

Anthony M Dean

List of Publications by Year in descending order

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102
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104
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104
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104
times ranked

3343
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of the Smokeless Rich Diesel Combustion by Reducing Temperature. , 0, , .		632
2	Forming benzene in flames by chemically activated isomerization. The Journal of Physical Chemistry, 1989, 93, 8171-8180.	2.9	328
3	Methane reforming kinetics within a Niâ€‘YSZ SOFC anode support. Applied Catalysis A: General, 2005, 295, 40-51.	4.3	290
4	High-Pressure Rate Rules for Alkyl + O ₂ Reactions. 1. The Dissociation, Concerted Elimination, and Isomerization Channels of the Alkyl Peroxy Radical. Journal of Physical Chemistry A, 2011, 115, 13425-13442.	2.5	223
5	O + NNH: A possible new route for NOX formation in flames. International Journal of Chemical Kinetics, 1995, 27, 1097-1109.	1.6	222
6	Rate-Based Construction of Kinetic Models for Complex Systems. Journal of Physical Chemistry A, 1997, 101, 3731-3740.	2.5	192
7	High-Pressure Rate Rules for Alkyl + O ₂ Reactions. 2. The Isomerization, Cyclic Ether Formation, and Î²-Scission Reactions of Hydroperoxy Alkyl Radicals. Journal of Physical Chemistry A, 2012, 116, 5068-5089.	2.5	172
8	Hydrogen Atom Bond Increments for Calculation of Thermodynamic Properties of Hydrocarbon Radical Species. The Journal of Physical Chemistry, 1995, 99, 14514-14527.	2.9	160
9	Direct Detection of Products from the Pyrolysis of 2-Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2011, 115, 428-438.	2.5	160
10	Detailed kinetic modeling of autocatalysis in methane pyrolysis. The Journal of Physical Chemistry, 1990, 94, 1432-1439.	2.9	151
11	Hydrocarbon radical reactions with oxygen: comparison of allyl, formyl, and vinyl to ethyl. The Journal of Physical Chemistry, 1993, 97, 4427-4441.	2.9	145
12	Bimolecular QRRK analysis of methyl radical reactions. International Journal of Chemical Kinetics, 1987, 19, 207-228.	1.6	142
13	Detailed Kinetics and Thermochemistry of C ₂ H ₅ + O ₂ :Â Reaction Kinetics of the Chemically-Activated and Stabilized CH ₃ CH ₂ OOâ€‘Adduct. Journal of Physical Chemistry A, 2002, 106, 7276-7293.	2.5	140
14	Combustion Chemistry of Nitrogen. , 2000, , 125-341.		136
15	Kinetic study on thermal decomposition of chlorobenzene diluted in hydrogen. The Journal of Physical Chemistry, 1990, 94, 2493-2504.	2.9	110
16	Chemical activation analysis of the reaction of ethyl radical with oxygen. The Journal of Physical Chemistry, 1990, 94, 3313-3317.	2.9	107
17	Prediction of rate constants for combustion and pyrolysis reactions by bimolecular QRRK. AIChE Journal, 1986, 32, 1971-1979.	3.6	101
18	Shock-tube studies of formaldehyde oxidation. Combustion and Flame, 1980, 37, 41-62.	5.2	100

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19	Rate Constant Rules for the Automated Generation of Gas-Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 367-380.	2.5	95
20	Mechanism Generation with Integrated Pressure Dependence: A New Model for Methane Pyrolysis. Journal of Physical Chemistry A, 2003, 107, 8552-8565.	2.5	94
21	Rate constants for the H abstraction from alkanes (R-H) by O_2 radicals: A systematic study on the impact of R and R^2 . Proceedings of the Combustion Institute, 2007, 31, 149-157.	3.9	89
22	Hydrocarbon Fuels in Solid Oxide Fuel Cells: In Situ Raman Studies of Graphite Formation and Oxidation. Journal of Physical Chemistry C, 2008, 112, 5232-5240.	3.1	88
23	Kinetics of rich ammonia flames. International Journal of Chemical Kinetics, 1984, 16, 633-653.	1.6	86
24	CHEMACT: A Computer Code to Estimate Rate Constants for Chemically-Activated Reactions. Combustion Science and Technology, 1991, 80, 63-85.	2.3	84
25	Computer Construction of Detailed Chemical Kinetic Models for Gas-Phase Reactors. Industrial & Engineering Chemistry Research, 2001, 40, 5362-5370.	3.7	78
26	Importance of Gas-Phase Kinetics within the Anode Channel of a Solid-Oxide Fuel Cell. Journal of Physical Chemistry A, 2004, 108, 3772-3783.	2.5	75
27	Homogeneous kinetics and equilibrium predictions of coking propensity in the anode channels of direct oxidation solid-oxide fuel cells using dry natural gas. Journal of Power Sources, 2003, 123, 182-189.	7.8	74
28	Detailed Modeling of Low-Temperature Propane Oxidation: 1. The Role of the Propyl + O_2 Reaction. Journal of Physical Chemistry A, 2010, 114, 6594-6607.	2.5	70
29	Detailed Modeling of the Reaction of $\text{C}_2\text{H}_5 + \text{O}_2$. Journal of Physical Chemistry A, 2005, 109, 2264-2281.	2.5	65
30	Molecular density of states from estimated vapor phase heat capacities. International Journal of Chemical Kinetics, 1997, 29, 161-170.	1.6	62
31	Numerical and Experimental Investigation of <i>n</i> -Heptane Autoignition in the Ignition Quality Tester (IQT). Energy & Fuels, 2011, 25, 5562-5572.	5.1	61
32	Energized complex quantum Rice-Ramsperger-Kassel analysis on reactions of amidogen with hydroperoxy, oxygen and oxygen atoms. The Journal of Physical Chemistry, 1989, 93, 1058-1065.	2.9	60
33	Reactivity-Structure-Based Rate Estimation Rules for Alkyl Radical H Atom Shift and Alkenyl Radical Cycloaddition Reactions. Journal of Physical Chemistry A, 2015, 119, 7205-7221.	2.5	60
34	The numerical solution of some kinetics models with VODE and CHEMKIN II. Computers & Chemistry, 1993, 17, 297-302.	1.2	59
35	Rate Rules, Branching Ratios, and Pressure Dependence of the $\text{HO}_2 + \text{Olefin}$ Addition Channels. Journal of Physical Chemistry A, 2013, 117, 6458-6473.	2.5	57
36	Fundamentally-based kinetic model for propene pyrolysis. Combustion and Flame, 2015, 162, 4456-4470.	5.2	57

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37	Comparison of conversion and deposit formation of ethanol and butane under SOFC conditions. <i>Journal of Power Sources</i> , 2006, 158, 497-503.	7.8	56
38	Ignition Quality Tester (IQT) Investigation of the Negative Temperature Coefficient Region of Alkane Autoignition. <i>Energy & Fuels</i> , 2013, 27, 1632-1642.	5.1	56
39	Laser induced fluorescence and absorption measurements of NO in NH ₃ /O ₂ and CH ₄ /air flames. <i>Journal of Chemical Physics</i> , 1983, 78, 5962-5970.	3.0	54
40	Detailed kinetic modeling of ethane oxidation. <i>Combustion and Flame</i> , 2006, 145, 16-37.	5.2	52
41	Master equation analysis of intermolecular energy transfer in multiple-well, multiple-channel unimolecular reactions. II. Numerical methods and application to the mechanism of the C ₂ H ₅ +O ₂ reaction. <i>Journal of Chemical Physics</i> , 1999, 111, 8313-8329.	3.0	51
42	Gas-phase reactions of methane and natural-gas with air and steam in non-catalytic regions of a solid-oxide fuel cell. <i>Journal of Power Sources</i> , 2006, 156, 434-447.	7.8	50
43	Reactions of allylic radicals that impact molecular weight growth kinetics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6255-6273.	2.8	49
44	Non-catalytic partial oxidation of bio-oil to synthesis gas for distributed hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2009, 34, 8519-8534.	7.1	45
45	A comparison of H ₂ S, SO ₂ , and COS poisoning on Ni/YSZ and Ni/K ₂ O-CaAl ₂ O ₄ during methane steam and dry reforming. <i>Applied Catalysis A: General</i> , 2015, 502, 399-409.	4.3	44
46	Rate constants for the abstraction reactions RO ₂ +C ₂ H ₆ ; R=H, CH ₃ , and C ₂ H ₅ . <i>Proceedings of the Combustion Institute</i> , 2005, 30, 995-1003.	3.9	41
47	Kinetic Modeling of Ethane Pyrolysis at High Conversion. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10470-10490.	2.5	41
48	Parameterization of pressure- and temperature-dependent kinetics in multiple well reactions. <i>AICHE Journal</i> , 1997, 43, 1331-1340.	3.6	40
49	A quantitative kinetic analysis of CO elimination from phenoxy radicals. <i>International Journal of Chemical Kinetics</i> , 2012, 44, 75-89.	1.6	40
50	Hydrocarbon fuel effects in solid-oxide fuel cell operation: an experimental and modeling study of n-hexane pyrolysis. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4245.	2.8	39
51	Analysis of the reactions H+N ₂ O and NH+NO: Pathways and rate constants over a wide range of temperature and pressure. <i>Proceedings of the Combustion Institute</i> , 1994, 25, 965-974.	0.3	35
52	Experiments and Computational Fluid Dynamics Modeling Analysis of Large <i>n</i> -Alkane Ignition Kinetics in the Ignition Quality Tester. <i>Energy & Fuels</i> , 2014, 28, 4781-4794.	5.1	35
53	Application of Computational Kinetic Mechanism Generation to Model the Autocatalytic Pyrolysis of Methane. <i>Industrial & Engineering Chemistry Research</i> , 2003, 42, 1000-1010.	3.7	32
54	Master equation analysis of intermolecular energy transfer in multiple-well, multiple-channel unimolecular reactions. I. Basic theory. <i>Journal of Chemical Physics</i> , 1997, 107, 8904-8916.	3.0	31

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55	Expanding the Experimental Capabilities of the Ignition Quality Tester for Autoigniting Fuels. SAE International Journal of Fuels and Lubricants, 0, 3, 353-367.	0.2	31
56	Experimental and kinetic modeling study of butene isomer pyrolysis: Part I. 1- and 2-Butene. Combustion and Flame, 2016, 173, 347-369.	5.2	31
57	Chapter 4 The Kinetics of Pressure-Dependent Reactions. Comprehensive Chemical Kinetics, 2007, 42, 101-184.	2.3	30
58	Insights into the Glycyl Radical Enzyme Active Site of Benzylsuccinate Synthase: A Computational Study. Journal of the American Chemical Society, 2013, 135, 12279-12288.	13.7	30
59	Hydrogen abstraction rates via density functional theory. Chemical Physics Letters, 1999, 312, 262-268.	2.6	26
60	A shock tube study of the recombination of carbon monoxide and oxygen atoms. Journal of Chemical Physics, 1977, 66, 598-604.	3.0	25
61	Shock tube studies of the N ₂ O/Ar and N ₂ O/H ₂ /Ar systems. International Journal of Chemical Kinetics, 1976, 8, 459-474.	1.6	24
62	Rate-based screening of pressure-dependent reaction networks. Computer Physics Communications, 2001, 138, 237-249.	7.5	24
63	Development of Detailed Kinetic Models for the Thermal Conversion of Biomass via First Principle Methods and Rate Estimation Rules. ACS Symposium Series, 2010, , 201-243.	0.5	23
64	The effects of multicomponent fuel droplet evaporation on the kinetics of strained opposed-flow diffusion flames. Combustion and Flame, 2013, 160, 265-275.	5.2	23
65	Dissociation of carbon dioxide behind reflected shock waves. Journal of Chemical Physics, 1973, 58, 5202-5208.	3.0	21
66	The Impact of Resonance Stabilization on the Intramolecular Hydrogen-Atom Shift Reactions of Hydrocarbon Radicals. ChemPhysChem, 2015, 16, 2635-2645.	2.1	21
67	Experimental and kinetic modeling study of butene isomer pyrolysis: Part II. Isobutene. Combustion and Flame, 2017, 176, 23-37.	5.2	21
68	Impact of gas-phase reactions in the mixing region upstream of a diesel fuel autothermal reformer. Journal of Power Sources, 2011, 196, 2020-2026.	7.8	20
69	Ab initio study of the influence of resonance stabilization on intramolecular ring closure reactions of hydrocarbon radicals. Physical Chemistry Chemical Physics, 2016, 18, 8437-8452.	2.8	20
70	Performance predictions of a tubular SOFC operating on a partially reformed JP-8 surrogate. Journal of Power Sources, 2006, 162, 553-562.	7.8	19
71	The effects of liquid-fuel thermophysical properties, carrier-gas composition, and pressure, on strained opposed-flow non-premixed flames. Combustion and Flame, 2011, 158, 1129-1139.	5.2	18
72	N ₂ O Dissociation behind reflected shock waves. International Journal of Chemical Kinetics, 1975, 7, 381-398.	1.6	16

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73	Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism – a gas-phase <i>ab initio</i> study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4054-4066.	2.8	14
74	Investigation of Iso-octane Ignition and Validation of a Multizone Modeling Method in an Ignition Quality Tester. <i>Energy & Fuels</i> , 2016, 30, 9761-9771.	5.1	14
75	Reaction of atomic oxygen with carbon dioxide behind reflected shock waves. <i>Journal of Chemical Physics</i> , 1974, 60, 307-313.	3.0	13
76	Nitrogen Chemistry in Flames. <i>ACS Symposium Series</i> , 1983, , 71-86.	0.5	13
77	Shock tube studies of the N ₂ O/CH ₄ /CO/Ar and N ₂ O/C ₂ H ₆ /CO/Ar systems. <i>Combustion and Flame</i> , 1980, 37, 109-123.	5.2	12
78	Selective Removal of Ethylene, a Deposit Precursor, from a –Dirty– Synthesis Gas Stream via Gas-Phase Partial Oxidation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6502-6514.	2.5	12
79	Bayesian method for global optimization. <i>Physical Review E</i> , 1997, 55, 6219-6232.	2.1	11
80	Modeling high pressure ethane oxidation and pyrolysis. <i>Proceedings of the Combustion Institute</i> , 2009, 32, 437-443.	3.9	11
81	Coupling Complex Reformer Chemical Kinetics with Three-Dimensional Computational Fluid Dynamics. <i>ECS Transactions</i> , 2009, 25, 1253-1262.	0.5	9
82	The impact of fuel evaporation on the gas-phase kinetics in the mixing region of a diesel autothermal reformer. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 15477-15490.	7.1	9
83	Excimer laser perturbations of methane flames: High temperature reactions of OH and CH. <i>International Journal of Chemical Kinetics</i> , 1985, 17, 1103-1118.	1.6	8
84	CHEBYSHEV EXPANSIONS AND SENSITIVITY ANALYSIS FOR APPROXIMATING THE TEMPERATURE- AND PRESSURE-DEPENDENCE OF CHEMICALLY-ACTIVATED REACTIONS. <i>Reviews in Chemical Engineering</i> , 1997, 13, 1-67.	4.4	8
85	Kinetic Analysis of C ₄ Alkane and Alkene Pyrolysis: Implications for SOFC Operation. <i>Journal of Fuel Cell Science and Technology</i> , 2010, 7, .	0.8	8
86	Investigation of gas-phase reactions in the mixing region for hydrocarbon autothermal reforming applications. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 7545-7553.	7.1	8
87	Comparative Kinetic Analysis of Ethane Pyrolysis at 0.1 and 2.0 MPa. <i>Energy & Fuels</i> , 2016, 30, 9703-9711.	5.1	8
88	On-Line Computer Acquisition of Data from a Shocktube Experiment*. <i>Instrumentation Science and Technology</i> , 1974, 5, 109-126.	1.8	7
89	Coupled transport and kinetics in the mixing region for hydrocarbon autothermal reforming applications. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 16140-16151.	7.1	7
90	Impact of the Molecular Structure on Olefin Pyrolysis. <i>Energy & Fuels</i> , 2017, 31, 6515-6524.	5.1	7

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91	RCARM: Reaction classification using automated reaction mapping. International Journal of Chemical Kinetics, 2013, 45, 125-139.	1.6	4
92	Rate rules and reaction classes. Computer Aided Chemical Engineering, 2019, 45, 203-257.	0.5	4
93	Microcanonical Transition State Theory Rate Coefficients from Thermal Rate Constants via Inverse Laplace Transformation. Journal of Physical Chemistry A, 1998, 102, 8104-8115.	2.5	3
94	Reactions of CH ₂ and CH with N ₂ and CH with NO. , 1993, , 101-116.		3
95	Variational optimisation by the solution of a series of Hamiltonian-Jacobi equations. Physica D: Nonlinear Phenomena, 2001, 154, 15-25.	2.8	2
96	The formation of ultrathin silicon oxide films using H ₂ /N ₂ O mixtures. Proceedings of the Combustion Institute, 2002, 29, 1055-1062.	3.9	2
97	Impact of Gas-Phase Reactions on SOFC Systems Operating on Diesel and Biomass-Derived Fuels. Materials Science Forum, 2010, 638-642, 1118-1124.	0.3	2
98	Simulation of n-Heptane and Surrogate Fuels for Advanced Combustion Engines (FACE) in a Single-Cylinder Compression Ignition Engine. , 2013, , . <small>Model-predicted effects of fuel droplet diameter and</small>		2
99	<small>xml:ns:xocs="http://www.elsevier.com/xml/xocs/dtd" xml:ns:xs="http://www.w3.org/2001/XMLSchema" xml:ns:xsi="http://www.w3.org/2001/XMLSchema-instance" xml:ns="http://www.elsevier.com/xml/ja/dtd" xml:ns:ja="http://www.elsevier.com/xml/ja/dtd" xml:ns:mml="http://www.w3.org/1998/Math/MathML" xml:ns:tb="http://www.elsevier.com/xml/common/table/dtd" xml:ns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xml:ns:ce="ht. Combustion and Flame,</small> Impact of Finite Mixing on Gas-Phase Partial Oxidation for Selective Removal of Deposit Precursors from Gasifier Outlet Streams. Energy & Fuels, 2015, 29, 6501-6511.	5.2	1
100	Impact of Finite Mixing on Gas-Phase Partial Oxidation for Selective Removal of Deposit Precursors from Gasifier Outlet Streams. Energy & Fuels, 2015, 29, 6501-6511.	5.1	1
101	Chemical Kinetics: A CS Perspective. Computing in Science and Engineering, 2016, 18, 48-55.	1.2	0
102	Ethanol Transport and Chemistry in Solid Oxide Fuel Cells. , 2008, , .		0