Role of O₂ + QOOH in Low-Temperature Ig Pressure Dependent Rate Coefficients

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Citation Report

#	Article	IF	Citations
1	High-Pressure Rate Rules for Alkyl + O₂ Reactions. 2. The Isomerization, Cyclic Ether Formation, and Î²-Scission Reactions of Hydroperoxy Alkyl Radicals. Journal of Physical Chemistry A, 2012, 116, 5068-5089.	2.5	172
2	MESMER: An Open-Source Master Equation Solver for Multi-Energy Well Reactions. Journal of Physical Chemistry A, 2012, 116, 9545-9560.	2.5	467
3	New Pathways for Formation of Acids and Carbonyl Products in Low-Temperature Oxidation: The Korcek Decomposition of Î³-Ketohydroperoxides. Journal of the American Chemical Society, 2013, 135, 11100-11114.	13.7	153
4	Rate Rules, Branching Ratios, and Pressure Dependence of the HO₂ + Olefin Addition Channels. Journal of Physical Chemistry A, 2013, 117, 6458-6473.	2.5	57
5	Directly measuring reaction kinetics of Ë™QOOH â€“ a crucial but elusive intermediate in hydrocarbon autoignition. Physical Chemistry Chemical Physics, 2013, 15, 10753.	2.8	58
6	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
7	A semi-detailed chemical kinetic model of a gasoline surrogate fuel for internal combustion engine applications. Fuel, 2013, 113, 347-356.	6.4	32
8	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 12146-12154.	2.5	461
9	Reaction Pathways for the Thermal Decomposition of Methyl Butanoate. Journal of Organic Chemistry, 2013, 78, 5898-5908.	3.2	35
10	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. Combustion and Flame, 2013, 160, 1907-1929.	5.2	65
11	Synchrotron Photoionization Mass Spectrometry Measurements of Product Formation in Low-Temperature n-Butane Oxidation: Toward a Fundamental Understanding of Autoignition Chemistry and n-C₄H₉ + O₂/s-C₄H₉ + O₂ Reactions. Journal of Physical Chemistry A, 2013, 117, 12216-12235.	2.5	33
12	A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi. Combustion and Flame, 2014, 161, 711-724.	5.2	54
13	Experiments and modeling of propane combustion with vitiation. Combustion and Flame, 2014, 161, 2038-2053.	5.2	58
14	Pathways, kinetics and thermochemistry of methyl-ester peroxy radical decomposition in the low-temperature oxidation of methyl butanoate: A computational study of a biodiesel fuel surrogate. Combustion and Flame, 2014, 161, 2270-2287.	5.2	29
15	An improved kinetic mechanism for 3-pentanone pyrolysis and oxidation developed using multispecies time histories in shock-tubes. Combustion and Flame, 2014, 161, 1135-1145.	5.2	23
16	Experimental and ab Initio Investigations of H₂S-Assisted Propane Oxidative Dehydrogenation Reactions. Journal of Physical Chemistry A, 2014, 118, 1541-1556.	2.5	11
17	Thermochemistry, Reaction Paths, and Kinetics on the Secondary Isooctane Radical Reaction with 3 O2. International Journal of Chemical Kinetics, 2014, 46, 71-103.	1.6	8
18	Ab Initio Investigation of the Thermal Decomposition of n-Butylcyclohexane. Journal of Physical Chemistry A, 2014, 118, 1067-1076.	2.5	15

#	Article	IF	Citations
19	Evaluation of Combustion Mechanisms Using Global Uncertainty and Sensitivity Analyses: A Case Study for Lowâ€Temperature Dimethyl Ether Oxidation. International Journal of Chemical Kinetics, 2014, 46, 662-682.	1.6	43
20	A shock tube laser schlieren study of methyl acetate dissociation in the fall-off regime. Physical Chemistry Chemical Physics, 2014, 16, 7241.	2.8	13
21	Analysis of the Kinetics and Yields of OH Radical Production from the CH₃OCH₂ + O₂ Reaction in the Temperature Range 195â€“650 K: An Experimental and Computational study. Journal of Physical Chemistry A, 2014, 118, 6773-6788.	2.5	58
23	Flow reactor studies of non-equilibrium plasma-assisted oxidation of n -alkanes. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2015, 373, 20140344.	3.4	23
24	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
25	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
26	Direct observation and kinetics of a hydroperoxyalkyl radical (QOOH). Science, 2015, 347, 643-646.	12.6	130
27	Detection and Identification of the Keto-Hydroperoxide (HOOCH₂OCHO) and Other Intermediates during Low-Temperature Oxidation of Dimethyl Ether. Journal of Physical Chemistry A, 2015, 119, 7361-7374.	2.5	143
28	Intricate Internal Rotation Surface and Fundamental Infrared Transitions of the n-Propyl Radical. Journal of Physical Chemistry B, 2015, 119, 728-735.	2.6	10
29	A rational strategy for the realization of chain-growth supramolecular polymerization. Science, 2015, 347, 646-651.	12.6	518
30	Quantum Chemical Study of Autoignition of Methyl Butanoate. Journal of Physical Chemistry A, 2015, 119, 7282-7292.	2.5	18
31	Computational Kinetic Study for the Unimolecular Decomposition of Cyclopentanone. International Journal of Chemical Kinetics, 2015, 47, 439-446.	1.6	16
32	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
33	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
34	New reaction classes in the kinetic modeling of low temperature oxidation of n-alkanes. Combustion and Flame, 2015, 162, 1679-1691.	5.2	214
35	Revisiting the Kinetics and Thermodynamics of the Low-Temperature Oxidation Pathways of Alkanes: A Case Study of the Three Pentane Isomers. Journal of Physical Chemistry A, 2015, 119, 7510-7527.	2.5	202
36	Mechanism and Kinetics of Low-Temperature Oxidation of a Biodiesel Surrogate: Methyl Propanoate Radicals with Oxygen Molecule. Journal of Physical Chemistry A, 2015, 119, 3689-3703.	2.5	24
37	Comparison of Three Isoelectronic Multiple-Well Reaction Systems: OH + CH₂O, OH + CH₂CH₂, and OH + CH₂NH. Journal of Physical Chemistry A, 2015, 119, 7578-7592.	2.5	47

#	Article	IF	Citations
38	Non-Equilibrium Plasma-Assisted Flow Reactor Studies of Highly Diluted Reactive Mixtures. , 2015, , .		4
39	An experimental and kinetic modeling study of n -hexane oxidation. Combustion and Flame, 2015, 162, 4194-4207.	5.2	124
40	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	5.2	122
41	Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. Proceedings of the Combustion Institute, 2015, 35, 283-290.	3.9	58
42	Explosive and general oxidative characteristics of fuels. , 2015, , 71-146.		3
43	Computational Kinetic Study for the Unimolecular Decomposition Pathways of Cyclohexanone. Journal of Physical Chemistry A, 2015, 119, 7138-7144.	2.5	17
44	Kinetic studies of methyl acetate pyrolysis and oxidation in a flow reactor and a low-pressure flat flame using molecular-beam mass spectrometry. Proceedings of the Combustion Institute, 2015, 35, 491-498.	3.9	45
45	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.	3.9	48
46	An ignition delay and kinetic modeling study of methane, dimethyl ether, and their mixtures at high pressures. Combustion and Flame, 2015, 162, 315-330.	5.2	364
47	Harnessing the Combined Power of Theoretical and Experimental Data through Multiscale Informatics. International Journal of Chemical Kinetics, 2016, 48, 212-235.	1.6	32
48	Infrared laser spectroscopy of the n-propyl and i-propyl radicals: Stretch-bend Fermi coupling in the alkyl CH stretch region. Journal of Chemical Physics, 2016, 145, 224304.	3.0	19
49	Investigating the ground-state rotamers of n-propylperoxy radical. Journal of Chemical Physics, 2016, 145, 174301.	3.0	7
50	Third O2 addition reactions promote the low-temperature auto-ignition of n-alkanes. Combustion and Flame, 2016, 165, 364-372.	5.2	66
51	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. Combustion and Flame, 2016, 168, 310-330.	5.2	85
52	Unimolecular HO₂ Loss from Peroxy Radicals Formed in Autoxidation Is Unlikely under Atmospheric Conditions. Journal of Physical Chemistry A, 2016, 120, 3588-3595.	2.5	21
53	Optimized reaction mechanism rate rules for ignition of normal alkanes. Combustion and Flame, 2016, 173, 468-482.	5.2	121
54	An updated experimental and kinetic modeling study of n-heptane oxidation. Combustion and Flame, 2016, 172, 116-135.	5.2	307
55	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.	2.5	40

#	Article	IF	Citations
56	Barrierless association of CF ₂ and dissociation of C ₂ F ₄ by variational transition-state theory and system-specific quantum Riceâ€“Ramspergerâ€“Kassel theory. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13606-13611.	7.1	28
57	The Stability of Î±â€Hydroperoxyalkyl Radicals. Chemistry - A European Journal, 2016, 22, 18092-18100.	3.3	24
58	Tunneling effect in 1,5 H-migration of a prototypical OOQOOH. Chemical Physics Letters, 2016, 646, 153-157.	2.6	9
59	A comprehensive experimental and modeling study of isobutene oxidation. Combustion and Flame, 2016, 167, 353-379.	5.2	282
60	Modeling Ignition of a Heptane Isomer: Improved Thermodynamics, Reaction Pathways, Kinetics, and Rate Rule Optimizations for 2-Methylhexane. Journal of Physical Chemistry A, 2016, 120, 2201-2217.	2.5	53
61	An experimental and modelling study of n-pentane oxidation in two jet-stirred reactors: The importance of pressure-dependent kinetics and new reaction pathways. Proceedings of the Combustion Institute, 2017, 36, 441-448.	3.9	92
62	A theoretical study of cyclic ether formation reactions. Proceedings of the Combustion Institute, 2017, 36, 161-167.	3.9	28
63	A comprehensive iso-octane combustion model with improved thermochemistry and chemical kinetics. Combustion and Flame, 2017, 178, 111-134.	5.2	164
64	Pressure-Dependent Rate Rules for Intramolecular H-Migration Reactions of Hydroperoxyalkylperoxy Radicals in Low Temperature. Journal of Physical Chemistry A, 2017, 121, 3001-3018.	2.5	20
65	Automatic Generation of Microkinetic Mechanisms for Heterogeneous Catalysis. Journal of Physical Chemistry C, 2017, 121, 9970-9981.	3.1	80
66	Revisiting 1-hexene low-temperature oxidation. Combustion and Flame, 2017, 181, 283-299.	5.2	29
67	An extensive experimental and modeling study of 1-butene oxidation. Combustion and Flame, 2017, 181, 198-213.	5.2	79
68	Calculation of the rate constants for concerted elimination reaction class of hydroperoxyl-alkyl-peroxyl radicals. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
69	Theoretical kinetic studies for low temperature oxidation of two typical methylcyclohexyl radicals. Combustion and Flame, 2017, 182, 216-224.	5.2	32
70	An Experimental and Theoretical Study of the Thermal Decomposition of C₄H₆ Isomers. Journal of Physical Chemistry A, 2017, 121, 3827-3850.	2.5	20
71	The fate of the tert-butyl radical in low-temperature autoignition reactions. Journal of Chemical Physics, 2017, 146, 194304.	3.0	17
72	Kinetic barriers, rate constants and branching ratios for unimolecular reactions of methyl octanoate peroxy radicals: A computational study of a mid-sized biodiesel fuel surrogate. Combustion and Flame, 2017, 180, 148-157.	5.2	15
73	Reaction Mechanisms on Multiwell Potential Energy Surfaces in Combustion (and Atmospheric) Chemistry. Annual Review of Physical Chemistry, 2017, 68, 233-260.	10.8	55

#	Article	IF	Citations
74	First kinetic study of the atmospherically important reactions BrHgË™ + NO2 and BrHgË™ + HOO. Physical Chemistry Chemical Physics, 2017, 19, 1826-1838.	2.8	51
75	Investigation of the two- and three-fragment photodissociation of the tert-butyl peroxy radical at 248 nm. Journal of Chemical Physics, 2017, 147, 134304.	3.0	5
76	RRKM and master equation kinetic analysis of parallel addition reactions of isomeric radical intermediates in hydrocarbon flames. Journal of Chemical Physics, 2017, 147, 054306.	3.0	5
77	Degradation of Carbonyl Hydroperoxides in the Atmosphere and in Combustion. Journal of the American Chemical Society, 2017, 139, 15821-15835.	13.7	34
78	A comprehensive experimental and kinetic modeling study of n-propylbenzene combustion. Combustion and Flame, 2017, 186, 178-192.	5.2	40
79	A chemical kinetic study of the oxidation of dibutyl-ether in a jet-stirred reactor. Combustion and Flame, 2017, 185, 4-15.	5.2	58
80	A Theoretical and Computational Analysis of the Methyl-Vinyl + O2 Reaction and Its Effects on Propene Combustion. Journal of Physical Chemistry A, 2017, 121, 9173-9184.	2.5	23
81	Advances in rapid compression machine studies of low- and intermediate-temperature autoignition phenomena. Progress in Energy and Combustion Science, 2017, 63, 1-78.	31.2	180
82	Experimental and modeling study of 1-octene jet-stirred reactor oxidation. Fuel, 2017, 207, 763-775.	6.4	10
83	Cyclopentane combustion chemistry. Part I: Mechanism development and computational kinetics. Combustion and Flame, 2017, 183, 358-371.	5.2	51
84	Theoretical studies for reaction kinetics of cy-C6H11CH2 radical with O2. Proceedings of the Combustion Institute, 2017, 36, 179-186.	3.9	25
85	From theoretical reaction dynamics to chemical modeling of combustion. Proceedings of the Combustion Institute, 2017, 36, 77-111.	3.9	199
86	Ignition of a lean PRF/air mixture under RCCI/SCCI conditions: Chemical aspects. Proceedings of the Combustion Institute, 2017, 36, 3587-3596.	3.9	52
87	Hot Î²-scission of radicals formed via hydrogen abstraction. Proceedings of the Combustion Institute, 2017, 36, 135-142.	3.9	12
88	Elucidating reactivity regimes in cyclopentane oxidation: Jet stirred reactor experiments, computational chemistry, and kinetic modeling. Proceedings of the Combustion Institute, 2017, 36, 469-477.	3.9	34
89	Photooxidation of cyclohexene in the presence of SO₂: SOA yield and chemical composition. Atmospheric Chemistry and Physics, 2017, 17, 13329-13343.	4.9	40
90	The multichannel n-propyl + O2 reaction surface: Definitive theory on a model hydrocarbon oxidation mechanism. Journal of Chemical Physics, 2018, 148, .	3.0	14
91	High-Pressure Limit Rate Rules for Î±-H Isomerization of Hydroperoxyalkylperoxy Radicals. Journal of Physical Chemistry A, 2018, 122, 3626-3639.	2.5	22

#	Article	IF	Citations
92	High temperature pyrolysis of 2-methyl furan. Physical Chemistry Chemical Physics, 2018, 20, 10826-10837.	2.8	17
93	A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants. Combustion and Flame, 2018, 191, 252-269.	5.2	36
94	Ab initio kinetics on low temperature oxidation of iso-pentane: The first oxygen addition. Combustion and Flame, 2018, 190, 119-132.	5.2	25
95	Assessing the Molecular Basis of the Fuel Octane Scale: A Detailed Investigation on the Rate Controlling Steps of the Autoignition of Heptane and Isooctane. Journal of Physical Chemistry A, 2018, 122, 610-630.	2.5	3
96	An experimental chemical kinetic study of the oxidation of diethyl ether in a jet-stirred reactor and comprehensive modeling. Combustion and Flame, 2018, 193, 453-462.	5.2	43
97	Relative Rates of Hydrogen Shift Isomerizations Depend Strongly on Multiple-Structure Anharmonicity. Journal of the American Chemical Society, 2018, 140, 17556-17570.	13.7	14
98	An experimental and chemical kinetic modeling study of 1,3-butadiene combustion: Ignition delay time and laminar flame speed measurements. Combustion and Flame, 2018, 197, 423-438.	5.2	432
99	Computational Kinetics of Hydroperoxybutylperoxy Isomerizations and Decompositions: A Study of the Effect of Hydrogen Bonding. Journal of Physical Chemistry A, 2018, 122, 6277-6291.	2.5	7
100	Hydrogen shift isomerizations in the kinetics of the second oxidation mechanism of alkane combustion. Reactions of the hydroperoxypentylperoxy OOQOOH radical. Combustion and Flame, 2018, 197, 88-101.	5.2	24
101	Sparsity Facilitates Chemical-Reaction Selection for Engine Simulations. Journal of Physical Chemistry A, 2018, 122, 7227-7237.	2.5	1
102	Methylcyclohexane pyrolysis and oxidation in a jet-stirred reactor. Proceedings of the Combustion Institute, 2019, 37, 409-417.	3.9	40
103	Investigation of the low-temperature oxidation of n-butanal in a jet-stirred reactor. Proceedings of the Combustion Institute, 2019, 37, 453-460.	3.9	12
104	Developing detailed chemical kinetic mechanisms for fuel combustion. Proceedings of the Combustion Institute, 2019, 37, 57-81.	3.9	228
105	New insights into propanal oxidation at low temperatures: An experimental and kinetic modeling study. Proceedings of the Combustion Institute, 2019, 37, 565-573.	3.9	21
106	High-pressure oxidation of propane. Proceedings of the Combustion Institute, 2019, 37, 461-468.	3.9	48
107	Kinetics and thermochemistry of the reaction of 3-methylpropargyl radical with molecular oxygen. Proceedings of the Combustion Institute, 2019, 37, 299-306.	3.9	4
108	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
109	Theoretical study on the gas phase reaction of CH2O + NH3: the formation of CH2Oâ‹¯NH3, NH2CH2OH, or CH2NH + H2O. Physical Chemistry Chemical Physics, 2019, 21, 19242-19251.	2.8	13

#	Article	IF	Citations
110	Influence of Different Core Mechanisms on Low-Temperature Combustion Characteristics of Large Hydrocarbon Fuels. Energy & Fuels, 2019, 33, 7835-7851.	5.1	3
111	Infrared spectroscopy of the n-propyl and i-propyl radicals in solid para-hydrogen. Journal of Molecular Spectroscopy, 2019, 363, 111170.	1.2	8
112	Chemical Kinetics of Hydrogen Atom Abstraction from Propargyl Sites by Hydrogen and Hydroxy Radicals. International Journal of Molecular Sciences, 2019, 20, 3227.	4.1	6
113	Oxidation Kinetics and Thermodynamics of Resonance-Stabilized Radicals: The Pent-1-en-3-yl + O₂ Reaction. Journal of Physical Chemistry A, 2019, 123, 7897-7910.	2.5	14
114	Reaction Pathways, Thermodynamics, and Kinetics of Cyclopentanone Oxidation Intermediates: A Theoretical Approach. Journal of Physical Chemistry A, 2019, 123, 9644-9657.	2.5	6
115	A detailed chemical mechanism for low to high temperature oxidation of n-butylcyclohexane and its validation. Combustion and Flame, 2019, 210, 360-373.	5.2	24
116	Chemical kinetic study of triptane (2,2,3-trimethylbutane) as an anti-knock additive. Combustion and Flame, 2019, 210, 399-412.	5.2	3
117	A chemical pathway perspective on the kinetics of low-temperature ignition of propane. Combustion and Flame, 2019, 202, 154-178.	5.2	6
118	Decomposition kinetics for HONO and HNO₂. Reaction Chemistry and Engineering, 2019, 4, 323-333.	3.7	52
119	Ignition Study of an Oxygenated and High-Alkene Light Petroleum Fraction Produced from Automotive Shredder Residues. Energy & Fuels, 2019, 33, 5664-5672.	5.1	7
120	Low to intermediate temperature oxidation studies of dimethoxymethane/n-heptane blends in a jet-stirred reactor. Combustion and Flame, 2019, 207, 20-35.	5.2	23
121	Theoretical Study on Reactions of Alkylperoxy Radicals. Journal of Physical Chemistry A, 2019, 123, 3949-3958.	2.5	11
122	2,5-Dimethyltetrahydrofuran combustion: Ignition delay times at high and low temperatures, speciation measurements and detailed kinetic modeling. Combustion and Flame, 2019, 203, 341-351.	5.2	19
123	Theoretical study of hydrogen abstraction by small radicals from cyclohexane-carbonyl-hydroperoxide. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
124	Temperature and Pressure Dependent Rate Coefficients for the Reaction of Ketene with Hydroxyl Radical. Journal of Physical Chemistry A, 2019, 123, 2483-2496.	2.5	13
125	High-pressure pyrolysis and oxidation of DME and DME/CH4. Combustion and Flame, 2019, 205, 80-92.	5.2	58
126	Exploring hydroperoxides in combustion: History, recent advances and perspectives. Progress in Energy and Combustion Science, 2019, 73, 132-181.	31.2	119
127	Reaction Mechanisms and Kinetics of the Hydrogen Abstraction Reactions of C4â€“C6 Alkenes with Hydroxyl Radical: A Theoretical Exploration. International Journal of Molecular Sciences, 2019, 20, 1275.	4.1	19

#	Article	IF	Citations
128	Computational study on the mechanism and kinetics for the reaction between HO₂ and n-propyl peroxy radical. RSC Advances, 2019, 9, 40437-40444.	3.6	5
129	Predictive kinetics for the thermal decomposition of RDX. Proceedings of the Combustion Institute, 2019, 37, 3167-3173.	3.9	34
130	Intramolecular Hydrogen Shift Chemistry of Hydroperoxy-Substituted Peroxy Radicals. Journal of Physical Chemistry A, 2019, 123, 590-600.	2.5	31
131	A computational investigation into the combustion byproducts of a liquid monopropellant. Proceedings of the Combustion Institute, 2019, 37, 5671-5677.	3.9	6
132	A computational investigation into the kinetics of NO + CH2CCH and its effect on NO reduction. Proceedings of the Combustion Institute, 2019, 37, 687-694.	3.9	6
133	Reactions of Î²-hydroxypropyl radicals with O2 on the HOC3H6OOâ€¢ potential energy surfaces: A theoretical study. Combustion and Flame, 2020, 211, 202-217.	5.2	10
134	A high pressure oxidation study of di-n-propyl ether. Fuel, 2020, 263, 116554.	6.4	14
135	Mechanisms and kinetics of the low-temperature oxidation of 2-methylfuran: insight from DFT calculations and kinetic simulations. Physical Chemistry Chemical Physics, 2020, 22, 3290-3303.	2.8	6
136	Comparative Chemical Kinetic Analysis and Skeletal Mechanism Generation for Syngas Combustion with NO_x Chemistry. Energy & Fuels, 2020, 34, 949-964.	5.1	19
137	The influence of iso-butene kinetics on the reactivity of di-isobutylene and iso-octane. Combustion and Flame, 2020, 222, 186-195.	5.2	31
138	Computational studies on the gas phase reaction of methylenimine (CH2NH) with water molecules. Scientific Reports, 2020, 10, 10995.	3.3	11
139	Kinetics of iso-butyl radical reaction with O2 in combustion: The first and second oxygen addition. Combustion and Flame, 2020, 220, 429-438.	5.2	8
140	An experimental and modeling study of ethyleneâ€“air combustion over a wide temperature range. Combustion and Flame, 2020, 221, 20-40.	5.2	22
141	Pressure-dependent kinetics of peroxy radicals formed in isobutanol combustion. Physical Chemistry Chemical Physics, 2020, 22, 19802-19815.	2.8	4
142	Ab initio kinetics predictions for the role of pre-reaction complexes in hydrogen abstraction from 2-butanone by OH radicals. RSC Advances, 2020, 10, 33205-33212.	3.6	6
143	Hindered rotor benchmarks for the transition states of free radical additions to unsaturated hydrocarbons. Physical Chemistry Chemical Physics, 2020, 22, 27241-27254.	2.8	2
144	Theoretical calculation of low-temperature oxidation of heptyl radicals and O2. Combustion and Flame, 2020, 217, 274-284.	5.2	14
145	Automatic construction of transition states and on-the-fly accurate kinetic calculations for reaction classes in automated mechanism generators. Computational and Theoretical Chemistry, 2020, 1184, 112852.	2.5	7

#	Article	IF	Citations
146	Study of low and high temperature oxidation of n-pentane at supercritical conditions in a jet stirred reactor. IOP Conference Series: Materials Science and Engineering, 2020, 715, 012065.	0.6	0
147	Energetics and mechanisms for the acetonyl radical + O2 reaction: An important system for atmospheric and combustion chemistry. Journal of Chemical Physics, 2020, 152, 114301.	3.0	5
148	Global uncertainty analysis for the RRKM/master equation modeling of a typical multi-well and multi-channel reaction system. Combustion and Flame, 2020, 216, 62-71.	5.2	13
149	Exploring the Chemistry of Lowâ€Temperature Ignition by Pressureâ€Accelerated Dynamics. ChemSystemsChem, 2020, 2, e1900043.	2.6	9
150	Experimental and modeling study of the low to high temperature oxidation of the linear pentanone isomers: 2-pentanone and 3-pentanone. Combustion and Flame, 2020, 216, 29-44.	5.2	14
151	Experimental and kinetic modeling investigation on ethylcyclohexane low-temperature oxidation in a jet-stirred reactor. Combustion and Flame, 2020, 214, 211-223.	5.2	31
152	An experimental and kinetic modeling study of the auto-ignition of natural gas blends containing C1â€“C7 alkanes. Proceedings of the Combustion Institute, 2021, 38, 365-373.	3.9	51
153	Insights on keto-hydroperoxide formation from O2 addition to the beta-tetrahydrofuran radical. Proceedings of the Combustion Institute, 2021, 38, 533-541.	3.9	5
154	A theoretical kinetics study on low-temperature oxidation of n-C4H9 radicals. Proceedings of the Combustion Institute, 2021, 38, 681-689.	3.9	12
155	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
156	Insight into the low-temperature oxidation of dimethylamine radicals. Proceedings of the Combustion Institute, 2021, 38, 853-860.	3.9	5
157	A chemical kinetic perspective on the low-temperature oxidation of propane/propene mixtures through experiments and kinetic analyses. Combustion and Flame, 2021, 223, 361-375.	5.2	52
158	Higher Alcohol and Ether Biofuels for Compression-Ignition Engine Application: A Review with Emphasis on Combustion Kinetics. Energy & Fuels, 2021, 35, 1890-1917.	5.1	42
159	Ab initio rate coefficients for reactions of 2,5-dimethylhexyl isomers with O₂: temperature- and pressure-dependent branching ratios. Physical Chemistry Chemical Physics, 2021, 23, 6225-6240.	2.8	3
160	Itâ€™s a Gas: Oxidative Dehydrogenation of Propane over Boron Nitride Catalysts. Journal of Physical Chemistry C, 2021, 125, 5623-5634.	3.1	28
161	Exploring the chemical kinetics on oxygen addition reactions of o-xylyl radical at the low temperature. Combustion and Flame, 2021, 227, 95-105.	5.2	5
162	Theoretical Study on Reactions of Î±-Site Hydroxyethyl and Hydroxypropyl Radicals with O2. Journal of Physical Chemistry A, 2021, 125, 5423-5437.	2.5	1
163	Hydrogen shift isomerizations in the kinetics of the first and second oxidation mechanism of diethyl ether combustion. Computational and Theoretical Chemistry, 2021, 1202, 113340.	2.5	1

#	Article	IF	Citations
164	A comprehensive study on low-temperature oxidation chemistry of cyclohexane. I. Conformational analysis and theoretical study of first and second oxygen addition. Combustion and Flame, 2022, 235, 111658.	5.2	6
165	Experimental and kinetic modeling studies of furfural pyrolysis at low and atmospheric pressures. Journal of Analytical and Applied Pyrolysis, 2021, 157, 105161.	5.5	11
166	Influence of functional groups on low-temperature combustion chemistry of biofuels. Progress in Energy and Combustion Science, 2021, 86, 100925.	31.2	58
167	High-Pressure-Limit and Pressure-Dependent Rate Rules for Unimolecular Reactions Related to Hydroperoxy Alkyl Radicals in Normal Alkyl Cyclohexane Combustion. 1. Concerted HO2 Elimination Reaction Class and Î²-Scission Reaction Class. Journal of Physical Chemistry A, 2021, 125, 8942-8958.	2.5	9
168	A theoretical study of Î²-hydroxybutenyl with O2 on the HOC4H6OOÂ· potential energy surface. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
169	Strong dependence on multistructural anharmonicity of the relative rates of intramolecular H-migration in alkylperoxyl and methylcyclohexylperoxyl radicals. Combustion and Flame, 2021, 231, 111503.	5.2	6
170	Furan formation pathways exploration in low temperature oxidation of 1,3-butadiene, trans-2-butene, and cis-2-butene. Combustion and Flame, 2021, 232, 111519.	5.2	9
171	An experimental and detailed kinetic modeling study of the pyrolysis and oxidation of allene and propyne over a wide range of conditions. Combustion and Flame, 2021, 233, 111578.	5.2	26
172	Experimental and kinetic modeling investigation on 2,5-hexanedione oxidation in a jet-stirred reactor. Combustion and Flame, 2021, 234, 111648.	5.2	2
173	Mechanistic insights of the degradation of an O-anisidine carcinogenic pollutant initiated by OH radical attack: theoretical investigations. New Journal of Chemistry, 2021, 45, 5907-5924.	2.8	10
174	From electronic structure to combustion model application for acrolein chemistry part I: AcroleinÂ+ÂH reactions and related chemistry. Combustion and Flame, 2022, 240, 111825.	5.2	3
175	Chemistry of Simple Organic Peroxy Radicals under Atmospheric through Combustion Conditions: Role of Temperature, Pressure, and NO_x Level. Journal of Physical Chemistry A, 2021, 125, 10303-10314.	2.5	7
176	A comprehensive experimental and modeling study of n-propylcyclohexane oxidation. Combustion and Flame, 2022, 238, 111944.	5.2	10
177	Conformation-dependent low-temperature oxidation chemistry of methylcyclohexane: First oxygen addition and chain-branching. Combustion and Flame, 2022, 243, 111963.	5.2	8
178	Infrared spectroscopic signature of a hydroperoxyalkyl radical (â€¢QOOH). Journal of Chemical Physics, 2022, 156, 014301.	3.0	8
179	CH₂ + O₂: reaction mechanism, biradical and zwitterionic character, and formation of CH₂OO, the simplest Criegee intermediate. Physical Chemistry Chemical Physics, 2022, 24, 914-927.	2.8	4
180	A detailed chemical insights into the kinetics of diethyl ether enhancing ammonia combustion and the importance of NOx recycling mechanism. Fuel Communications, 2022, 10, 100051.	5.2	46
181	Combustion chemistry of alkenes and alkadienes. Progress in Energy and Combustion Science, 2022, 90, 100983.	31.2	28

#	Article	IF	Citations
182	A Hierarchical Theoretical Study of the Hydrogen Abstraction Reactions of H₂/C₁â€“C₄ Molecules by the Methyl Peroxy Radical and Implications for Kinetic Modeling. ACS Omega, 2022, 7, 8675-8685.	3.5	2
183	Revisiting low temperature oxidation chemistry of n-heptane. Combustion and Flame, 2022, 242, 112177.	5.2	15
184	Dissociation-Induced Depletion of High-Energy Reactant Molecules as a Mechanism for Pressure-Dependent Rate Constants for Bimolecular Reactions. Faraday Discussions, 0, , .	3.2	1
185	Kinetic insights into plasma-assisted low-temperature oxidation of propane with synchrotron photoionization mass spectrometry. Proceedings of the Combustion Institute, 2023, 39, 5499-5509.	3.9	2
186	Helium droplet infrared spectroscopy of the butyl radicals. Journal of Chemical Physics, 2022, 157, 084311.	3.0	0
187	Characterization of the low-temperature oxidation chemistry of an unsaturated aldehyde 2-butenal in a Jet-stirred reactor. Proceedings of the Combustion Institute, 2022, , .	3.9	2
188	A comprehensive experimental and kinetic modeling study of di-isobutylene isomers: Part 1. Combustion and Flame, 2023, 251, 112301.	5.2	2
189	Experimental and kinetic studies of extinction limits of counterflow cool and hot diffusion flames of ammonia/n-dodecane. Combustion and Flame, 2022, 245, 112316.	5.2	11
190	The effect of the addition of nitrogen oxides on the oxidation of propane: An experimental and modeling study. Combustion and Flame, 2022, 245, 112306.	5.2	17
191	The kinetic model of ethylcyclohexane combustion over a wide temperature range and its comprehensive validation. Combustion and Flame, 2022, 245, 112307.	5.2	2
192	An experimental and kinetic modeling investigation on lowâ€temperature oxidation chemistry of 1,3,5â€trimethylcyclohexane in a jetâ€stirred reactor. Combustion and Flame, 2022, 245, 112365.	5.2	1
193	Recent advances in oxidative dehydrogenation of propane to propylene on boron-based catalysts. Catalysis Reviews - Science and Engineering, 0, , 1-80.	12.9	4
194	Effects of Oxygen: Experimental and VTST/DFT Studies on Cumene Autoxidation with Air under Atmospheric Pressure. ACS Omega, 2022, 7, 34547-34553.	3.5	1
195	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.	3.9	2
196	Experimental and modeling study of the low to high-temperature oxidation of the methyl isopropyl ketone in O2/N2/Ar and O2/CO2/Ar atmospheres. Proceedings of the Combustion Institute, 2023, 39, 315-324.	3.9	2
197	Modeling Formic Acid Combustion. Energy & Fuels, 2022, 36, 14382-14392.	5.1	2
198	Exploring low-temperature oxidation of methacrolein with insights into fuel molecular structure effects. Combustion and Flame, 2023, 248, 112528.	5.2	0
199	A wide range experimental study and further development of a kinetic model describing propane oxidation. Combustion and Flame, 2023, 248, 112562.	5.2	10

#	Article	IF	Citations
200	A workflow for automatic generation and efficient refinement of individual pressure-dependent networks. Combustion and Flame, 2023, 257, 112516.	5.2	3
201	Green synthesis of propylene oxide directly from propane. Nature Communications, 2022, 13, .	12.8	10
202	From electronic structure to model application for alkyl cyclohexane combustion chemistry: H-atom abstraction reactions by HÈ®₂radical. Physical Chemistry Chemical Physics, 2023, 25, 10795-10810.	2.8	3
203	Modelling of acetaldehyde and acetic acid combustion. Combustion Theory and Modelling, 2023, 27, 536-557.	1.9	2
204	Experimental and Updated Kinetic Modeling Study of Neopentane Low Temperature Oxidation. Journal of Physical Chemistry A, 2023, 127, 2113-2122.	2.5	4
205	Measurement of the Intramolecular Hydrogen-Shift Rate Coefficient for the CH₃SCH₂OO Radical between 314 and 433 K. Journal of Physical Chemistry A, 2023, 127, 2336-2350.	2.5	5
206	Effect of formic acid on O₂ + OHË™CHOH â†' HCOOH + HO₂ reaction under tropospheric condition: kinetics of cis and trans isomers. Physical Chemistry Chemical Physics, 2023, 25, 9965-9978.	2.8	2
207	Theoretical Study of Intramolecular H-Migration Reactions of Peroxyl Radicals of JP-10 (Exo-Tetrahydrodicyclopentadiene). Combustion Science and Technology, 0, , 1-18.	2.3	0
208	An experimental and theoretical kinetic modeling study of the thermal decomposition of methyl-2-methyl butanoate behind shock waves. Combustion and Flame, 2023, 254, 112835.	5.2	0
209	Temperature -and pressure-dependent branching ratios for 2,6-dimethylheptyl radicals (C9H19)Â+ÂO2 reaction: An ab initio and RRKM/ME approach on a key component of bisabolane biofuel. Fuel, 2023, 351, 128969.	6.4	0
210	Experimental and kinetic modeling study of low-temperature oxidation of n-pentane. Combustion and Flame, 2023, 254, 112813.	5.2	3
211	Isomeric effects on the reactivity of branched alkenes: An experimental and kinetic modeling study of methylbutenes. Combustion and Flame, 2023, 254, 112849.	5.2	1
212	The multichannel i-propyl + O2 reaction system: A model of secondary alkyl radical oxidation. Journal of Chemical Physics, 2023, 159, .	3.0	0
213	Highâ€pressure oxidation of nâ€butane. International Journal of Chemical Kinetics, 0, , .	1.6	1
214	A Theoretical Kinetic Study on Concerted Elimination Reaction Class of Peroxyl-hydroperoxyl-alkyl Radicals (â€¢OOQOOH) in Normal-alkyl Cyclohexanes. Molecules, 2023, 28, 6612.	3.8	1
215	Can a single ammonia and water molecule enhance the formation of methanimine under tropospheric conditions?: kinetics of â€¢CH2NH2 + O2 (+NH3/H2O). Frontiers in Chemistry, 0, 11, .	3.6	0
216	Elucidating the mechanism of 1,3-butadiene oxidation with O2: A DFT study. Journal of Molecular Structure, 2024, 1298, 137109.	3.6	0
217	An experimental and chemical kinetic modeling study of octane isomer oxidation. Part 1: 2,3,4-trimethyl pentane. Combustion and Flame, 2023, , 113226.	5.2	1

#	Article	IF	Citations
218	Development of a Gasoline and Jet Fuel Blend Kinetic Mechanism using Hybrid Response Surface Networks. , 2024, , .		0
219	An experimental and chemical kinetic modeling study of octane isomer oxidation. Part 2: 223- and 224-trimethylpentane. Combustion and Flame, 2024, 263, 113341.	5.2	0
220	A comprehensive experimental and kinetic modeling study of p-cymene oxidation. Combustion and Flame, 2024, 262, 113337.	5.2	0
221	Multichannel kinetics of methoxymethyl + O2 in combustion. Combustion and Flame, 2024, 262, 113339.	5.2	0
222	A machine learning method to predict rate constants for various reactions in combustion kinetic models. Combustion and Flame, 2024, 263, 113375.	5.2	0
223	Intramolecular Catalytic Hydrogen Atom Transfer (CHAT). Journal of Physical Chemistry A, 2024, 128, 2169-2190.	2.5	0