

John M Simmie

List of Publications by Year in descending order

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122
papers

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38742

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133
docs citations

133
times ranked

3379
citing authors

#	ARTICLE	IF	CITATIONS
1	A comprehensive modeling study of hydrogen oxidation. <i>International Journal of Chemical Kinetics</i> , 2004, 36, 603-622.	1.6	833
2	Detailed chemical kinetic models for the combustion of hydrocarbon fuels. <i>Progress in Energy and Combustion Science</i> , 2003, 29, 599-634.	31.2	410
3	Bio-butanol: Combustion properties and detailed chemical kinetic model. <i>Combustion and Flame</i> , 2010, 157, 363-373.	5.2	267
4	Autoignition measurements and a validated kinetic model for the biodiesel surrogate, methyl butanoate. <i>Combustion and Flame</i> , 2008, 153, 2-32.	5.2	228
5	Methane/propane oxidation at high pressures: Experimental and detailed chemical kinetic modeling. <i>Proceedings of the Combustion Institute</i> , 2007, 31, 447-454.	3.9	216
6	Benchmarking Compound Methods (CBS-QB3, CBS-APNO, G3, G4, W1BD) against the Active Thermochemical Tables: A Litmus Test for Cost-Effective Molecular Formation Enthalpies. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7235-7246.	2.5	174
7	Experimental and Modeling Study of C ₅ H ₁₀ O ₂ Ethyl and Methyl Esters. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4001-4014.	2.5	157
8	Experimental and Modeling Study of Methyl Cyclohexane Pyrolysis and Oxidation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 114-131.	2.5	146
9	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels: Ethyl Propanoate and Methyl Butanoate. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3727-3739.	2.5	145
10	A comprehensive experimental and detailed chemical kinetic modelling study of 2,5-dimethylfuran pyrolysis and oxidation. <i>Combustion and Flame</i> , 2013, 160, 2291-2318.	5.2	143
11	The oxidation and ignition of dimethylether from low to high temperature (500–1600 K): Experiments and kinetic modeling. <i>Proceedings of the Combustion Institute</i> , 1998, 27, 361-369.	0.3	141
12	Burning velocities of dimethyl ether and air. <i>Combustion and Flame</i> , 2001, 125, 1329-1340.	5.2	141
13	Methyl formate oxidation: Speciation data, laminar burning velocities, ignition delay times, and a validated chemical kinetic model. <i>International Journal of Chemical Kinetics</i> , 2010, 42, 527-549.	1.6	134
14	Benchmarking Compound Methods (CBS-QB3, CBS-APNO, G3, G4, W1BD) against the Active Thermochemical Tables: Formation Enthalpies of Radicals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8922-8933.	2.5	126
15	A rapid compression machine study of the oxidation of propane in the negative temperature coefficient regime. <i>Combustion and Flame</i> , 2008, 153, 316-333.	5.2	123
16	A high temperature and atmospheric pressure experimental and detailed chemical kinetic modelling study of 2-methyl furan oxidation. <i>Proceedings of the Combustion Institute</i> , 2013, 34, 225-232.	3.9	121
17	The influence of fuel structure on combustion as demonstrated by the isomers of heptane: a rapid compression machine study. <i>Proceedings of the Combustion Institute</i> , 2005, 30, 2639-2647.	3.9	118
18	Methane/ethane/propane mixture oxidation at high pressures and at high, intermediate and low temperatures. <i>Combustion and Flame</i> , 2008, 155, 441-448.	5.2	111

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19	A Multiple Shock Tube and Chemical Kinetic Modeling Study of Diethyl Ether Pyrolysis and Oxidation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9098-9109.	2.5	108
20	Accurate Benchmark Calculation of the Reaction Barrier Height for Hydrogen Abstraction by the Hydroperoxyl Radical from Methane. Implications for C_nH_{2n+2} where $n = 2-4$. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7047-7054.	2.5	105
21	The pyrolysis of 2-methylfuran: a quantum chemical, statistical rate theory and kinetic modelling study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5349.	2.8	104
22	Enthalpies of Formation and Bond Dissociation Energies of Lower Alkyl Hydroperoxides and Related Hydroperoxy and Alkoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2008, 112, 5010-5016.	2.5	98
23	The combustion chemistry of a fuel tracer: Measured flame speeds and ignition delays and a detailed chemical kinetic model for the oxidation of acetone. <i>Combustion and Flame</i> , 2009, 156, 494-504.	5.2	98
24	Critical Evaluation of Thermochemical Properties of C_1-C_4 Species: Updated Group-Contributions to Estimate Thermochemical Properties. <i>Journal of Physical and Chemical Reference Data</i> , 2015, 44, .	4.2	93
25	Shock tube ignition of ethanol, isobutene and MTBE: Experiments and modeling. <i>Proceedings of the Combustion Institute</i> , 1992, 24, 769-776.	0.3	89
26	Simulation of methane autoignition in a rapid compression machine with creviced pistons. <i>Combustion and Flame</i> , 2001, 124, 326-329.	5.2	87
27	A shock tube and chemical kinetic modeling study of the pyrolysis and oxidation of butanols. <i>Combustion and Flame</i> , 2012, 159, 2009-2027.	5.2	87
28	CFD studies of a twin-piston rapid compression machine. <i>Combustion and Flame</i> , 2005, 141, 417-430.	5.2	84
29	Barrier heights for H-atom abstraction by H_2O_2 from <i>n</i> -butanol: A simple yet exacting test for model chemistries?. <i>Journal of Computational Chemistry</i> , 2010, 31, 1236-1248.	3.3	80
30	Formation Enthalpies and Bond Dissociation Energies of Alkylfurans. The Strongest C-X Bonds Known?. <i>Journal of Physical Chemistry A</i> , 2009, 113, 5128-5137.	2.5	80
31	Ab Initio Study of the Decomposition of 2,5-Dimethylfuran. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8877-8888.	2.5	80
32	Rate constants for hydrogen-abstraction by O from <i>n</i> -butanol. <i>Combustion and Flame</i> , 2011, 158, 726-731.	5.2	78
33	Oxidation of dimethoxymethane in a jet-stirred reactor. <i>Combustion and Flame</i> , 2001, 125, 1106-1117.	5.2	77
34	A high pressure shock tube study of <i>n</i> -propylbenzene oxidation and its comparison with <i>n</i> -butylbenzene. <i>Combustion and Flame</i> , 2012, 159, 2219-2232.	5.2	76
35	High-temperature oxidation of ethanol. Part 1. Ignition delays in shock waves. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1991, 87, 1691-1696.	1.7	74
36	Kinetics and Thermochemistry of 2,5-Dimethyltetrahydrofuran and Related Oxolanes: Next-Generation Biofuels. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4528-4538.	2.5	74

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37	The development of a detailed chemical kinetic mechanism for diisobutylene and comparison to shock tube ignition times. Proceedings of the Combustion Institute, 2007, 31, 377-384.	3.9	73
38	The effect of diluent gases on ignition delay times in the shock tube and in the rapid compression machine. Combustion and Flame, 2007, 151, 289-302.	5.2	72
39	Methane/propane mixture oxidation at high pressures and at high, intermediate and low temperatures. Combustion and Flame, 2008, 155, 451-461.	5.2	71
40	A jet-stirred reactor and kinetic modeling study of ethyl propanoate oxidation. Combustion and Flame, 2009, 156, 250-260.	5.2	64
41	Detailed chemical kinetic mechanisms of ethyl methyl, methyl tert-butyl and ethyl tert-butyl ethers: The importance of uni-molecular elimination reactions. Combustion and Flame, 2011, 158, 1032-1036.	5.2	64
42	High-temperature oxidation of ethanol. Part 2. Kinetic modelling. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 2549-2559.	1.7	63
43	Autoignition of heptanes; experiments and modeling. International Journal of Chemical Kinetics, 2005, 37, 728-736.	1.6	63
44	Rate constants for hydrogen abstraction by H_2O_2 from <i>n</i> -butanol. International Journal of Chemical Kinetics, 2012, 44, 155-164.	1.6	62
45	Experimental and modeling study of the oxidation of <i>n</i> -butylbenzene. Combustion and Flame, 2012, 159, 1399-1416.	5.2	59
46	Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine. , 0, , .		57
47	Ab initio and kinetic study of the reaction of ketones with OH for $T = 500\text{--}2000\text{ K}$. Part I: hydrogen-abstraction from $\text{H}_3\text{CC}(\text{O})\text{CH}_2(\text{CH}_2)_x$, $x = 0\text{--}2$. Physical Chemistry Chemical Physics, 2011, 13, 11175.	2.8	56
48	Uniqueness in the low temperature oxidation of cycloalkanes. Combustion and Flame, 2010, 157, 2357-2368.	5.2	54
49	The elimination of water from a conformationally complex alcohol: A computational study of the gas phase dehydration of <i>n</i> -butanol. Journal of Molecular Structure, 2009, 928, 149-157.	3.6	53
50	Thermochemistry of Acetylonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	2.5	52
51	Effects of molecular structure on oxidation reactivity of cyclic hydrocarbons: Experimental observations and conformational analysis. Combustion and Flame, 2010, 157, 2369-2379.	5.2	51
52	Ab Initio Chemical Kinetics of Methyl Formate Decomposition: The Simplest Model Biodiesel. Journal of Physical Chemistry A, 2010, 114, 5478-5484.	2.5	50
53	An ab initio/Rice-Ramsperger-Kassel-Marcus study of the hydrogen-abstraction reactions of methyl ethers, $\text{H}_3\text{COCH}_2(\text{CH}_2)_x$, $x = 0\text{--}2$, by H_2O ; mechanism and kinetics. Physical Chemistry Chemical Physics, 2010, 12, 7221.	2.8	50
54	Kinetics of the dehydrofluorination of vinyl fluoride in a single-pulse shock tube. The Journal of Physical Chemistry, 1970, 74, 992-994.	2.9	49

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55	Acetaldehyde Oxidation in a JSR and Ignition in Shock Waves: Experimental and Comprehensive Kinetic Modeling. <i>Combustion Science and Technology</i> , 1995, 107, 301-316.	2.3	46
56	A Database of Formation Enthalpies of Nitrogen Species by Compound Methods (CBS-QB3, CBS-APNO, Tj ETQq0 0.0 rgBT /Overlock 10	2.5	46
57	Experimental and Chemical Kinetic Modeling Study of 3-Pentanone Oxidation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12176-12186.	2.5	45
58	Thermochemistry of Methyl and Ethyl Nitro, RNO_2 , and Nitrite, RONO , Organic Compounds. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3172-3185.	2.5	44
59	Thermochemistry of C_7H_{16} to $\text{C}_{10}\text{H}_{22}$ Alkane Isomers: Primary, Secondary, and Tertiary C-H Bond Dissociation Energies and Effects of Branching. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9364-9379.	2.5	44
60	Chemical Kinetics of Hydrogen Atom Abstraction from Allylic Sites by HO_2 ; Implications for Combustion Modeling and Simulation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1890-1899.	2.5	44
61	The Ignition and Oxidation of Tetrahydrofuran: Experiments and Kinetic Modeling. <i>Combustion Science and Technology</i> , 1998, 135, 3-29.	2.3	43
62	Quantitative Structure-Activity Relationship Studies of Sulfamates RNHSO_3Na : Distinction between Sweet, Sweet-Bitter, and Bitter Molecules. <i>Journal of Agricultural and Food Chemistry</i> , 1998, 46, 3016-3026.	5.2	43
63	Energy Barriers for the Addition of H, H_3 , and H_5 to $\text{CH}_2\text{-CHX}$ [X = H, CH_3 , OH] and for H-Atom Addition to $\text{RCH}_2\text{-O}$ [R = H, CH_3 , H_5 , n-C $_3$ H $_7$]: Implications for the Gas-Phase Chemistry of Enols. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7834-7845.	2.5	40
64	The reaction of 2,5-dimethylfuran with hydrogen atoms: An experimental and theoretical study. <i>Proceedings of the Combustion Institute</i> , 2013, 34, 233-239.	3.9	40
65	Hydrogen Abstraction from n-Butanol by the Hydroxyl Radical: High Level Ab Initio Study of the Relative Significance of Various Abstraction Channels and the Role of Weakly Bound Intermediates. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5558-5564.	2.5	38
66	High-Level ab Initio Enthalpies of Formation of 2,5-Dimethylfuran, 2-Methylfuran, and Furan. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11768-11775.	2.5	38
67	Thermochemistry for enthalpies and reaction paths of nitrous acid isomers. <i>International Journal of Chemical Kinetics</i> , 2007, 39, 378-398.	1.6	35
68	A Shock Tube and Chemical Kinetic Modeling Study of Methyl Ethyl Ketone Oxidation. <i>Combustion Science and Technology</i> , 2010, 182, 574-587.	2.3	34
69	Substituent effects in the thermochemistry of furans: A theoretical (CBS-QB3, CBS-APNO and G3) study. <i>Journal of Chemical Thermodynamics</i> , 2013, 58, 117-128.	2.0	33
70	Kinetics of 1,2-Dimethylbenzene Oxidation and Ignition: Experimental and Detailed Chemical Kinetic Modeling. <i>Combustion Science and Technology</i> , 2008, 180, 1748-1771.	2.3	32
71	Modeling Nitrogen Species as Pollutants: Thermochemical Influences. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7192-7197.	2.5	32
72	The ignition and oxidation of allene and propyne: Experiments and kinetic modeling. <i>Proceedings of the Combustion Institute</i> , 1996, 26, 613-620.	0.3	31

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91	Combined Experimental and Theoretical Study of the Reactivity of $\hat{\text{I}}^3$ -Butyro- and Related Lactones, with the OH Radical at Room Temperature. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5013-5019.	2.5	14
92	The comparison of detailed chemical kinetic mechanisms: Application to the combustion of methane. <i>International Journal of Chemical Kinetics</i> , 2004, 36, 467-471.	1.6	13
93	An Organized Collection of Theoretical Gas-Phase Geometric, Spectroscopic, and Thermochemical Data of Oxygenated Hydrocarbons, $\text{C}_x\text{H}_y\text{O}_z$ ($x, y = 1, 2; z = 1 \hat{\text{a}}^{\text{c}}8$), of Relevance to Atmospheric, Astrochemical, and Combustion Sciences. <i>Journal of Physical and Chemical Reference Data</i> , 2020, 49, .	4.2	13
94	Preliminary observations on the high temperature oxidation of ethyltert-butyl ether. <i>International Journal of Chemical Kinetics</i> , 1991, 23, 553-558.	1.6	11
95	Ketene Thermochemistry. <i>ChemPhysChem</i> , 2008, 9, 700-702.	2.1	11
96	The Unimolecular Decomposition and H Abstraction Reactions by HO and HO[sub 2] from n-Butanol. , 2009, , .		11
97	Thermochemistry and Kinetics of Angelica and Cognate Lactones. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4172-4183.	2.5	11
98	An experimental and kinetic modeling study of $\hat{\text{I}}^3$ -valerolactone pyrolysis. <i>Combustion and Flame</i> , 2016, 164, 183-200.	5.2	11
99	Allene isomerisation. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1978, 74, 1337.	1.0	10
100	Kinetic study of a retro Diels-Alder reaction in a single-pulse shock tube: Decyclization of 1-methylcyclohex-1-ene. <i>International Journal of Chemical Kinetics</i> , 1978, 10, 227-231.	1.6	9
101	A Quantum Chemical Study of the Abnormal Reactivity of 2 $\hat{\text{a}}$ Methoxyfuran. <i>International Journal of Chemical Kinetics</i> , 2013, 45, 531-541.	1.6	9
102	Pyrolysis Pathways of the Furanic Ether 2-Methoxyfuran. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9962-9977.	2.5	9
103	Barriometry $\hat{\text{a}}^{\text{c}}$ an enhanced database of accurate barrier heights for gas-phase reactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10732-10740.	2.8	9
104	The reactions of sulfuryl chloride with $[\text{Fe}_2(\hat{\text{I}}\text{-C}_5\text{H}_5)_2(\text{CO})_4\text{-n}(\text{CNMe})_n]$ ($n = 0, 1, 2$ and 4) and related complexes. The crystal structure of $[\text{Fe}(\hat{\text{I}}\text{-C}_9\text{H}_7)(\text{CO})_3][\text{FeCl}_4]$. <i>Journal of Organometallic Chemistry</i> , 1988, 338, 383-392.	1.8	8
105	The taste of monosubstituted phenylsulphamates. <i>Journal of the Chemical Society Chemical Communications</i> , 1989, , 545.	2.0	8
106	High-temperature oxidation of ethylene oxide in shock waves. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 715-721.	1.7	8
107	The ignition of oxetane in shock waves and oxidation in a jet-stirred reactor: An experimental and kinetic modeling study. <i>Combustion and Flame</i> , 1997, 110, 409-417.	5.2	8
108	Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the estimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1 $\hat{\text{a}}$ C5 oxygenates. <i>Molecular Physics</i> , 2015, 113, 1630-1635.	1.7	8

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109	A W1 computational study on the kinetics of initial pyrolysis of a biodiesel model: methyl propanoate. <i>New Journal of Chemistry</i> , 2021, 45, 19531-19541.	2.8	7
110	Thermal Decomposition of 2(3H) and 2(5H) Furanones: Theoretical Aspects. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6919-6927.	2.5	6
111	H-Atom Abstraction Reactions by Ground-State Ozone from Saturated Oxygenates. <i>Journal of Physical Chemistry A</i> , 2017, 121, 8053-8060.	2.5	6
112	Snakes on the Rungs of Jacob's Ladder: Anomalous Vibrational Spectra from Double-Hybrid DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6899-6902.	2.5	6
113	C ₂ H ₅ NO Isomers: From Acetamide to 1,2-Oxazetidine and Beyond. <i>Journal of Physical Chemistry A</i> , 2022, 126, 924-939.	2.5	5
114	The thermolysis of hexamethyldisilane. <i>Chemical Communications / Chemical Society, London</i> , 1968, , 1426.	0.1	4
115	Vibrational relaxation in OCS mixtures. Part 1. "Measured relaxation times for pure OCS and for OCS in mixtures with helium-4, helium-3, normal deuterium, ortho-deuterium, HD, normal hydrogen and para-hydrogen. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1976, 72, 417-422.	1.1	4
116	Crystallization of Organic Salts from the Gas Phase: When Does Proton Transfer Take Place?. <i>Crystal Growth and Design</i> , 2021, 21, 23-27.	3.0	4
117	Differences in Coformer Interactions of the 2,4-Diaminopyrimidines Pyrimethamine and Trimethoprim. <i>Crystal Growth and Design</i> , 2022, 22, 3163-3173.	3.0	4
118	Automatic comparison of thermodynamic data for species in detailed chemical kinetic modeling. <i>International Journal of Chemical Kinetics</i> , 2005, 37, 341-345.	1.6	3
119	Ethyl lactate: a sinister molecule exhibiting high chemical diversity with potential as a "green" solvent. <i>International Journal of Chemical Kinetics</i> , 2021, 53, 457-464.	1.6	3
120	Comment on "Vibrational Relaxation Studies of the 10 ⁰ and 02 ⁰ States of Shock-Heated CO ₂ ". <i>Journal of Chemical Physics</i> , 1971, 55, 5842-5842.	3.0	2
121	Thermal decomposition of vinylidene fluoride behind reflected shock waves. <i>Challenge</i> , 1970, , 773.	0.4	1
122	Unknown Knowns: Case studies in uncertainties in the computation of thermochemical parameters. <i>Chemical Physics</i> , 2021, 550, 111251.	1.9	0