations for unimolecular dissociations with no reverse barrier. Journal of Chemical Physics, 1992, 96, 367-371.	3.1	279
14	Long-range transition state theory. Journal of Chemical Physics, 2005, 122, 194103.	3.1	243
15	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
16	A Two Transition State Model for Radicalâˆ’Molecule Reactions:Â A Case Study of the Addition of OH to C2H4. Journal of Physical Chemistry A, 2005, 109, 6031-6044.	2.6	223
17	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
18	From the Multiple-Well Master Equation to Phenomenological Rate Coefficients:â€‰ Reactions on a C3H4 Potential Energy Surface. Journal of Physical Chemistry A, 2003, 107, 2680-2692.	2.6	219

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19	From theoretical reaction dynamics to chemical modeling of combustion. Proceedings of the Combustion Institute, 2017, 36, 77-111.	4.5	215
20	Predictive theory for the combination kinetics of two alkyl radicals. Physical Chemistry Chemical Physics, 2006, 8, 1133.	2.9	209
21	Kinetics of the Reaction of Methyl Radical with Hydroxyl Radical and Methanol Decompositionâ€. Journal of Physical Chemistry A, 2007, 111, 3932-3950.	2.6	191
22	From the Time-Dependent, Multiple-Well Master Equation to Phenomenological Rate Coefficients. Journal of Physical Chemistry A, 2002, 106, 9267-9277.	2.6	188
23	Predictive Theory for Hydrogen Atomâ^'Hydrocarbon Radical Association Kinetics. Journal of Physical Chemistry A, 2005, 109, 4646-4656.	2.6	183
24	High-pressure oxidation of methane. Combustion and Flame, 2016, 172, 349-364.	5.3	168
25	An Efficient Procedure for Evaluating the Number of Available States within a Variably Defined Reaction Coordinate Framework. The Journal of Physical Chemistry, 1994, 98, 11459-11464.	2.9	167
26	Measurements, Theory, and Modeling of OH Formation in Ethyl + O2 and Propyl + O2 Reactions. Journal of Physical Chemistry A, 2003, 107, 4415-4427.	2.6	163
27	Reaction of Ethylene with Hydroxyl Radicals:Â A Theoretical Studyâ€. Journal of Physical Chemistry A, 2006, 110, 6960-6970.	2.6	161
28	Exploring the Role of PAHs in the Formation of Soot: Pyrene Dimerization. Journal of Physical Chemistry Letters, 2010, 1, 2962-2967.	4.9	161
29	Ab initio methods for reactive potential surfaces. Physical Chemistry Chemical Physics, 2007, 9, 4055.	2.9	160
30	Vibrational Spectroscopy and Density Functional Theory of Transition-Metal Ionâ^'Benzene and Dibenzene Complexes in the Gas Phase. Journal of the American Chemical Society, 2004, 126, 10981-10991.	14.6	159
31	Transition State Theory for Multichannel Addition Reactions:â€‰ Multifaceted Dividing Surfaces. Journal of Physical Chemistry A, 2003, 107, 9776-9781.	2.6	156
32	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
33	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
34	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.	2.6	146
35	The Hâ€‰+â€‰C2H2(+M)â€‰â‡„â€‰C2H3(+M) and Hâ€‰+â€‰C2H2(+M)â€‰â‡„â€‰C2H5(+M) reactions: Electronic structure transition-state theory, and solutions to a two-dimensional master equation. Physical Chemistry Chemical Physics, 2004, 6, 1192-1202.	2.9	144
36	Identification and Chemistry of C4H3and C4H5Isomers in Fuel-Rich Flames. Journal of Physical Chemistry A, 2006, 110, 3670-3678.	2.6	143

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37	Association rate constants for reactions between resonance-stabilized radicals: C3H3 + C3H3, C3H3 + C3H5, and C3H5 + C3H5. Physical Chemistry Chemical Physics, 2007, 9, 4259.	2.9	143
38	Variable reaction coordinate transition state theory: Analytic results and application to the C2H3+Hâ†'C2H4 reaction. Journal of Chemical Physics, 2003, 118, 5442-5455.	3.1	140
39	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
40	A bond length reaction coordinate for unimolecular reactions. II. Microcanonical and canonical implementations with application to the dissociation of NCNO. Journal of Chemical Physics, 1991, 94, 6469-6482.	3.1	135
41	Understanding Reactivity at Very Low Temperatures: The Reactions of Oxygen Atoms with Alkenes. Science, 2007, 317, 102-105.	20.9	132
42	The Recombination of Propargyl Radicals:Â Solving the Master Equation. Journal of Physical Chemistry A, 2001, 105, 7254-7266.	2.6	130
43	Application of unimolecular reaction rate theory for highly flexible transition states to the dissociation of NCNO into NC and NO. Journal of Chemical Physics, 1988, 89, 4761-4770.	3.1	129
44	Roaming Radical Kinetics in the Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 765-777.	2.6	129
45	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	5.3	128
46	Solution of Some One- and Two-Dimensional Master Equation Models for Thermal Dissociation:â€‰ The Dissociation of Methane in the Low-Pressure Limit. Journal of Physical Chemistry A, 2002, 106, 4904-4913.	2.6	127
47	The reaction between ethyl and molecular oxygen II: Further analysis. International Journal of Chemical Kinetics, 2001, 33, 654-668.	1.7	126
48	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
49	Identification of C5HxIsomers in Fuel-Rich Flames by Photoionization Mass Spectrometry and Electronic Structure Calculations. Journal of Physical Chemistry A, 2006, 110, 4376-4388.	2.6	124
50	The spin-forbidden reaction CH(2Î)+N2â†'HCN+N(4S) revisited. II. Nonadiabatic transition state theory and application. Journal of Chemical Physics, 1999, 110, 9469-9482.	3.1	121
51	Implementation of RRKM theory for highly flexible transition states with a bond length as the reaction coordinate. Chemical Physics Letters, 1990, 170, 71-77.	2.7	118
52	Application of unimolecular reaction rate theory for highly flexible transition states to the dissociation of CH2CO into CH2 and CO. Journal of Chemical Physics, 1989, 91, 2280-2292.	3.1	116
53	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
54	Synchrotron photoionization measurements of combustion intermediates: Photoionization efficiency and identification of C3H2 isomers. Physical Chemistry Chemical Physics, 2005, 7, 806.	2.9	114

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55	On the Combination Reactions of Hydrogen Atoms with Resonance-Stabilized Hydrocarbon Radicalsâ€. Journal of Physical Chemistry A, 2007, 111, 3789-3801.	2.6	113
56	Direct Observation of Roaming Radicals in the Thermal Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 755-764.	2.6	112
57	High pressure rate constants for unimolecular dissociation/free radical recombination: Determination of the quantum correction via quantum Monte Carlo path integration. Journal of Chemical Physics, 1987, 87, 3410-3417.	3.1	107
58	The anharmonic force field and equilibrium molecular structure of ketene. Journal of Chemical Physics, 1995, 102, 8506-8532.	3.1	107
59	A theoretical analysis of the reaction between ethyl and molecular oxygen. Proceedings of the Combustion Institute, 2000, 28, 1479-1486.	4.5	106
60	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
61	Binding Energy of Al(C6H6)+from Analysis of Radiative Association Kinetics. Journal of the American Chemical Society, 1996, 118, 5277-5283.	14.6	104
62	Communication: Real time observation of unimolecular decay of Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 144, 061102.	3.1	104
63	Initial Steps of Aromatic Ring Formation in a Laminar Premixed Fuel-Rich Cyclopentene Flameâ€. Journal of Physical Chemistry A, 2007, 111, 4081-4092.	2.6	103
64	On the formation and decomposition of C7H8. Proceedings of the Combustion Institute, 2007, 31, 221-229.	4.5	102
65	Theory, measurements, and modeling of OH and HO2 formation in the reaction of cyclohexyl radicals with O2. Physical Chemistry Chemical Physics, 2007, 9, 4315.	2.9	96
66	A theoretical analysis of the reaction between propargyl and molecular oxygen. Faraday Discussions, 2001, 119, 79-100.	3.7	95
67	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
68	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.	2.6	94
69	Ephemeral collision complexes mediate chemically termolecular transformations that affect system chemistry. Nature Chemistry, 2017, 9, 1078-1082.	14.3	93
70	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
71	Binding Energies of Ag+ and Cd+ Complexes from Analysis of Radiative Association Kinetics. Journal of Physical Chemistry A, 1997, 101, 3338-3347.	2.6	92
72	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.	2.6	92

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73	Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory. Combustion and Flame, 2011, 158, 618-632.	5.3	92
74	A Theoretical Analysis of the Reaction between Vinyl and Acetylene:Â Quantum Chemistry and Solution of the Master Equation. Journal of Physical Chemistry A, 2000, 104, 7525-7536.	2.6	91
75	Shock Tube and Theory Investigation of Cyclohexane and 1-Hexene Decomposition. Journal of Physical Chemistry A, 2009, 113, 13570-13583.	2.6	91
76	Binding Energies of Gas-Phase Metal Ions with Pyrrole:â€‰ Experimental and Quantum Chemical Results. Journal of Physical Chemistry A, 2000, 104, 3246-3256.	2.6	89
77	Energy-Resolved Photoionization of Alkylperoxy Radicals and the Stability of Their Cations. Journal of the American Chemical Society, 2006, 128, 13559-13567.	14.6	89
78	Strange Kinetics of the C2H6+ CN Reaction Explainedâ€. Journal of Physical Chemistry A, 2007, 111, 3802-3811.	2.6	89
79	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
80	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.	4.5	88
81	Infrared frequency-modulation probing of product formation in alkyl + O2 reactions. Part IV.For Part III see ref. 12. Reactions of propyl and butyl radicals with O2Electronic Supplementary Information available. See http://www.rsc.org/suppdata/fd/b1/b102237g/. Faraday Discussions, 2001, 119, 101-120.	3.7	87
82	Theoretical and Experimental Investigation of the Dynamics of the Production of CO from the CH3 + O and CD3 + O Reactions. Journal of Physical Chemistry A, 2001, 105, 8361-8369.	2.6	87
83	The Reaction of Acetylene with Hydroxyl Radicals. Journal of Physical Chemistry A, 2005, 109, 6045-6055.	2.6	87
84	Density functional theory predictions for the binding of transition metal cations to pi systems: from acetylene to coronene and tribenzocyclyne. International Journal of Mass Spectrometry, 2000, 201, 253-267.	1.6	85
85	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	2.6	84
86	A high level ab initio map and direct statistical treatment of the fragmentation of singlet ketene. Journal of Chemical Physics, 1996, 105, 118-140.	3.1	83
87	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. Faraday Discussions, 2016, 195, 637-670.	3.7	81
88	A Direct Transition State Theory Based Study of Methyl Radical Recombination Kinetics. Journal of Physical Chemistry A, 1999, 103, 9388-9398.	2.6	78
89	Theory and Modeling of the Binding in Cationic Transition-Metalâ^'Benzene Complexes. Journal of Physical Chemistry A, 1999, 103, 1094-1103.	2.6	78
90	Statistical Theory for the Kinetics and Dynamics of Roaming Reactions. Journal of Physical Chemistry A, 2011, 115, 14370-14381.	2.6	77

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91	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	4.5	77
92	Dissociation of Propyl Radicals and Other Reactions on a C₃H₇ Potential. Journal of Physical Chemistry A, 2013, 117, 2718-2727.	2.6	77
93	High-pressure oxidation of ethane. Combustion and Flame, 2017, 182, 150-166.	5.3	77
94	Theoretical Considerations in the NH2 + NO Reaction. Journal of Physical Chemistry A, 2000, 104, 2061-2069.	2.6	76
95	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
96	A combined theoretical and experimental study of the dissociation of benzene cation. Journal of Chemical Physics, 1993, 98, 243-256.	3.1	75
97	Pathways and Rate Coefficients for the Decomposition of Vinoxy and Acetyl Radicals. Journal of Physical Chemistry A, 2006, 110, 5772-5781.	2.6	75
98	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
99	Reactions over Multiple, Interconnected Potential Wells: Unimolecular and Bimolecular Reactions on a C₃H₅Potential. Journal of Physical Chemistry A, 2008, 112, 9429-9438.	2.6	74
100	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.	2.6	73
101	Roaming Radical Pathways for the Decomposition of Alkanes. Journal of Physical Chemistry Letters, 2010, 1, 3016-3020.	4.9	73
102	Theory and modeling of ionâ€“molecule radiative association kinetics. Journal of Chemical Physics, 1996, 104, 4502-4516.	3.1	71
103	A combined ab initio and photoionization mass spectrometric study of polyynes in fuel-rich flames. Physical Chemistry Chemical Physics, 2008, 10, 366-374.	2.9	71
104	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
105	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
106	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
107	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
108	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	2.6	67

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109	Formation of NH3 and CH2NH in Titan's upper atmosphere. Faraday Discussions, 2010, 147, 31.	3.7	66
110	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
111	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
112	Experimental and theoretical rate constants for CH4 + O2 â†' CH3 + HO2. Combustion and Flame, 2007, 149, 104-111.	5.3	64
113	Kinetics of CH + N₂ Revisited with Multireference Methods. Journal of Physical Chemistry A, 2008, 112, 522-532.	2.6	64
114	Experimental and Theoretical Investigation of the Self-Reaction of Phenyl Radicals. Journal of Physical Chemistry A, 2010, 114, 8240-8261.	2.6	64
115	Dissociation, relaxation, and incubation in the high-temperature pyrolysis of ethane, and a successful RRKM modeling. Proceedings of the Combustion Institute, 2005, 30, 1129-1135.	4.5	63
116	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	14.3	62
117	The Addition of Hydrogen Atoms to Diacetylene and the Heats of Formation ofi-C4H3andn-C4H3. Journal of Physical Chemistry A, 2005, 109, 4285-4295.	2.6	61
118	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.6	61
119	Deep tunneling in the unimolecular decay of CH3CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 234308.	3.1	61
120	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
121	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
122	Theory and modeling of relevance to prompt-NO formation at high pressure. Combustion and Flame, 2018, 195, 3-17.	5.3	60
123	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
124	Experiments and Theory on the Thermal Decomposition of CHCl3and the Reactions of CCl2. Journal of Physical Chemistry A, 1997, 101, 8653-8661.	2.6	58
125	Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. Proceedings of the Combustion Institute, 2015, 35, 283-290.	4.5	58
126	Application of unimolecular reaction rate theory for highly flexible transition states to the dissociation of CH2CO into CH2 and CO. II. Photofragment excitation spectra for vibrationallyâ€excited fragments. Journal of Chemical Physics, 1990, 93, 2418-2424.	3.1	56

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127	Pressure-Dependent OH Yields in Alkene + HO₂ Reactions: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10218-10225.	2.6	56
128	RAPID ASSOCIATION REACTIONS AT LOW PRESSURE: IMPACT ON THE FORMATION OF HYDROCARBONS ON TITAN. Astrophysical Journal, 2012, 744, 11.	4.7	56
129	Reactions of oxygen atoms with hydrocarbon radicals: a priori kinetic predictions for the CH3+O, C2H5+O, and C2H3+O reactions. Proceedings of the Combustion Institute, 2005, 30, 985-993.	4.5	55
130	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
131	A theoretical study of the dissociation of NO2. Journal of Chemical Physics, 1993, 99, 3644-3653.	3.1	52
132	A kinetic issue in reburning: the fate of HCNO. Combustion and Flame, 2003, 135, 357-362.	5.3	51
133	Resolving the mystery of prompt CO2: The HCCO+O2 reaction. Proceedings of the Combustion Institute, 2002, 29, 1209-1217.	4.5	50
134	Direct observation of unimolecular decay of CH3CH2CHOO Criegee intermediates to OH radical products. Journal of Chemical Physics, 2016, 145, 044312.	3.1	50
135	High-pressure oxidation of propane. Proceedings of the Combustion Institute, 2019, 37, 461-468.	4.5	50
136	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	2.6	49
137	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
138	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
139	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	4.5	48
140	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
141	Unimolecular reaction rate theory for highly flexible transition states: use of conventional coordinates. The Journal of Physical Chemistry, 1988, 92, 3105-3109.	2.9	47
142	Variational statistical study of the CN+O2 reaction employing ab initio determined properties for the transition state. Journal of Chemical Physics, 1993, 99, 5790-5799.	3.1	47
143	First-principles binary diffusion coefficients for H, H2, and four normal alkanes + N2. Journal of Chemical Physics, 2014, 141, 124313.	3.1	45
144	Theoretical kinetics predictions for NH2Â+ÂHO2. Combustion and Flame, 2022, 236, 111787.	5.3	45

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145	Comparisons between statistics, dynamics, and experiment for the H+O2â†'OH+O reaction. Journal of Chemical Physics, 1995, 103, 7287-7298.	3.1	44
146	Detailed balance in multiple-well chemical reactions. Physical Chemistry Chemical Physics, 2009, 11, 1128.	2.9	44
147	Temperature Dependence of Two Key Interstellar Reactions of H₃⁺: O(³P) + H₃⁺ and CO + H₃⁺. Journal of Physical Chemistry A, 2010, 114, 278-290.	2.6	44
148	Unimolecular reaction rate theory for highly flexible transition states. 2. Conventional coordinate formulas for the various possible fragment combinations: miscellaneous topics. The Journal of Physical Chemistry, 1988, 92, 5412-5417.	2.9	43
149	Rate Constant and Branching Fraction for the NH₂ + NO₂ Reaction. Journal of Physical Chemistry A, 2013, 117, 9011-9022.	2.6	43
150	Decomposition of acetaldehyde: Experiment and detailed theory. Proceedings of the Combustion Institute, 2007, 31, 167-174.	4.5	42
151	Propargyl + O₂ Reaction in Helium Droplets: Entrance Channel Barrier or Not?. Journal of Physical Chemistry A, 2013, 117, 13626-13635.	2.6	41
152	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
153	A complete statistical analysis of the reaction between OH and CO. Proceedings of the Combustion Institute, 2005, 30, 945-953.	4.5	40
154	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
155	Measurements and Modeling of HO2Formation in the Reactions ofn-C3H7andi-C3H7Radicals with O2â€. Journal of Physical Chemistry B, 2005, 109, 8374-8387.	2.7	39
156	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	4.9	39
157	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
158	Intramolecular dynamics. I. Curvilinear normal modes, local modes, molecular anharmonic Hamiltonian, and application to benzene. Journal of Chemical Physics, 1991, 94, 7319-7334.	3.1	38
159	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.	4.5	38
160	Ramifications of including non-equilibrium effects for HCO in flame chemistry. Proceedings of the Combustion Institute, 2017, 36, 525-532.	4.5	38
161	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
162	Watching a hydroperoxyalkyl radical (â€¢QOOH) dissociate. Science, 2021, 373, 679-682.	20.9	38

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163	Variational calculation of the rate of dissociation of ethenone into methylene and carbon monoxide on an ab initio determined potential energy surface. The Journal of Physical Chemistry, 1991, 95, 9882-9889.	2.9	37
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