James A Miller

List of Publications by Citations

137 papers	15,726 citations	64 h-index	124 g-index
142 ext. papers	17,352 ext. citations	5.5 avg, IF	6.69 L-index

#	Paper	IF	Citations
137	Mechanism and modeling of nitrogen chemistry in combustion. *Progress in Energy and Combustion Science*, **1989**, 15, 287-338	33.6	2243
136	Kinetic and thermodynamic issues in the formation of aromatic compounds in flames of aliphatic fuels. *Combustion and Flame*, **1992**, 91, 21-39	5.3	738
135	Searches for ultimate chemical carcinogens and their reactions with cellular macromolecules. *Cancer*, **1981**, 47, 2327-45	6.4	704
134	Modeling the kinetics of bimolecular reactions. *Chemical Reviews*, **2006**, 106, 4518-84	68.1	464
133	Modeling nitrogen chemistry in combustion. *Progress in Energy and Combustion Science*, **2018**, 67, 31-68	33.6	449
132	Kinetic Modeling of Hydrocarbon/Nitric Oxide Interactions in a Flow Reactor. *Combustion and Flame* , **1998**, 115, 1-27	5.3	417
131	Unravelling combustion mechanisms through a quantitative understanding of elementary reactions. *Proceedings of the Combustion Institute*, **2005**, 30, 43-88	5.9	369
130	Kinetic modeling and sensitivity analysis of nitrogen oxide formation in well-stirred reactors. *Combustion and Flame*, **1986**, 65, 177-202	5.3	328
129	Master equation methods in gas phase chemical kinetics. *Journal of Physical Chemistry A*, **2006**, 110, 10528-44	2.8	325
128	A computational model of the structure and extinction of strained, opposed flow, premixed methane-air flames. *Proceedings of the Combustion Institute*, **1989**, 22, 1479-1494		317
127	The Recombination of Propargyl Radicals and Other Reactions on a C6H6Potential. *Journal of Physical Chemistry A*, **2003**, 107, 7783-7799	2.8	315
126	Reformulation and solution of the master equation for multiple-well chemical reactions. *Journal of Physical Chemistry A*, **2013**, 117, 12146-54	2.8	297
125	A Mathematical Model of the Coupled Fluid Mechanics and Chemical Kinetics in a Chemical Vapor Deposition Reactor. *Journal of the Electrochemical Society*, **1984**, 131, 425-434	3.9	296
124	Enols are common intermediates in hydrocarbon oxidation. *Science*, **2005**, 308, 1887-9	33.3	277
123	Mechanisms of chemical carcinogenesis. *Cancer*, **1981**, 47, 1055-64	6.4	274
122	A Mathematical Model of Silicon Chemical Vapor Deposition: Further Refinements and the Effects of Thermal Diffusion. *Journal of the Electrochemical Society*, **1986**, 133, 1206-1213	3.9	244
121	The carcinogenic aminoazo dyes. *Advances in Cancer Research*, **1953**, 1, 339-96	5.9	230

120	Kinetic Modeling of the Oxidation of Ammonia in Flames. *Combustion Science and Technology*, **1983**, 34, 149-176	1.5	201
119	From the Multiple-Well Master Equation to Phenomenological Rate Coefficients: Reactions on a C3H4 Potential Energy Surface. *Journal of Physical Chemistry A*, **2003**, 107, 2680-2692	2.8	191
118	The role of NNH in NO formation and control. *Combustion and Flame*, **2011**, 158, 774-789	5.3	180
117	From the Time-Dependent, Multiple-Well Master Equation to Phenomenological Rate Coefficients. *Journal of Physical Chemistry A*, **2002**, 106, 9267-9277	2.8	150
116	Kinetic modeling of the reduction of nitric oxide in combustion products by isocyanic acid. *International Journal of Chemical Kinetics*, **1991**, 23, 289-313	1.4	146
115	Measurements, Theory, and Modeling of OH Formation in Ethyl + O2 and Propyl + O2 Reactions. *Journal of Physical Chemistry A*, **2003**, 107, 4415-4427	2.8	144
114	Identification and chemistry of C4H3 and C4H5 isomers in fuel-rich flames. *Journal of Physical Chemistry A*, **2006**, 110, 3670-8	2.8	137
113	Reaction of ethylene with hydroxyl radicals: a theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 6960-70	2.8	137
112	Modeling the thermal DENOx process in flow reactors. Surface effects and Nitrous Oxide formation. *International Journal of Chemical Kinetics*, **1994**, 26, 421-436	1.4	130
111	Collisional energy transfer in the low-pressure-limit unimolecular dissociation of HO2. *Journal of Chemical Physics*, **1984**, 80, 5568-5580	3.9	129
110	Exploring old and new benzene formation pathways in low-pressure premixed flames of aliphatic fuels. *Proceedings of the Combustion Institute*, **2000**, 28, 1519-1527	5.9	125
109	The reaction between propene and hydroxyl. *Physical Chemistry Chemical Physics*, **2009**, 11, 11040-53	3.6	121
108	Association rate constants for reactions between resonance-stabilized radicals: C3H3 + C3H3, C3H3 + C3H5, and C3H5 + C3H5. *Physical Chemistry Chemical Physics*, **2007**, 9, 4259-68	3.6	121
107	The H + C2H2 (+M) ? C2H3 (+M) and H + C2H2 (+M) ? C2H5 (+M) reactions: Electronic structure, variational transition-state theory, and solutions to a two-dimensional master equation. *Physical Chemistry Chemical Physics*, **2004**, 6, 1192-1202	3.6	121
106	Theoretical unimolecular kinetics for CH4 + M ? CH3 + H + M in eight baths, M = He, Ne, Ar, Kr, H2, N2, CO, and CH4. *Journal of Physical Chemistry A*, **2011**, 115, 6438-55	2.8	118
105	Predictive a priori pressure-dependent kinetics. *Science*, **2014**, 346, 1212-5	33.3	115
104	Solution of Some One- and Two-Dimensional Master Equation Models for Thermal Dissociation: The Dissociation of Methane in the Low-Pressure Limit. *Journal of Physical Chemistry A*, **2002**, 106, 4904-4913	2.8	115
103	Lennard□ones parameters for combustion and chemical kinetics modeling from full-dimensional intermolecular potentials. *Combustion and Flame*, **2014**, 161, 101-110	5.3	112

102	Identification of C5Hx isomers in fuel-rich flames by photoionization mass spectrometry and electronic structure calculations. *Journal of Physical Chemistry A*, **2006**, 110, 4376-88	2.8	112
101	The reaction between ethyl and molecular oxygen II: Further analysis. *International Journal of Chemical Kinetics*, **2001**, 33, 654-668	1.4	111
100	The Recombination of Propargyl Radicals: Solving the Master Equation. *Journal of Physical Chemistry A*, **2001**, 105, 7254-7266	2.8	110
99	Synchrotron photoionization measurements of combustion intermediates: photoionization efficiency and identification of C3H2 isomers. *Physical Chemistry Chemical Physics*, **2005**, 7, 806-13	3.6	107
98	Isomer-specific combustion chemistry in allene and propyne flames. *Combustion and Flame*, **2009**, 156, 2153-2164	5.3	102
97	Determination of Adiabatic Flame Speeds by Boundary Value Methods. *Combustion Science and Technology*, **1983**, 34, 79-90	1.5	100
96	Collision dynamics and the thermal rate coefficient for the reaction H+O2->OH+O. *Journal of Chemical Physics*, **1981**, 74, 5120-5132	3.9	97
95	A theoretical analysis of the reaction between ethyl and molecular oxygen. *Proceedings of the Combustion Institute*, **2000**, 28, 1479-1486	5.9	94
94	Theory and modeling in combustion chemistry. *Proceedings of the Combustion Institute*, **1996**, 26, 461-480		93
93	The reaction of ammonia with nitrogen dioxide in a flow reactor: Implications for the NH2 + NO2 reaction. *International Journal of Chemical Kinetics*, **1995**, 27, 1207-1220	1.4	92
92	Toward a comprehensive chemical kinetic mechanism for the oxidation of acetylene: Comparison of model predictions with results from flame and shock tube experiments. *Proceedings of the Combustion Institute*, **1982**, 19, 181-196		90
91	Combustion chemistry of enols: possible ethenol precursors in flames. *Journal of Physical Chemistry A*, **2006**, 110, 3254-60	2.8	89
90	A Theoretical Analysis of the Reaction between Vinyl and Acetylene:Quantum Chemistry and Solution of the Master Equation. *Journal of Physical Chemistry A*, **2000**, 104, 7525-7536	2.8	82
89	Nonstatistical effects and detailed balance in quasiclassical trajectory calculations of the thermal rate coefficient for O+OH->O2+H. *Journal of Chemical Physics*, **1986**, 84, 6170-6177	3.9	82
88	Third-Body collision efficiencies for combustion modeling: Hydrocarbons in atomic and diatomic baths. *Proceedings of the Combustion Institute*, **2015**, 35, 197-204	5.9	80
87	Benzene formation in premixed fuel-rich 1,3-butadiene flames. *Proceedings of the Combustion Institute*, **2009**, 32, 623-630	5.9	80
86	Infrared frequency-modulation probing of product formation in alkyl + O2 reactions. Part IV. Reactions of propyl and butyl radicals with O2. *Faraday Discussions*, **2001**, 101-20; discussion 121-43	3.6	80
85	A theoretical analysis of the reaction between propargyl and molecular oxygen. *Faraday Discussions* , **2001**, 79-100; discussion 121-43	3.6	80

84	The reaction of acetylene with hydroxyl radicals. *Journal of Physical Chemistry A*, **2005**, 109, 6045-55	2.8	79
83	The reaction of hydroxyethyl radicals with O2: A theoretical analysis and experimental product study. *Proceedings of the Combustion Institute*, **2009**, 32, 271-277	5.9	78
82	Collisional energy transfer in unimolecular reactions: direct classical trajectories for CH4 CH3 + H in helium. *Journal of Physical Chemistry A*, **2009**, 113, 5612-9	2.8	77
81	Mechanism and modeling of hydrogen cyanide oxidation in a flow reactor. *Combustion and Flame*, **1994**, 99, 475-483	5.3	75
80	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. *Journal of Physical Chemistry A*, **2015**, 119, 7766-79	2.8	74
79	The reaction of n- and i-C4H5 radicals with acetylene. *Journal of Physical Chemistry A*, **2007**, 111, 3740-7	2.8	73
78	Pathways and rate coefficients for the decomposition of vinoxy and acetyl radicals. *Journal of Physical Chemistry A*, **2006**, 110, 5772-81	2.8	69
77	Improved simulations of snow extent in the second phase of the Atmospheric Model Intercomparison Project (AMIP-2). *Journal of Geophysical Research*, **2003**, 108,		69
76	Reactions over multiple, interconnected potential wells: unimolecular and bimolecular reactions on a C3H5 potential. *Journal of Physical Chemistry A*, **2008**, 112, 9429-38	2.8	66
75	Formally direct pathways and low-temperature chain branching in hydrocarbon autoignition: the cyclohexyl + O2 reaction at high pressure. *Physical Chemistry Chemical Physics*, **2009**, 11, 1320-7	3.6	65
74	Reactions between resonance-stabilized radicals: propargyl + allyl. *Journal of Physical Chemistry A*, **2010**, 114, 4881-90	2.8	64
73	A hybrid Newton/time-integration procedure for the solution of steady, laminar, one-dimensional, premixed flames. *Proceedings of the Combustion Institute*, **1988**, 21, 1773-1782		64
72	Dissociation of propyl radicals and other reactions on a C3H7 potential. *Journal of Physical Chemistry A*, **2013**, 117, 2718-27	2.8	63
71	Theoretical Considerations in the NH2 + NO Reaction. *Journal of Physical Chemistry A*, **2000**, 104, 2061-2069	2.8	63
70	The temperature and pressure dependence of the reactions H + O2 (+M) --> HO2 (+M) and H + OH (+M) --> H2O (+M). *Journal of Physical Chemistry A*, **2008**, 112, 5085-95	2.8	60
69	Collision efficiency of water in the unimolecular reaction CH4 (+H2O) ? CH3 + H (+H2O): one-dimensional and two-dimensional solutions of the low-pressure-limit master equation. *Journal of Physical Chemistry A*, **2013**, 117, 12243-55	2.8	59
68	Kinetics of CH + N2 revisited with multireference methods. *Journal of Physical Chemistry A*, **2008**, 112, 522-32	2.8	59
67	Photoionization mass spectrometric studies and modeling of fuel-rich allene and propyne flames. *Proceedings of the Combustion Institute*, **2007**, 31, 1157-1164	5.9	58

66	The effect of allene addition on the structure of a rich C2H2/O2/Ar flame. *Combustion and Flame*, **1996**, 105, 451-461	5.3	58
65	Unimolecular reaction mechanisms involving C3H4, C4H4, and C6H6 hydrocarbon species. *Proceedings of the Combustion Institute*, **1992**, 24, 621-628		58
64	Chemical nonequilibrium effects in hydrogen-air laminar jet diffusion flames. *The Journal of Physical Chemistry*, **1977**, 81, 2534-2542		58
63	The addition of hydrogen atoms to diacetylene and the heats of formation of i-C4H3 and n-C4H3. *Journal of Physical Chemistry A*, **2005**, 109, 4285-95	2.8	57
62	First-Principles Insight into the Hydration Ability and Proton Conduction of the Solid State Proton Conductor, Y and Sn Co-Doped BaZrO3. *Chemistry of Materials*, **2015**, 27, 901-908	9.6	56
61	Determining phenomenological rate coefficients from a time-dependent, multiple-well master equation: "species reduction" at high temperatures. *Physical Chemistry Chemical Physics*, **2013**, 15, 4744-53	3.6	53
60	Kinetics of the reaction between oxygen atoms and ethyl radicals. *Journal of the Chemical Society, Faraday Transactions 2*, **1988**, 84, 491-503		53
59	The conversion of HCN to NO and N2 in H2O2HCNAr flames at low pressure. *Proceedings of the Combustion Institute*, **1985**, 20, 673-684		51
58	A kinetic issue in reburning: the fate of HCNO. *Combustion and Flame*, **2003**, 135, 357-362	5.3	50
57	Quantifying the non-RRKM effect in the H + O2 ? OH + O reaction. *International Journal of Chemical Kinetics*, **1997**, 29, 275-287	1.4	49
56	Weakly Bound Free Radicals in Combustion: "Prompt" Dissociation of Formyl Radicals and Its Effect on Laminar Flame Speeds. *Journal of Physical Chemistry Letters*, **2016**, 7, 85-9	6.4	47
55	Resolving the mystery of prompt CO2: The HCCO+O2 reaction. *Proceedings of the Combustion Institute*, **2002**, 29, 1209-1217	5.9	47
54	Role of Microstructure and Surface Defects on the Dissolution Kinetics of CeO2, a UO2 Fuel Analogue. *ACS Applied Materials & Interfaces*, **2016**, 8, 10562-71	9.5	46
53	Pressure-dependent OH yields in alkene + HO2 reactions: a theoretical study. *Journal of Physical Chemistry A*, **2011**, 115, 10218-25	2.8	45
52	A statistical-theoretical investigation of the thermal rate coefficient and branching ratio for the reaction atomic oxygen + hydrogen cyanide .fwdarw. products. *The Journal of Physical Chemistry*, **1986**, 90, 3339-3345		43
51	Prompt NO: Theoretical prediction of the high-temperature rate coefficient for CH + N2 -> HCN + N. *International Journal of Chemical Kinetics*, **1997**, 29, 253-259	1.4	40
50	Snow Mass over North America: Observations and Results from the Second Phase of the Atmospheric Model Intercomparison Project. *Journal of Hydrometeorology*, **2005**, 6, 681-695	3.7	40
49	The Oxidation of Allene in a Low-Pressure H2 / O2 / Ar-C3 H4 Flame. *Combustion Science and Technology*, **1995**, 110-111, 249-276	1.5	40

48	Branching Fraction of the NH2 + NO Reaction between 1210 and 1370 K. *Journal of Physical Chemistry A*, **1997**, 101, 3741-3745	2.8	39
47	Detailed balance in multiple-well chemical reactions. *Physical Chemistry Chemical Physics*, **2009**, 11, 1128-37	3.6	38
46	Dynamics of the unimolecular dissociation of hydroperoxo. Phase space coupling, microcanonical rate coefficients, and rotational effects. *The Journal of Physical Chemistry*, **1982**, 86, 772-784		35
45	Kinetics of the gas-phase recombination reaction of hydroxyl radicals to form hydrogen peroxide. *Journal of Physical Chemistry A*, **2009**, 113, 4457-67	2.8	34
44	A complete statistical analysis of the reaction between OH and CO. *Proceedings of the Combustion Institute*, **2005**, 30, 945-953	5.9	34
43	An exploratory investigation of the use of alkali metals in nitrous oxide control. *International Journal of Chemical Kinetics*, **1996**, 28, 217-234	1.4	34
42	A Theoretical Investigation of Mixing Effects in the Selective Reduction of Nitric Oxide by Ammonia. *Combustion Science and Technology*, **1982**, 29, 147-165	1.5	33
41	Theoretical kinetics of O + C2H4. *Proceedings of the Combustion Institute*, **2017**, 36, 219-227	5.9	32
40	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. *Progress in Energy and Combustion Science*, **2021**, 83, 100886	33.6	31
39	Adventures on the C3H5O potential energy surface: OH + propyne, OH + allene and related reactions. *Proceedings of the Combustion Institute*, **2015**, 35, 181-188	5.9	30
38	Research in chemical carcinogenesis with Elizabeth Miller--a trail of discovery with our associates. *Drug Metabolism Reviews*, **1994**, 26, 1-36	7	30
37	First-principles binary diffusion coefficients for H, H$_2$ and four normal alkanes + N$_2$ *Journal of Chemical Physics*, **2014**, 141, 124313	3.9	29
36	The recombination of hydrogen atoms with nitric oxide at high temperatures. *Proceedings of the Combustion Institute*, **1998**, 27, 219-226		29
35	The reactions of imidogen with nitric oxide and molecular oxygen. *Proceedings of the Combustion Institute*, **1992**, 24, 719-726		29
34	The measurement of relative concentration profiles of NH2 using laser absorption spectroscopy. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **1981**, 26, 313-327	2.1	28
33	Kinetics of Propargyl Radical Dissociation. *Journal of Physical Chemistry A*, **2015**, 119, 7780-91	2.8	27
32	Ramifications of including non-equilibrium effects for HCO in flame chemistry. *Proceedings of the Combustion Institute*, **2017**, 36, 525-532	5.9	26
31	A theoretical analysis of the overtone-induced isomerization of methyl isocyanide. *Journal of Chemical Physics*, **1986**, 85, 4502-4508	3.9	25

30	Comment on "When Rate Constants Are Not Enough". *Journal of Physical Chemistry A*, **2016**, 120, 306-122.8		23
29	Some Observations Concerning Detailed Balance in Association/Dissociation Reactions. *Journal of Physical Chemistry A*, **2004**, 108, 8296-8306	2.8	23
28	Hydrocarbon/nitric oxide interactions in low-pressure flames. *Proceedings of the Combustion Institute*, **1988**, 21, 965-977		23
27	Some chemical kinetics issues in reburning: The branching fraction of the HCCO+NO reaction. *Proceedings of the Combustion Institute*, **1998**, 27, 235-243		22
26	Combustion chemistry: important features of the C3H5 potential energy surface, including allyl radical, propargyl + H2, allene + H, and eight transition states. *Journal of Physical Chemistry A*, **2011**, 115, 14209-14	2.8	21
25	Kinetic isotope effects: Theoretical prediction of the thermal rate coefficient for the reaction D+O2->OD+O. *Journal of Chemical Physics*, **1981**, 75, 5349-5354	3.9	21
24	Unimolecular dissociation of hydroxypropyl and propoxy radicals. *Proceedings of the Combustion Institute*, **2013**, 34, 519-526	5.9	20
23	A direct transition state theory based analysis of the branching in NH2 + NO. *Faraday Discussions*, **2001**, 207-22; discussion 255-74	3.6	20
22	A theoretical analysis of photoactivated unimolecular dissociation: The overtone dissociation of t-butyl hydroperoxide. *Journal of Chemical Physics*, **1984**, 81, 455-464	3.9	20
21	High-temperature measurements and a theoretical study of the reaction of OH with 1,3-butadiene. *Journal of Physical Chemistry A*, **2010**, 114, 8312-8	2.8	19
20	The CH3+NO rate coefficient at high temperatures: Theoretical analysis and comparison with experiment. *International Journal of Chemical Kinetics*, **1998**, 30, 223-228	1.4	19
19	A theoretical analysis of the reaction between hydrogen atoms and isocyanic acid. *International Journal of Chemical Kinetics*, **1992**, 24, 421-432	1.4	19
18	Oxidation pathways in the reaction of diacetylene with OH radicals. *Proceedings of the Combustion Institute*, **2007**, 31, 185-192	5.9	17
17	Angular momentum conservation in the O + OH <-> O2 + H reaction. *International Journal of Chemical Kinetics*, **1999**, 31, 753-756	1.4	17
16	The need for epidemiological studies of the medical exposures of Japanese patients to the carcinogen ethyl carbamate (urethane) from 1950 to 1975. *Japanese Journal of Cancer Research*, **1991**, 82, 1323-4		17
15	Methyl isocyanaide isomerization. Determination of collisional deactivation parameters following carbon-hydrogen overtone excitation. *The Journal of Physical Chemistry*, **1986**, 90, 3544-3549		17
14	Solution of Premixed and Counterflow Diffusion Flame Problems by Adaptive Boundary Value Methods **1985**, 303-317		16
13	Pressure effects on the thermal de-NOx process. *Proceedings of the Combustion Institute*, **1996**, 26, 2067-2074		15

12	Initiation Reactions in Acetylene Pyrolysis. *Journal of Physical Chemistry A*, **2017**, 121, 4203-4217	2.8	14
11	Reference natural gas flames at nominally autoignitive engine-relevant conditions. *Proceedings of the Combustion Institute*, **2019**, 37, 1631-1638	5.9	14
10	The structure and reaction mechanism of rich, non-sooting C2H2/O2/Ar flames. *Proceedings of the Combustion Institute*, **1991**, 23, 187-194		13
9	A theoretical analysis of the reaction between hydroxyl and hydrogen cyanide at high temperature. *Proceedings of the Combustion Institute*, **1988**, 21, 919-927		9
8	Comment on "Automatic estimation of pressure-dependent rate coefficients" (J. W. Allen, C. F. Goldsmith, and W. H. Green, Phys. Chem. Chem. Phys., 2011, 14, 1131-1155). *Physical Chemistry Chemical Physics*, **2012**, 14, 8431-3; discussion 8434	3.6	8
7	Computational modeling of flame structure. *Physica D: Nonlinear Phenomena*, **1984**, 12, 198-211	3.3	8
6	Inhibitory effects of chlorophyllin on micronucleus formation induced by ethyl carbamate and its proximate and ultimate carcinogenic forms in mouse peripheral reticulocytes. *Environmental and Molecular Mutagenesis*, **1999**, 34, 57-60	3.2	7
5	Rich methane/air flames: Burning velocities, extinction limits, and flammability limit. *Proceedings of the Combustion Institute*, **1994**, 25, 1309-1315		7
4	Secondary decomposition of C3H5 radicals formed by the photodissociation of 2-bromopropene. *Journal of Chemical Physics*, **2007**, 127, 144301	3.9	6
3	Synthesis of the hepatocarcinogen N-methyl-4-aminoazobenzene with tritium in the prime ring. *Journal of Labelled Compounds*, **1969**, 5, 257-260		3
2	Comparative carcinogenicities and reactivities of N-myristoyloxy-N-acetyl-2-aminofluorene and its 7-iodo derivative. *Carcinogenesis*, **1981**, 2, 655-9	4.6	2
1	Comment on "Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals". *Journal of Physical Chemistry A*, **2019**, 123, 1129-1130	2.8	1