James A Miller

List of Publications by Year
in descending order

138 papers	18,996 citations	12322 69 h-index	11303 136 g-index
142 all docs	142 docs citations	142 times ranked	6440 citing authors

#	Article	IF	Citations
1	Mechanism and modeling of nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 1989, 15, 287-338.	15.8	2,716
2	Modeling nitrogen chemistry in combustion. Progress in Energy and Combustion Science, 2018, 67, 31-68.	15.8	980
3	Kinetic and thermodynamic issues in the formation of aromatic compounds in flames of aliphatic fuels. Combustion and Flame, 1992, 91, 21-39.	2.8	813
4	Searches for ultimate chemical carcinogens and their reactions with cellular macromolecules. Cancer, 1981, 47, 2327-2345.	2.0	761
5	Modeling the Kinetics of Bimolecular Reactions. Chemical Reviews, 2006, 106, 4518-4584.	23.0	533
6	Kinetic Modeling of Hydrocarbon/Nitric Oxide Interactions in a Flow Reactor. Combustion and Flame, 1998, 115, 1-27.	2.8	475
7	Reformulation and Solution of the Master Equation for Multiple-Well Chemical Reactions. Journal of Physical Chemistry A, 2013, 117, 12146-12154.	1.1	461
8	Unravelling combustion mechanisms through a quantitative understanding of elementary reactions. Proceedings of the Combustion Institute, 2005, 30, 43-88.	2.4	417
9	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.	0.3	416
10	Kinetic modeling and sensitivity analysis of nitrogen oxide formation in well-stirred reactors. Combustion and Flame, 1986, 65, 177-202.	2.8	398
11	Master Equation Methods in Gas Phase Chemical Kinetics. Journal of Physical Chemistry A, 2006, 110, 10528-10544.	1.1	386
12	The Recombination of Propargyl Radicals and Other Reactions on a C6H6Potential. Journal of Physical Chemistry A, 2003, 107, 7783-7799.	1.1	368
13	Mechanisms of chemical carcinogenesis. Cancer, 1981, 47, 1055-1064.	2.0	327
14	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.	1.3	326
15	Enols Are Common Intermediates in Hydrocarbon Oxidation. Science, 2005, 308, 1887-1889.	6.0	306
16	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	2.8	304
17	Kinetic Modeling of the Oxidation of Ammonia in Flames. Combustion Science and Technology, 1983, 34, 149-176.	1.2	280
18	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.	1.3	268

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19	The Carcinogenic Aminoazo Dyes. Advances in Cancer Research, 1953, 1, 339-396.	1.9	263
20	From the Multiple-Well Master Equation to Phenomenological Rate Coefficients:â€‰ Reactions on a C3H4 Potential Energy Surface. Journal of Physical Chemistry A, 2003, 107, 2680-2692.	1.1	216
21	From the Time-Dependent, Multiple-Well Master Equation to Phenomenological Rate Coefficients. Journal of Physical Chemistry A, 2002, 106, 9267-9277.	1.1	184
22	Kinetic modeling of the reduction of nitric oxide in combustion products by isocyanic acid. International Journal of Chemical Kinetics, 1991, 23, 289-313.	1.0	161
23	Measurements, Theory, and Modeling of OH Formation in Ethyl + O2 and Propyl + O2 Reactions. Journal of Physical Chemistry A, 2003, 107, 4415-4427.	1.1	160
24	Modeling the thermal DENOx process in flow reactors. Surface effects and Nitrous Oxide formation. International Journal of Chemical Kinetics, 1994, 26, 421-436.	1.0	156
25	Reaction of Ethylene with Hydroxyl Radicals:Â A Theoretical Studyâ€. Journal of Physical Chemistry A, 2006, 110, 6960-6970.	1.1	156
26	The reaction between propene and hydroxyl. Physical Chemistry Chemical Physics, 2009, 11, 11040.	1.3	147
27	Lennardâ€“Jones parameters for combustion and chemical kinetics modeling from full-dimensional intermolecular potentials. Combustion and Flame, 2014, 161, 101-110.	2.8	147
28	Exploring old and new benzene formation pathways in low-pressure premixed flames of aliphatic fuels. Proceedings of the Combustion Institute, 2000, 28, 1519-1527.	2.4	144
29	Identification and Chemistry of C4H3and C4H5Isomers in Fuel-Rich Flames. Journal of Physical Chemistry A, 2006, 110, 3670-3678.	1.1	143
30	Predictive a priori pressure-dependent kinetics. Science, 2014, 346, 1212-1215.	6.0	142
31	Association rate constants for reactions between resonance-stabilized radicals: C3H3 + C3H3, C3H3 + C3H5, and C3H5 + C3H5. Physical Chemistry Chemical Physics, 2007, 9, 4259.	1.3	141
32	The Hâ€‰+â€‰C2H2(+M)â€‰â‡„â€‰C2H3(+M) and Hâ€‰+â€‰C2H2(+M)â€‰â‡„â€‰C2H5(+M) reactions: Electronic structure transition-state theory, and solutions to a two-dimensional master equation. Physical Chemistry Chemical Physics, 2004, 6, 1192-1202.	1.3	139
33	Collisional energy transfer in the lowâ€pressureâ€limit unimolecular dissociation of HO2. Journal of Chemical Physics, 1984, 80, 5568-5580.	1.2	138
34	Theoretical Unimolecular Kinetics for CH₄ + M â‡„ CH₃ + H + M in Eight Baths, M = He, Ne, Ar, Kr, H₂, N₂, CO, and CH₄. Journal of Physical Chemistry A, 2011, 115, 6438-6455.	1.1	132
35	The Recombination of Propargyl Radicals:Â Solving the Master Equation. Journal of Physical Chemistry A, 2001, 105, 7254-7266.	1.1	127
36	Solution of Some One- and Two-Dimensional Master Equation Models for Thermal Dissociation:â€‰ The Dissociation of Methane in the Low-Pressure Limit. Journal of Physical Chemistry A, 2002, 106, 4904-4913.	1.1	127

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37	The reaction between ethyl and molecular oxygen II: Further analysis. International Journal of Chemical Kinetics, 2001, 33, 654-668.	1.0	124
38	Identification of C5HxIsomers in Fuel-Rich Flames by Photoionization Mass Spectrometry and Electronic Structure Calculations. Journal of Physical Chemistry A, 2006, 110, 4376-4388.	1.1	122
39	Determination of Adiabatic Flame Speeds by Boundary Value Methods. Combustion Science and Technology, 1983, 34, 79-90.	1.2	118
40	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.	0.3	116
41	Isomer-specific combustion chemistry in allene and propyne flames. Combustion and Flame, 2009, 156, 2153-2164.	2.8	115
42	Synchrotron photoionization measurements of combustion intermediates: Photoionization efficiency and identification of C3H2 isomers. Physical Chemistry Chemical Physics, 2005, 7, 806.	1.3	113
43	Collision dynamics and the thermal rate coefficient for the reaction H+O2â†'OH+O. Journal of Chemical Physics, 1981, 74, 5120-5132.	1.2	110
44	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.	1.0	110
45	A theoretical analysis of the reaction between ethyl and molecular oxygen. Proceedings of the Combustion Institute, 2000, 28, 1479-1486.	2.4	105
46	Theory and modeling in combustion chemistry. Proceedings of the Combustion Institute, 1996, 26, 461-480.	0.3	103
47	â€œThird-Bodyâ€•collision efficiencies for combustion modeling: Hydrocarbons in atomic and diatomic baths. Proceedings of the Combustion Institute, 2015, 35, 197-204.	2.4	97
48	Combustion Chemistry of Enols:â€‰ Possible Ethenol Precursors in Flames. Journal of Physical Chemistry A, 2006, 110, 3254-3260.	1.1	96
49	A theoretical analysis of the reaction between propargyl and molecular oxygen. Faraday Discussions, 2001, 119, 79-100.	1.6	93
50	A Theoretical Analysis of the Reaction between Vinyl and Acetylene:Â Quantum Chemistry and Solution of the Master Equation. Journal of Physical Chemistry A, 2000, 104, 7525-7536.	1.1	91
51	Benzene formation in premixed fuel-rich 1,3-butadiene flames. Proceedings of the Combustion Institute, 2009, 32, 623-630.	2.4	91
52	The reaction of hydroxyethyl radicals with O2: A theoretical analysis and experimental product study. Proceedings of the Combustion Institute, 2009, 32, 271-277.	2.4	90
53	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. Progress in Energy and Combustion Science, 2021, 83, 100886.	15.8	89
54	Nonstatistical effects and detailed balance in quasiclassical trajectory calculations of the thermal rate coefficient for O+OHâ†'O2+H. Journal of Chemical Physics, 1986, 84, 6170-6177.	1.2	88

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55	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	1.1	88
56	Mechanism and modeling of hydrogen cyanide oxidation in a flow reactor. Combustion and Flame, 1994, 99, 475-483.	2.8	87
57	Collisional Energy Transfer in Unimolecular Reactions: Direct Classical Trajectories for CH₄ â‡„ CH₃ + H in Helium. Journal of Physical Chemistry A, 2009, 113, 5612-5619.	1.1	87
58	Infrared frequency-modulation probing of product formation in alkyl + O2 reactions. Part IV.For Part III see ref. 12. Reactions of propyl and butyl radicals with O2Electronic Supplementary Information available. See http://www.rsc.org/suppdata/fd/b1/b102237g/. Faraday Discussions, 2001, 119, 101-120.	1.6	86
59	The Reaction of Acetylene with Hydroxyl Radicals. Journal of Physical Chemistry A, 2005, 109, 6045-6055.	1.1	86
60	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	1.1	84
61	The Reaction ofn- andi-C4H5Radicals with Acetyleneâ€. Journal of Physical Chemistry A, 2007, 111, 3740-3747.	1.1	83
62	Improved simulations of snow extent in the second phase of the Atmospheric Model Intercomparison Project (AMIP-2). Journal of Geophysical Research, 2003, 108, .	3.3	79
63	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.	1.3	76
64	Theoretical Considerations in the NH2 + NO Reaction. Journal of Physical Chemistry A, 2000, 104, 2061-2069.	1.1	74
65	Pathways and Rate Coefficients for the Decomposition of Vinoxy and Acetyl Radicals. Journal of Physical Chemistry A, 2006, 110, 5772-5781.	1.1	74
66	Dissociation of Propyl Radicals and Other Reactions on a C₃H₇ Potential. Journal of Physical Chemistry A, 2013, 117, 2718-2727.	1.1	74
67	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.	0.3	73
68	Reactions over Multiple, Interconnected Potential Wells: Unimolecular and Bimolecular Reactions on a C3H5 Potential. Journal of Physical Chemistry A, 2008, 112, 9429-9438.	1.1	73
69	Determining phenomenological rate coefficients from a time-dependent, multiple-well master equation: â€œspecies reductionâ€•at high temperatures. Physical Chemistry Chemical Physics, 2013, 15, 4744.	1.3	73
70	Chemical nonequilibrium effects in hydrogen-air laminar jet diffusion flames. The Journal of Physical Chemistry, 1977, 81, 2534-2542.	2.9	69
71	Combustion Chemistry. Chemical & Engineering News, 1987, 65, 22-46.	0.2	68
72	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.	3.2	67

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73	The conversion of HCN to NO and N2 in H2â^'O2â^'HCNâ^'Ar flames at low pressure. Proceedings of the Combustion Institute, 1985, 20, 673-684.	0.3	65
74	Collision Efficiency of Water in the Unimolecular Reaction CH₄ (+H₂O) â‡† CH₃ + H (+H₂O): One-Dimensional and Two-Dimensional Solutions of the Low-Pressure-Limit Master Equation. Journal of Physical Chemistry A, 2013, 117, 12243-12255.	1.1	65
75	Unimolecular reaction mechanisms involving C3H4, C4H4, and C6H6 hydrocarbon species. Proceedings of the Combustion Institute, 1992, 24, 621-628.	0.3	63
76	Photoionization mass spectrometric studies and modeling of fuel-rich allene and propyne flames. Proceedings of the Combustion Institute, 2007, 31, 1157-1164.	2.4	63
77	The Temperature and Pressure Dependence of the Reactions H + O2 (+M) â†' HO2 (+M) and H + OH (+M) â†' H2O (+M). Journal of Physical Chemistry A, 2008, 112, 5085-5095.	1.1	63
78	Weakly Bound Free Radicals in Combustion: â€œPromptâ€•Dissociation of Formyl Radicals and Its Effect on Laminar Flame Speeds. Journal of Physical Chemistry Letters, 2016, 7, 85-89.	2.1	63
79	The effect of allene addition on the structure of a rich C2H2/O2/Ar flame. Combustion and Flame, 1996, 105, 451-461.	2.8	62
80	Kinetics of CH + N₂ Revisited with Multireference Methods. Journal of Physical Chemistry A, 2008, 112, 522-532.	1.1	62
81	The Addition of Hydrogen Atoms to Diacetylene and the Heats of Formation ofi-C4H3andn-C4H3. Journal of Physical Chemistry A, 2005, 109, 4285-4295.	1.1	61
82	Kinetics of the reaction between oxygen atoms and ethyl radicals. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 491-503.	1.1	56
83	Pressure-Dependent OH Yields in Alkene + HO₂ Reactions: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 10218-10225.	1.1	56
84	Role of Microstructure and Surface Defects on the Dissolution Kinetics of CeO₂, a UO₂ Fuel Analogue. ACS Applied Materials & Interfaces, 2016, 8, 10562-10571.	4.0	56
85	Quantifying the non-RRKM effect in the H + O2 ? OH + O reaction. International Journal of Chemical Kinetics, 1997, 29, 275-287.	1.0	55
86	A kinetic issue in reburning: the fate of HCNO. Combustion and Flame, 2003, 135, 357-362.	2.8	51
87	Resolving the mystery of prompt CO2: The HCCO+O2 reaction. Proceedings of the Combustion Institute, 2002, 29, 1209-1217.	2.4	50
88	Branching Fraction of the NH2 + NO Reaction between 1210 and 1370 K. Journal of Physical Chemistry A, 1997, 101, 3741-3745.	1.1	49
89	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.	2.9	47
90	Prompt NO: Theoretical prediction of the high-temperature rate coefficient for CH + N2 ? HCN + N. International Journal of Chemical Kinetics, 1997, 29, 253-259.	1.0	44

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91	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.	0.7	43
92	Detailed balance in multiple-well chemical reactions. Physical Chemistry Chemical Physics, 2009, 11, 1128.	1.3	43
93	First-principles binary diffusion coefficients for H, H2, and four normal alkanes + N2. Journal of Chemical Physics, 2014, 141, 124313.	1.2	42
94	Adventures on the C3H5O potential energy surface: OH + propyne, OH + allene and related reactions. Proceedings of the Combustion Institute, 2015, 35, 181-188.	2.4	42
95	Theoretical kinetics of O + C2H4. Proceedings of the Combustion Institute, 2017, 36, 219-227.	2.4	42
96	An exploratory investigation of the use of alkali metals in nitrous oxide control. International Journal of Chemical Kinetics, 1996, 28, 217-234.	1.0	41
97	The recombination of hydrogen atoms with nitric oxide at high temperatures. Proceedings of the Combustion Institute, 1998, 27, 219-226.	0.3	41
98	The Oxidation of Allene in a Low-Pressure H2/ O2/ Ar-C3H4Flame. Combustion Science and Technology, 1995, 110-111, 249-276.	1.2	40
99	A complete statistical analysis of the reaction between OH and CO. Proceedings of the Combustion Institute, 2005, 30, 945-953.	2.4	40
100	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.	2.9	39
101	Kinetics of the Gas-Phase Recombination Reaction of Hydroxyl Radicals to Form Hydrogen Peroxide. Journal of Physical Chemistry A, 2009, 113, 4457-4467.	1.1	38
102	Research in Chemical Carcinogenesis with Elizabeth Millerâ€"A Trail of Discovery with Our Associates. Drug Metabolism Reviews, 1994, 26, 1-36.	1.5	36
103	Ramifications of including non-equilibrium effects for HCO in flame chemistry. Proceedings of the Combustion Institute, 2017, 36, 525-532.	2.4	36
104	A Theoretical Investigation of Mixing Effects in the Selective Reduction of Nitric Oxide by Ammonia. Combustion Science and Technology, 1982, 29, 147-165.	1.2	35
105	Kinetics of Propargyl Radical Dissociation. Journal of Physical Chemistry A, 2015, 119, 7780-7791.	1.1	35
106	The reactions of imidogen with nitric oxide and molecular oxygen. Proceedings of the Combustion Institute, 1992, 24, 719-726.	0.3	33
107	Hydrocarbon/nitric oxide interactions in low-pressure flames. Proceedings of the Combustion Institute, 1988, 21, 965-977.	0.3	31
108	Some Observations Concerning Detailed Balance in Association/Dissociation Reactions. Journal of Physical Chemistry A, 2004, 108, 8296-8306.	1.1	31

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109	The measurement of relative concentration profiles of NH2 using laser absorption spectroscopy. Journal of Quantitative Spectroscopy and Radiative Transfer, 1981, 26, 313-327.	1.1	30
110	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	1.1	30
111	A theoretical analysis of the overtoneâ€induced isomerization of methyl isocyanide. Journal of Chemical Physics, 1986, 85, 4502-4508.	1.2	27
112	A direct transition state theory based analysis of the branching in NH2 + NO. Faraday Discussions, 2001, 119, 207-222.	1.6	27
113	Some chemical kinetics issues in reburning: The branching fraction of the HCCO+NO reaction. Proceedings of the Combustion Institute, 1998, 27, 235-243.	0.3	26
114	Reference natural gas flames at nominally autoignitive engine-relevant conditions. Proceedings of the Combustion Institute, 2019, 37, 1631-1638.	2.4	26
115	Kinetic isotope effects: Theoretical prediction of the thermal rate coefficient for the reaction D+O2â†'OD+O. Journal of Chemical Physics, 1981, 75, 5349-5354.	1.2	25
116	A theoretical analysis of photoactivated unimolecular dissociation: The overtone dissociation of tâ€butyl hydroperoxide. Journal of Chemical Physics, 1984, 81, 455-464.	1.2	25
117	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, 14209-14214.	1.1	25
118	High-Temperature Measurements and a Theoretical Study of the Reaction of OH with 1,3-Butadiene. Journal of Physical Chemistry A, 2010, 114, 8312-8318.	1.1	24
119	The CH3+NO rate coefficient at high temperatures: Theoretical analysis and comparison with experiment. International Journal of Chemical Kinetics, 1998, 30, 223-228.	1.0	23
120	Initiation Reactions in Acetylene Pyrolysis. Journal of Physical Chemistry A, 2017, 121, 4203-4217.	1.1	22
121	A theoretical analysis of the reaction between hydrogen atoms and isocyanic acid. International Journal of Chemical Kinetics, 1992, 24, 421-432.	1.0	21
122	Unimolecular dissociation of hydroxypropyl and propoxy radicals. Proceedings of the Combustion Institute, 2013, 34, 519-526.	2.4	21
123	Solution of Premixed and Counterflow Diffusion Flame Problems by Adaptive Boundary Value Methods. , 1985, , 303-317.		20
124	The Need for Epidemiological Studies of the Medical Exposures of Japanese Patients to the Carcinogen Ethyl Carhamate (Urethane) from 1950 to 1975. Japanese Journal of Cancer Research, 1991, 82, 1323-1324.	1.7	20
125	Oxidation pathways in the reaction of diacetylene with OH radicals. Proceedings of the Combustion Institute, 2007, 31, 185-192.	2.4	20
126	Pressure effects on the thermal de-NOx process. Proceedings of the Combustion Institute, 1996, 26, 2067-2074.	0.3	18

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127	Angular momentum conservation in the O + OH ? O2 + H reaction. International Journal of Chemical Kinetics, 1999, 31, 753-756.	1.0	18
128	Methyl isocyanaide isomerization. Determination of collisional deactivation parameters following carbon-hydrogen overtone excitation. The Journal of Physical Chemistry, 1986, 90, 3544-3549.	2.9	17
129	The structure and reaction mechanism of rich, non-sooting C2H2/O2/Ar flames. Proceedings of the Combustion Institute, 1991, 23, 187-194.	0.3	14
130	A theoretical analysis of the reaction between hydroxyl and hydrogen cyanide at high temperature. Proceedings of the Combustion Institute, 1988, 21, 919-927.	0.3	11
131	Computational modeling of flame structure. Physica D: Nonlinear Phenomena, 1984, 12, 198-211.	1.3	10
132	Rich methane/air flames: Burning velocities, extinction limits, and flammability limit. Proceedings of the Combustion Institute, 1994, 25, 1309-1315.	0.3	8
133	Comment on â€œAutomatic estimation of pressure-dependent rate coefficientsâ€•(J. W. Allen, C. F.) Tj ETQq1 1 0.784314 rgBT /Over Physics, 2012, 14, 8431.	1.3	8
134	Inhibitory effects of chlorophyllin on micronucleus formation induced by ethyl carbamate and its proximate and ultimate carcinogenic forms in mouse peripheral reticulocytes. , 1999, 34, 57-60.		7
135	Comparative carcinogeniocities and reactivities of N-myristoyloxy-N-acetyl-2-aminofluorene and its 7-iodo derivative. Carcinogenesis, 1981, 2, 655-659.	1.3	6
136	Secondary decomposition of C3H5 radicals formed by the photodissociation of 2-bromopropene. Journal of Chemical Physics, 2007, 127, 144301.	1.2	6
137	Synthesis of the hepatocarcinogen N-methyl-4-aminoazobenzene with tritium in the prime ring. Journal of Labelled Compounds, 1969, 5, 257-260.	0.3	3
138	Comment on â€œInfluence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicalsâ€• Journal of Physical Chemistry A, 2019, 123, 1129-1130.	1.1	1