Paul Marshall

List of Publications by Year
in descending order

78 papers	2,411 citations	185998 28 h-index	214527 47 g-index
80 all docs	80 docs citations	80 times ranked	2064 citing authors

#	Article	IF	Citations
1	Ammonia oxidation at high pressure and intermediate temperatures. Fuel, 2016, 181, 358-365.	3.4	223
2	Mechanism and modeling of the formation of gaseous alkali sulfates. Combustion and Flame, 2005, 141, 22-39.	2.8	203
3	Experimental measurements and kinetic modeling of CO/H₂/O₂/NO_x conversion at high pressure. International Journal of Chemical Kinetics, 2008, 40, 454-480.	1.0	164
4	Ignition delay times of NH3 /DME blends at high pressure and low DME fraction: RCM experiments and simulations. Combustion and Flame, 2021, 227, 120-134.	2.8	97
5	An exploratory study of alkali sulfate aerosol formation during biomass combustion. Fuel, 2008, 87, 1591-1600.	3.4	95
6	An ab Initio Investigation of Halocarbenes. Journal of Physical Chemistry A, 1999, 103, 7900-7906.	1.1	93
7	Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes. Journal of Physical Chemistry A, 2017, 121, 2552-2557.	1.1	72
8	Rate coefficients for the hydrogen atom + ammonia reaction over a wide temperature range. The Journal of Physical Chemistry, 1990, 94, 1401-1404.	2.9	69
9	Experimental and Kinetic Modeling Study of C₂H₂ Oxidation at High Pressure. International Journal of Chemical Kinetics, 2016, 48, 724-738.	1.0	67
10	Experimental and kinetic modeling study of C2H4 oxidation at high pressure. Proceedings of the Combustion Institute, 2009, 32, 367-375.	2.4	66
11	Kinetic studies of the reactions of atomic chlorine and bromine with silane. The Journal of Physical Chemistry, 1992, 96, 2197-2201.	2.9	64
12	Characterization of Reaction Pathways on the Potential Energy Surfaces for H + SO2 and HS + O2. Journal of Physical Chemistry A, 1999, 103, 11328-11335.	1.1	63
13	Experimental and ab Initio Investigations of the Kinetics of the Reaction of H Atoms with H2S. Journal of Physical Chemistry A, 1999, 103, 5307-5311.	1.1	49
14	Enthalpy of Formation of the Cyclohexadienyl Radical and the Câ^'H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-Evaluation. Journal of Physical Chemistry A, 2009, 113, 6955-6963.	1.1	47
15	The reaction of OH with acetone and acetone-d6 from 298 to 832 K: Rate coefficients and mechanism. Journal of Chemical Physics, 2003, 119, 10600-10606.	1.2	46
16	Computational studies of the potential energy surface for O(3P)+H2S: Characterization of transition states and the enthalpy of formation of HSO and HOS. Journal of Chemical Physics, 1995, 102, 161-169.	1.2	43
17	A Computational Study of the Thermochemistry of Bromine- and Iodine-Containing Methanes and Methyl Radicals. Journal of Physical Chemistry A, 2005, 109, 6371-6379.	1.1	42
18	A kinetic study of the recombination reaction sodium + sulfur dioxide + argon. The Journal of Physical Chemistry, 1991, 95, 1654-1658.	2.9	40

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19	Thermochemistry of the Ethyl Radical and the Câ”H Bond Strength in Ethane. Journal of Physical Chemistry A, 1999, 103, 4560-4563.	1.1	38
20	Oxidation of Reduced Sulfur Species: Carbonyl Sulfide. International Journal of Chemical Kinetics, 2013, 45, 429-439.	1.0	38
21	An Exploratory Flow Reactor Study of H₂S Oxidation at 30â€“100 Bar. International Journal of Chemical Kinetics, 2017, 49, 37-52.	1.0	38
22	Oxidation of Reduced Sulfur Species: Carbon Disulfide. Journal of Physical Chemistry A, 2014, 118, 6798-6809.	1.1	37
23	High-accuracy coupled-cluster computations of bond dissociation energies in SH, H2S, and H2O. Journal of Chemical Physics, 2002, 117, 3132-3138.	1.2	35
24	An experimental and modeling study on auto-ignition kinetics of ammonia/methanol mixtures at intermediate temperature and high pressure. Combustion and Flame, 2022, 242, 112160.	2.8	34
25	Computational studies of the potential energy surface for O(1D)+H2S: Characterization of pathways involving H2SO, HOSH, and H2OS. Journal of Chemical Physics, 1994, 101, 9405-9411.	1.2	32
26	Global warming potential estimates for the C₁â€“C₃ hydrochlorofluorocarbons (HCFCs) included in the Kigali Amendment to the Montreal Protocol. Atmospheric Chemistry and Physics, 2018, 18, 6317-6330.	1.9	32
27	A kinetic study of the reaction of atomic oxygen with SO2. Proceedings of the Combustion Institute, 2005, 30, 1219-1225.	2.4	31
28	An ab initio study of the reaction of atomic hydrogen with sulfur dioxide. Journal of Chemical Physics, 1991, 95, 4940-4947.	1.2	30
29	The reaction of OH with acetaldehyde and deuterated acetaldehyde: Further insight into the reaction mechanism at both low and elevated temperatures. International Journal of Chemical Kinetics, 2006, 38, 489-495.	1.0	28
30	Kinetic studies and ab initio investigations of the reactions of atomic bromine with methylsilane and dimethylsilane. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 419.	1.7	25
31	Experimental and theoretical studies of the reaction of atomic oxygen with silane. Journal of Chemical Physics, 1993, 98, 8545-8550.	1.2	25
32	Experimental and Computational Investigations of the Reaction of OH with CF3I and the Enthalpy of Formation of HOI. Journal of Physical Chemistry A, 1998, 102, 5182-5188.	1.1	24
33	A computational study of chlorofluoro-methyl radicals. Journal of Chemical Physics, 2003, 118, 557-564.	1.2	24
34	Studies of the Kinetics and Thermochemistry of the Forward and Reverse Reaction Cl + C6H6= HCl + C6H5â€. Journal of Physical Chemistry A, 2007, 111, 3970-3976.	1.1	24
35	Glyoxal Oxidation Mechanism: Implications for the Reactions HCO + O2and OCHCHO + HO2. Journal of Physical Chemistry A, 2015, 119, 7305-7315.	1.1	24
36	Oxidation of methylamine. International Journal of Chemical Kinetics, 2020, 52, 893-906.	1.0	24

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37	Importance of the Hydrogen Isocyanide Isomer in Modeling Hydrogen Cyanide Oxidation in Combustion. Energy & Fuels, 2017, 31, 2156-2163.	2.5	22
38	Rate Constant and Thermochemistry for K + O₂ + N₂ = KO₂ + N₂. Journal of Physical Chemistry A, 2015, 119, 3329-3336.	1.1	20
39	Investigation of the gas-phase kinetics of the reaction potassium + sulfur dioxide + argon. The Journal of Physical Chemistry, 1993, 97, 5295-5297.	2.9	18
40	Atmospheric chemistry of isopropyl formate and tertâ€butyl formate. International Journal of Chemical Kinetics, 2010, 42, 479-498.	1.0	18
41	Laser-Induced Fluorescence and Mass Spectrometric Studies of the Cu + HCl Reaction over a Wide Temperature Range. Formation of HCuCl. The Journal of Physical Chemistry, 1996, 100, 17835-17839.	2.9	17
42	Reaction kinetics of the addition of atomic sulfur to nitric oxide. Journal of Chemical Physics, 2004, 121, 9999-10005.	1.2	17
43	New reactions of diazene and related species for modelling combustion of amine fuels. Molecular Physics, 2021, 119, .	0.8	15
44	Experimental and Computational Studies of the Kinetics of the Reaction of Atomic Hydrogen with Methanethiol. Journal of Physical Chemistry A, 2015, 119, 7352-7360.	1.1	14
45	The C2H2 + NO2 reaction: Implications for high pressure oxidation of C2H2/NOx mixtures. Proceedings of the Combustion Institute, 2019, 37, 469-476.	2.4	14
46	Experimental and kinetic modeling study of oxidation of acetonitrile. Proceedings of the Combustion Institute, 2021, 38, 575-583.	2.4	13
47	Computational Studies of the Thermochemistry of the Atmospheric Iodine Reservoirs HOI and IONO2. Advances in Quantum Chemistry, 2008, 55, 159-175.	0.4	10
48	Rate Coefficient Measurements and Theoretical Analysis of the OH + (E)-CF₃CHâ•CHCF₃ Reaction. Journal of Physical Chemistry A, 2018, 122, 4635-4646.	1.1	10
49	A computational study of the reaction kinetics of methyl radicals with trifluorohalomethanes. International Journal of Chemical Kinetics, 1998, 30, 179-184.	1.0	9
50	Anabinitiostudy of the ionization of sodium superoxide. Journal of Chemical Physics, 1991, 95, 7773-7774.	1.2	8
51	Ab initio calculations and kinetic modeling of thermal conversion of methyl chloride: implications for gasification of biomass. Physical Chemistry Chemical Physics, 2018, 20, 10741-10752.	1.3	8
52	UV and infrared absorption spectra and 248 nm photolysis of maleic anhydride (C4H2O3). Journal of Photochemistry and Photobiology A: Chemistry, 2019, 382, 111953.	2.0	8
53	Acetaldehyde oxidation at elevated pressure. Proceedings of the Combustion Institute, 2021, 38, 269-278.	2.4	7
54	Selective Noncatalytic Reduction of NO_x Using Ammonium Sulfate. Energy & Fuels, 2021, 35, 12392-12402.	2.5	7

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55	Participation of alkali and sulfur in ammonia combustion chemistry: Investigation for ammonia/solid fuel co-firing applications. Combustion and Flame, 2022, 244, 112236.	2.8	7
56	Discharge-flow/chemiluminescence and flash-photolysis/resonance fluorescence studies of the reaction O + SiH4 at room temperature. International Journal of Chemical Kinetics, 1993, 25, 183-191.	1.0	6
57	The Reaction Kinetics of Amino Radicals with Sulfur Dioxide. Zeitschrift Fur Physikalische Chemie, 2015, 229, 1649-1661.	1.4	6
58	Experimental and theoretical studies of the reactions of ground-state sulfur atoms with hydrogen and deuterium. Journal of Chemical Physics, 2017, 147, 134302.	1.2	6
59	Temperatureâ€dependent rate coefficients for the gasâ€phase OH + furanâ€2,5â€dione (C₄H₂O₃, maleic anhydride) reaction. International Journal of Chemical Kinetics, 2020, 52, 623-631.	1.0	6
60	An experimental and computational study of the reaction of ground-state sulfur atoms with carbon disulfide. Journal of Chemical Physics, 2011, 135, 144306.	1.2	5
61	High-temperature kinetics of the reaction between chlorine atoms and hydrogen sulfide. Chemical Physics Letters, 2015, 624, 83-86.	1.2	5
62	Climate Metrics for C1â€“C4 Hydrofluorocarbons (HFCs). Journal of Physical Chemistry A, 2020, 124, 4793-4800.	1.1	5
63	The Gas-Phase Kinetics of Reactions of Alkali Metal Atoms with Nitric Oxide. Journal of Physical Chemistry A, 1999, 103, 9252-9258.	1.1	4
64	Kinetics and thermochemistry of the addition of atomic chlorine to acetylene. Proceedings of the Combustion Institute, 2007, 31, 193-200.	2.4	4
65	Kinetic and theoretical investigations of the S + NO2 reaction. International Journal of Chemical Kinetics, 2012, 44, 90-99.	1.0	4
66	Kinetic studies of the reaction of atomic sulfur with acetylene. Proceedings of the Combustion Institute, 2015, 35, 215-222.	2.4	4
67	Temperature and Pressure Dependence of the Reaction S + CS (+M) â† CS₂ (+M). Journal of Physical Chemistry A, 2015, 119, 7277-7281.	1.1	4
68	Relative Rate and Product Studies of the Reactions of Atomic Chlorine with Tetrafluoroethylene, 1,2-Dichloro-1,2-difluoroethylene, 1,1-Dichloro-2,2-difluoroethylene, and Hexafluoro-1,3-butadiene in the Presence of Oxygen. Journal of Physical Chemistry A, 2016, 120, 7311-7319.	1.1	4
69	Kinetic Studies of the Cl + HI Reaction Using Three Techniques. Journal of Physical Chemistry A, 2004, 108, 6857-6862.	1.1	3
70	Predicted thermochemistry and unimolecular kinetics of nitrous sulfide. Journal of Chemical Physics, 2011, 135, 094301.	1.2	3
71	Experimental and computational studies of the kinetics of the reaction of hydrogen atoms with carbon disulfide. Proceedings of the Combustion Institute, 2019, 37, 373-379.	2.4	3
72	Experimental and computational studies of the kinetics of the reaction of hydrogen peroxide with the amidogen radical. Journal of Chemical Physics, 2022, 157, .	1.2	3

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73	The Kinetics of the Reaction of H Atoms with C4F6. Journal of Physical Chemistry A, 2001, 105, 11220-11225.	1.1	2
74	Relative Rate Studies of the Reactions of Atomic Chlorine with Acetone and Cyclic Ketones. International Journal of Chemical Kinetics, 2018, 50, 41-46.	1.0	2
75	Reply to the Comment on: An ab initio study of the ionization of sodium superoxide. Journal of Chemical Physics, 1992, 96, 7872-7872.	1.2	1
76	The Spinâ€Forbidden Reaction of Groundâ€State Sulfur Atoms with Ethylene. International Journal of Chemical Kinetics, 2016, 48, 124-130.	1.0	1
77	Kinetic fall-off behavior for the Cl + Furan-2,5-dione (C₄H₂O₃,) Tj ETQq1 1 0.784314 rgBT /Ov	1.3	1
78	Theoretical modeling study of the reaction H + CF 4 â† ' HF + CF 3. International Journal of Chemical Kinetics, 2021, 53, 939-945.	1.0	0