John M Simmie

List of Publications by Year
in descending order

122 papers	7,758 citations	38742 50 h-index	53230 85 g-index
133 all docs	133 docs citations	133 times ranked	3379 citing authors

#	Article	IF	Citations
1	C₂H₅NO Isomers: From Acetamide to 1,2-Oxazetidine and Beyond. Journal of Physical Chemistry A, 2022, 126, 924-939.	2.5	5
2	Differences in Coformer Interactions of the 2,4-Diaminopyrimidines Pyrimethamine and Trimethoprim. Crystal Growth and Design, 2022, 22, 3163-3173.	3.0	4
3	Ethyl lactate: a sinister molecule exhibiting high chemical diversity with potential as a â€œgreenâ€• solvent. International Journal of Chemical Kinetics, 2021, 53, 457-464.	1.6	3
4	Crystallization of Organic Salts from the Gas Phase: When Does Proton Transfer Take Place?. Crystal Growth and Design, 2021, 21, 23-27.	3.0	4
5	A W1 computational study on the kinetics of initial pyrolysis of a biodiesel model: methyl propanoate. New Journal of Chemistry, 2021, 45, 19531-19541.	2.8	7
6	Unknown Knowns: Case studies in uncertainties in the computation of thermochemical parameters. Chemical Physics, 2021, 550, 111251.	1.9	0
7	Snakes on the Rungs of Jacobâ€™s Ladder: Anomalous Vibrational Spectra from Double-Hybrid DFT Methods. Journal of Physical Chemistry A, 2020, 124, 6899-6902.	2.5	6
8	An Organized Collection of Theoretical Gas-Phase Geometric, Spectroscopic, and Thermochemical Data of Oxygenated Hydrocarbons, CxHyOz (x, y = 1, 2; z = 1â€“8), of Relevance to Atmospheric, Astrochemical, and Combustion Sciences. Journal of Physical and Chemical Reference Data, 2020, 49, .	4.2	13
9	Barriometry â€“ an enhanced database of accurate barrier heights for gas-phase reactions. Physical Chemistry Chemical Physics, 2018, 20, 10732-10740.	2.8	9
10	Chemical Kinetics of Hydrogen Atom Abstraction from Allylic Sites by ³O₂; Implications for Combustion Modeling and Simulation. Journal of Physical Chemistry A, 2017, 121, 1890-1899.	2.5	44
11	H-Atom Abstraction Reactions by Ground-State Ozone from Saturated Oxygenates. Journal of Physical Chemistry A, 2017, 121, 8053-8060.	2.5	6
12	Validation of a Database of Formation Enthalpies and of Mid-Level Model Chemistries. Journal of Physical Chemistry A, 2016, 120, 7370-7384.	2.5	26
13	Toward the Development of a Fundamentally Based Chemical Model for Cyclopentanone: High-Pressure-Limit Rate Constants for H Atom Abstraction and Fuel Radical Decomposition. Journal of Physical Chemistry A, 2016, 120, 7037-7044.	2.5	20
14	Modeling Nitrogen Species as Pollutants: Thermochemical Influences. Journal of Physical Chemistry A, 2016, 120, 7192-7197.	2.5	32
15	An experimental and kinetic modeling study of Î³-valerolactone pyrolysis. Combustion and Flame, 2016, 164, 183-200.	5.2	11
16	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 C1â€“C5 oxygenates. Molecular Physics, 2015, 113, 1630-1635.	1.7	8
17	Experimental and computational study of the initial decomposition of gamma-valerolactone. Proceedings of the Combustion Institute, 2015, 35, 515-523.	3.9	17
18	Benchmarking Compound Methods (CBS-QB3, CBS-APNO, G3, G4, W1BD) against the Active Thermochemical Tables: A Litmus Test for Cost-Effective Molecular Formation Enthalpies. Journal of Physical Chemistry A, 2015, 119, 7235-7246.	2.5	174

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19	Benchmarking Compound Methods (CBS-QB3, CBS-APNO, G3, G4, W1BD) against the Active Thermochemical Tables: Formation Enthalpies of Radicals. Journal of Physical Chemistry A, 2015, 119, 8922-8933.	2.5	126
20	Thermal Decomposition of 2(3H) and 2(5H) Furanones: Theoretical Aspects. Journal of Physical Chemistry A, 2015, 119, 6919-6927.	2.5	6
21	A Database of Formation Enthalpies of Nitrogen Species by Compound Methods (CBS-QB3, CBS-APNO,) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	46
22	Critical Evaluation of Thermochemical Properties of C1â€“C4 Species: Updated Group-Contributions to Estimate Thermochemical Properties. Journal of Physical and Chemical Reference Data, 2015, 44, .	4.2	93
23	Pyrolysis Pathways of the Furanic Ether 2-Methoxyfuran. Journal of Physical Chemistry A, 2015, 119, 9962-9977.	2.5	9
24	The pyrolysis of 2-methylfuran: a quantum chemical, statistical rate theory and kinetic modelling study. Physical Chemistry Chemical Physics, 2014, 16, 5349.	2.8	104
25	Thermochemistry of C₇H₁₆ to C₁₀H₂₂ Alkane Isomers: Primary, Secondary, and Tertiary Câ€“H Bond Dissociation Energies and Effects of Branching. Journal of Physical Chemistry A, 2014, 118, 9364-9379.	2.5	44
26	Combined Experimental and Theoretical Study of the Reactivity of Î³-Butyro- and Related Lactones, with the OH Radical at Room Temperature. Journal of Physical Chemistry A, 2014, 118, 5013-5019.	2.5	14
27	Thermochemistry and Kinetics of Angelica and Cognate Lactones. Journal of Physical Chemistry A, 2014, 118, 4172-4183.	2.5	11
28	A high temperature and atmospheric pressure experimental and detailed chemical kinetic modelling study of 2-methyl furan oxidation. Proceedings of the Combustion Institute, 2013, 34, 225-232.	3.9	121
29	Harmonising Production, Properties and Environmental Consequences of Liquid Transport Fuels from Biomassâ€”2,5â€Dimethylfuran as a Case Study. ChemSusChem, 2013, 6, 36-41.	6.8	30
30	Substituent effects in the thermochemistry of furans: A theoretical (CBS-QB3, CBS-APNO and G3) study. Journal of Chemical Thermodynamics, 2013, 58, 117-128.	2.0	33
31	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>	3.9	16
32	A comprehensive experimental and detailed chemical kinetic modelling study of 2,5-dimethylfuran pyrolysis and oxidation. Combustion and Flame, 2013, 160, 2291-2318.	5.2	143
33	The reaction of 2,5-dimethylfuran with hydrogen atoms â€“ An experimental and theoretical study. Proceedings of the Combustion Institute, 2013, 34, 233-239.	3.9	40
34	A Quantum Chemical Study of the Abnormal Reactivity of 2â€Methoxyfuran. International Journal of Chemical Kinetics, 2013, 45, 531-541.	1.6	9
35	High-Level ab Initio Enthalpies of Formation of 2,5-Dimethylfuran, 2-Methylfuran, and Furan. Journal of Physical Chemistry A, 2012, 116, 11768-11775.	2.5	38
36	Kinetics and Thermochemistry of 2,5-Dimethyltetrahydrofuran and Related Oxolanes: Next Next-Generation Biofuels. Journal of Physical Chemistry A, 2012, 116, 4528-4538.	2.5	74

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37	Experimental and modeling study of the oxidation of n-butylbenzene. Combustion and Flame, 2012, 159, 1399-1416.	5.2	59
38	A shock tube and chemical kinetic modeling study of the pyrolysis and oxidation of butanols. Combustion and Flame, 2012, 159, 2009-2027.	5.2	87
39	A high pressure shock tube study of n-propylbenzene oxidation and its comparison with n-butylbenzene. Combustion and Flame, 2012, 159, 2219-2232.	5.2	76
40	Rate constants for hydrogen abstraction by HÈ®₂ from nâ€butanol. International Journal of Chemical Kinetics, 2012, 44, 155-164.	1.6	62
41	Ab initio and kinetic study of the reaction of ketones with OÌ‡H for T = 500â€“2000 K. Part I: hydrogen-abstraction from H3CC(O)CH3â€“x(CH3)x, x = 0 â† 2. Physical Chemistry Chemical Physics, 2011, 13, 11175.	2.8	56
42	Ab Initio Study of the Decomposition of 2,5-Dimethylfuran. Journal of Physical Chemistry A, 2011, 115, 8877-8888.	2.5	80
43	Reduction of a detailed kinetic model for the ignition of methane/propane mixtures at gas turbine conditions using simulation error minimization methods. Combustion and Flame, 2011, 158, 1469-1479.	5.2	27
44	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
45	Rate constants for hydrogen-abstraction by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.gif" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mo>Ë™</mml:mo></mml:mrow></mml:mover><mml:mi mathvariant="normal">H</mml:mi></mml:mrow></mml:math>from n-butanol. Combustion and Flame, 2011, 158, 726-731.	5.2	78
46	Barrier heights for Hâ€atom abstraction by HÈ®₂ from nâ€butanolâ€”A simple yet exacting test for model chemistries?. Journal of Computational Chemistry, 2010, 31, 1236-1248.	3.3	80
47	Methyl formate oxidation: Speciation data, laminar burning velocities, ignition delay times, and a validated chemical kinetic model. International Journal of Chemical Kinetics, 2010, 42, 527-549.	1.6	134
48	Bio-butanol: Combustion properties and detailed chemical kinetic model. Combustion and Flame, 2010, 157, 363-373.	5.2	267
49	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
50	Uniqueness in the low temperature oxidation of cycloalkanes. Combustion and Flame, 2010, 157, 2357-2368.	5.2	54
51	A Multiple Shock Tube and Chemical Kinetic Modeling Study of Diethyl Ether Pyrolysis and Oxidation. Journal of Physical Chemistry A, 2010, 114, 9098-9109.	2.5	108
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	Experimental and Chemical Kinetic Modeling Study of 3-Pentanone Oxidation. Journal of Physical Chemistry A, 2010, 114, 12176-12186.	2.5	45
54	Oxidation of Acetone and Its Interaction with Nitric Oxide. Energy & Fuels, 2010, 24, 1511-1520.	5.1	16

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55	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. Journal of Physical Chemistry A, 2010, 114, 5558-5564.	2.5	38
56	An ab initio/Rice-Ramsperger-Kassel-Marcus study of the hydrogen-abstraction reactions of methyl ethers, H3COCH3â˜x(CH3)x, x = 0â€“2, by Ë™OH; mechanism and kinetics. Physical Chemistry Chemical Physics, 2010, 12, 7221.	2.8	50
57	A Shock Tube and Chemical Kinetic Modeling Study of Methy Ethyl Ketone Oxidation. Combustion Science and Technology, 2010, 182, 574-587.	2.3	34
58	The elimination of water from a conformationally complex alcohol: A computational study of the gas phase dehydration of n-butanol. Journal of Molecular Structure, 2009, 928, 149-157.	3.6	53
59	A jet-stirred reactor and kinetic modeling study of ethyl propanoate oxidation. Combustion and Flame, 2009, 156, 250-260.	5.2	64
60	The combustion chemistry of a fuel tracer: Measured flame speeds and ignition delays and a detailed chemical kinetic model for the oxidation of acetone. Combustion and Flame, 2009, 156, 494-504.	5.2	98
61	Formation Enthalpies and Bond Dissociation Energies of Alkylfurans. The Strongest Câ€”X Bonds Known?. Journal of Physical Chemistry A, 2009, 113, 5128-5137.	2.5	80
62	Energy Barriers for the Addition of H, ĂŠH3, and ĂŠ2H5 to CH2â•CHX [X = H, CH3, OH] and for H-Atom Addition to RCHâ•O [R = H, CH3, ĂŠ2H5, n-C3H7]: Implications for the Gas-Phase Chemistry of Enols. Journal of Physical Chemistry A, 2009, 113, 7834-7845.	2.5	40
63	The Unimolecular Decomposition and H Abstraction Reactions by HO and HO[sub 2] from n-Butanol. , 2009, , .		11
64	Methane/ethane/propane mixture oxidation at high pressures and at high, intermediate and low temperatures. Combustion and Flame, 2008, 155, 441-448.	5.2	111
65	Ketene Thermochemistry. ChemPhysChem, 2008, 9, 700-702.	2.1	11
66	A rapid compression machine study of the oxidation of propane in the negative temperature coefficient regime. Combustion and Flame, 2008, 153, 316-333.	5.2	123
67	Autoignition measurements and a validated kinetic model for the biodiesel surrogate, methyl butanoate. Combustion and Flame, 2008, 153, 2-32.	5.2	228
68	Methane/propane mixture oxidation at high pressures and at high, intermediate and low temperatures. Combustion and Flame, 2008, 155, 451-461.	5.2	71
69	Thermochemistry of Methyl and Ethyl Nitro, RNO₂, and Nitrite, RONO, Organic Compounds. Journal of Physical Chemistry A, 2008, 112, 3172-3185.	2.5	44
70	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 â† 4. Journal of Physical Chemistry A, 2008, 112, 7047-7054.	2.5	105
71	Enthalpies of Formation and Bond Dissociation Energies of Lower Alkyl Hydroperoxides and Related Hydroperoxy and Alkoxy Radicals. Journal of Physical Chemistry A, 2008, 112, 5010-5016.	2.5	98
72	Thermochemistry and kinetics of acetonylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. Physical Chemistry Chemical Physics, 2008, 10, 7139.	2.8	19

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73	Kinetics of 1,2-Dimethylbenzene Oxidation and Ignition: Experimental and Detailed Chemical Kinetic Modeling. Combustion Science and Technology, 2008, 180, 1748-1771.	2.3	32
74	Studying the chemistry of HCCI in rapid compression machines. International Journal of Vehicle Design, 2007, 44, 84.	0.3	25
75	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels:Â Ethyl Propanoate and Methyl Butanoateâ€. Journal of Physical Chemistry A, 2007, 111, 3727-3739.	2.5	145
76	Experimental and Modeling Study of C5H10O2Ethyl and Methyl Estersâ€. Journal of Physical Chemistry A, 2007, 111, 4001-4014.	2.5	157
77	Thermochemistry for enthalpies and reaction paths of nitrous acid isomers. International Journal of Chemical Kinetics, 2007, 39, 378-398.	1.6	35
78	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
79	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
80	Methane/propane oxidation at high pressures: Experimental and detailed chemical kinetic modeling. Proceedings of the Combustion Institute, 2007, 31, 447-454.	3.9	216
81	Experimental and Modeling Study of Methyl Cyclohexane Pyrolysis and Oxidation. Journal of Physical Chemistry A, 2006, 110, 114-131.	2.5	146
82	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	2.5	52
83	The influence of fuel structure on combustion as demonstrated by the isomers of heptane: a rapid compression machine study. Proceedings of the Combustion Institute, 2005, 30, 2639-2647.	3.9	118
84	CFD studies of a twin-piston rapid compression machine. Combustion and Flame, 2005, 141, 417-430.	5.2	84
85	The comparison of detailed chemical kinetic mechanisms; forward versus reverse rates with CHEMRev. International Journal of Chemical Kinetics, 2005, 37, 119-125.	1.6	18
86	Automatic comparison of thermodynamic data for species in detailed chemical kinetic modeling. International Journal of Chemical Kinetics, 2005, 37, 341-345.	1.6	3
87	Autoignition of heptanes; experiments and modeling. International Journal of Chemical Kinetics, 2005, 37, 728-736.	1.6	63
88	The comparison of detailed chemical kinetic mechanisms: Application to the combustion of methane. International Journal of Chemical Kinetics, 2004, 36, 467-471.	1.6	13
89	A comprehensive modeling study of hydrogen oxidation. International Journal of Chemical Kinetics, 2004, 36, 603-622.	1.6	833
90	The high temperature oxidation of pyrrole and pyridine; ignition delay times measured behind reflected shock waves. Combustion and Flame, 2003, 133, 231-239.	5.2	21

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91	Detailed chemical kinetic models for the combustion of hydrocarbon fuels. Progress in Energy and Combustion Science, 2003, 29, 599-634.	31.2	410
92	Simulation of methane autoignition in a rapid compression machine with creviced pistons. Combustion and Flame, 2001, 124, 326-329.	5.2	87
93	Oxidation of dimethoxymethane in a jet-stirred reactor. Combustion and Flame, 2001, 125, 1106-1117.	5.2	77
94	Burning velocities of dimethyl ether and air. Combustion and Flame, 2001, 125, 1329-1340.	5.2	141
95	The oxidation and ignition of dimethylether from low to high temperature (500â€“1600 K): Experiments and kinetic modeling. Proceedings of the Combustion Institute, 1998, 27, 361-369.	0.3	141
96	The Ignition and Oxidation of Tetrahydrofuran: Experiments and Kinetic Modeling. Combustion Science and Technology, 1998, 135, 3-29.	2.3	43
97	Quantitative Structureâ”Activity Relationship Studies of Sulfamates RNHSO3Na: Distinction between Sweet, Sweet-Bitter, and Bitter Molecules. Journal of Agricultural and Food Chemistry, 1998, 46, 3016-3026.	5.2	43
98	The Ignition and Oxidation of Tetrahydropyran: Experiments and Kinetic Modeling. Combustion Science and Technology, 1997, 129, 1-16.	2.3	16
99	The ignition of oxetane in shock waves and oxidation in a jet-stirred reactor: An experimental and kinetic modeling study. Combustion and Flame, 1997, 110, 409-417.	5.2	8
100	High-temperature oxidation of ethylene oxide in shock waves. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 715-721.	1.7	8
101	The oxidation of ethylene oxide in a jet-stirred reactor and its ignition in shock waves. Combustion and Flame, 1996, 106, 62-68.	5.2	30
102	The ignition and oxidation of allene and propyne: Experiments and kinetic modeling. Proceedings of the Combustion Institute, 1996, 26, 613-620.	0.3	31
103	Acetaldehyde Oxidation in a JSR and Ignition in Shock Waves: Experimental and Comprehensive Kinetic Modeling. Combustion Science and Technology, 1995, 107, 301-316.	2.3	46
104	Shock tube ignition of ethanol, isobutene and MTBE: Experiments and modeling. Proceedings of the Combustion Institute, 1992, 24, 769-776.	0.3	89
105	High-temperature oxidation of ethanol. Part 1.â€”Ignition delays in shock waves. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1691-1696.	1.7	74
106	High-temperature oxidation of ethanol. Part 2.â€”Kinetic modelling. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 2549-2559.	1.7	63
107	Combustion of methyl tert-butyl ether. Part I: Ignition in Shock waves. Combustion and Flame, 1991, 85, 489-498.	5.2	18
108	Preliminary observations on the high temperature oxidation of ethyltert-butyl ether. International Journal of Chemical Kinetics, 1991, 23, 553-558.	1.6	11

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109	The taste of monosubstituted phenylsulphamates. Journal of the Chemical Society Chemical Communications, 1989, , 545.	2.0	8
110	The reactions of sulfuryl chloride with [Fe2(Î·-C5H5)2(CO)4-n(CNMe)n] (n = 0, 1, 2 and 4) and related complexes. The crystal structure of [Fe(Î·5-C9H7)(CO)3] [FeCl4]. Journal of Organometallic Chemistry, 1988, 338, 383-392.	1.8	8
111	Falloff behavior in propane thermal decomposition at high temperature. The Journal of Physical Chemistry, 1982, 86, 799-802.	2.9	29
112	Kinetic study of a retro Diels-Alder reaction in a single-pulse shock tube: Decyclization of 1-methylcyclohex-1-ene. International Journal of Chemical Kinetics, 1978, 10, 227-231.	1.6	9
113	Allene isomerisation. Journal of the Chemical Society Faraday Transactions I, 1978, 74, 1337.	1.0	10
114	The vibrational deactivation of the bending mode of CO2 by O2 and by N2. Chemical Physics Letters, 1977, 47, 133-136.	2.6	25
115	Vibrational relaxation in OCS mixtures. Part 1.â€”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. Journal of the Chemical Society, Faraday Transactions 2, 1976, 72, 417-422.	1.1	4
116	Kinetics of the thermal isomerisation of hexamethyldisilane. Journal of the Chemical Society Faraday Transactions I, 1974, 70, 249.	1.0	20
117	Comment on ``Vibrational Relaxation Studies of the 10Â°0 and 02Â°0 States of Shockâ€Heated CO2''. Journal of Chemical Physics, 1971, 55, 5842-5842.	3.0	2
118	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
119	Thermal decomposition of vinylidene fluoride behind reflected shock waves. Challenge, 1970, , 773.	0.4	1
120	Thermal decomposition of perfluorocyclobutane in a single-pulse shock tube. The Journal of Physical Chemistry, 1969, 73, 3830-3833.	2.9	21
121	The thermolysis of hexamethyldisilane. Chemical Communications / Chemical Society, London, 1968, , 1426.	0.1	4
122	Detailed Chemical Kinetic Modeling of Surrogate Fuels for Gasoline and Application to an HCCI Engine. , 0, , .		57