William H Green

List of Publications by Year
in descending order

297 papers	16,892 citations	11639 70 h-index	22147 113 g-index
306 all docs	306 docs citations	306 times ranked	10937 citing authors

#	Article	IF	Citations
1	A robotic platform for flow synthesis of organic compounds informed by AI planning. Science, 2019, 365, .	6.0	548
2	Reaction Mechanism Generator: Automatic construction of chemical kinetic mechanisms. Computer Physics Communications, 2016, 203, 212-225.	3.0	515
3	Prediction of Organic Reaction Outcomes Using Machine Learning. ACS Central Science, 2017, 3, 434-443.	5.3	477
4	Machine Learning in Computer-Aided Synthesis Planning. Accounts of Chemical Research, 2018, 51, 1281-1289.	7.6	430
5	A graph-convolutional neural network model for the prediction of chemical reactivity. Chemical Science, 2019, 10, 370-377.	3.7	430
6	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 1757-1772.	2.5	317
7	Detailed modeling of PAH and soot formation in a laminar premixed benzene/oxygen/argon low-pressure flame. Proceedings of the Combustion Institute, 2005, 30, 1397-1405.	2.4	251
8	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. ACS Central Science, 2018, 4, 1465-1476.	5.3	245
9	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. Combustion and Flame, 2011, 158, 16-41.	2.8	240
10	Intramolecular Hydrogen Migration in Alkylperoxy and Hydroperoxyalkylperoxy Radicals: Accurate Treatment of Hindered Rotors. Journal of Physical Chemistry A, 2010, 114, 5689-5701.	1.1	225
11	Role of O₂ + QOOH in Low-Temperature Ignition of Propane. 1. Temperature and Pressure Dependent Rate Coefficients. Journal of Physical Chemistry A, 2012, 116, 3325-3346.	1.1	223
12	High-gradient magnetic separation of coated magnetic nanoparticles. AICHE Journal, 2004, 50, 2835-2848.	1.8	221
13	Computational Investigation of Thermochemistry and Kinetics of Steam Methane Reforming on Ni(111) under Realistic Conditions. Journal of Physical Chemistry C, 2009, 113, 4898-4908.	1.5	220
14	Reactivity and stability investigation of supported molybdenum oxide catalysts for the hydrodeoxygenation (HDO) of m-cresol. Journal of Catalysis, 2015, 331, 86-97.	3.1	205
15	Computer-Assisted Retrosynthesis Based on Molecular Similarity. ACS Central Science, 2017, 3, 1237-1245.	5.3	200
16	Rate-Based Construction of Kinetic Models for Complex Systems. Journal of Physical Chemistry A, 1997, 101, 3731-3740.	1.1	192
17	Database of Small Molecule Thermochemistry for Combustion. Journal of Physical Chemistry A, 2012, 116, 9033-9057.	1.1	178
18	SCScore: Synthetic Complexity Learned from a Reaction Corpus. Journal of Chemical Information and Modeling, 2018, 58, 252-261.	2.5	176

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19	Dramatic Solvent Effects on the Absolute Rate Constants for Abstraction of the Hydroxylic Hydrogen Atom from tert-Butyl Hydroperoxide and Phenol by the Cumyloxyl Radical. The Role of Hydrogen Bonding. Journal of the American Chemical Society, 1995, 117, 2929-2930.	6.6	160
20	New Pathways for Formation of Acids and Carbonyl Products in Low-Temperature Oxidation: The Korcek Decomposition of Î³-Ketohydroperoxides. Journal of the American Chemical Society, 2013, 135, 11100-11114.	6.6	153
21	Transition States and Rate Constants for Unimolecular Reactions. Annual Review of Physical Chemistry, 1992, 43, 591-626.	4.8	151
22	Optimally-reduced kinetic models: reaction elimination in large-scale kinetic mechanisms. Combustion and Flame, 2003, 135, 191-208.	2.8	147
23	Reaction Rate Prediction via Group Additivity Part 1:â€‰ H Abstraction from Alkanes by H and CH3. Journal of Physical Chemistry A, 2001, 105, 6910-6925.	1.1	136
24	Bond breaking without barriers: Photofragmentation of ketene at the singlet threshold. Journal of Chemical Physics, 1988, 89, 314-328.	1.2	134
25	Water-Based Magnetic Fluids as Extractants for Synthetic Organic Compounds. Industrial & Engineering Chemistry Research, 2002, 41, 4739-4749.	1.8	133
26	Upper bound on the yield for oxidative coupling of methane. Journal of Catalysis, 2003, 218, 321-333.	3.1	133
27	Anharmonic corrections to vibrational transition intensities. The Journal of Physical Chemistry, 1990, 94, 5608-5616.	2.9	132
28	Automated Discovery of Elementary Chemical Reaction Steps Using Freezing String and Berny Optimization Methods. Journal of Chemical Theory and Computation, 2015, 11, 4248-4259.	2.3	127
29	Formation of polycyclic aromatic hydrocarbons and their radicals in a nearly sooting premixed benzene flame. Proceedings of the Combustion Institute, 2000, 28, 2609-2618.	2.4	126
30	Electronic Structures and Geometries of C60Anions via Density Functional Calculations. The Journal of Physical Chemistry, 1996, 100, 14892-14898.	2.9	125
31	Capturing pressure-dependence in automated mechanism generation: Reactions through cycloalkyl intermediates. International Journal of Chemical Kinetics, 2003, 35, 95-119.	1.0	123
32	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	2.8	122
33	Automatic reaction network generation using RMG for steam cracking of n-hexane. AICHE Journal, 2006, 52, 718-730.	1.8	119
34	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. Journal of Medicinal Chemistry, 2020, 63, 8667-8682.	2.9	118
35	Reaction Mechanism Generator v3.0: Advances in Automatic Mechanism Generation. Journal of Chemical Information and Modeling, 2021, 61, 2686-2696.	2.5	116
36	Anharmonic vibrational properties of CH2F2: A comparison of theory and experiment. Journal of Chemical Physics, 1991, 95, 8323-8336.	1.2	115

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37	Learning only buys you so much: Practical limits on battery price reduction. Applied Energy, 2019, 239, 218-224.	5.1	115
38	Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. Journal of Chemical Information and Modeling, 2020, 60, 2697-2717.	2.5	113
39	Thermodynamic Properties and Kinetic Parameters for Cyclic Ether Formation from Hydroperoxyalkyl Radicals. Journal of Physical Chemistry A, 2003, 107, 4908-4920.	1.1	110
40	Upgrading and desulfurization of heavy oils by supercritical water. Journal of Supercritical Fluids, 2015, 96, 114-123.	1.6	109
41	Reaction Rate Prediction via Group Additivity, Part 2:Â H-Abstraction from Alkenes, Alkynes, Alcohols, Aldehydes, and Acids by H Atoms. Journal of Physical Chemistry A, 2001, 105, 8969-8984.	1.1	103
42	Deep Learning of Activation Energies. Journal of Physical Chemistry Letters, 2020, 11, 2992-2997.	2.1	102
43	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. Journal of Chemical Physics, 1990, 93, 4965-4981.	1.2	101
44	RPMDrate: Bimolecular chemical reaction rates from ring polymer molecular dynamics. Computer Physics Communications, 2013, 184, 833-840.	3.0	101
45	Detailed Kinetic Study of the Growth of Small Polycyclic Aromatic Hydrocarbons. 1. 1-Naphthyl + Ethyneâ€. Journal of Physical Chemistry A, 2001, 105, 1561-1573.	1.1	97
46	Automatic estimation of pressure-dependent rate coefficients. Physical Chemistry Chemical Physics, 2012, 14, 1131-1155.	1.3	96
47	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. Journal of Chemical Information and Modeling, 2019, 59, 2529-2537.	2.5	96
48	Mechanism Generation with Integrated Pressure Dependence:Â A New Model for Methane Pyrolysis. Journal of Physical Chemistry A, 2003, 107, 8552-8565.	1.1	94
49	Supercritical Water Desulfurization of Organic Sulfides Is Consistent with Free-Radical Kinetics. Energy & Fuels, 2013, 27, 6108-6117.	2.5	90
50	An adaptive chemistry approach to modeling complex kinetics in reacting flows. Combustion and Flame, 2003, 133, 451-465.	2.8	89
51	Computational Investigation of the Thermochemistry and Kinetics of Steam Methane Reforming Over a Multi-Faceted Nickel Catalyst. Topics in Catalysis, 2011, 54, 828-844.	1.3	89
52	Accurate and Efficient Method for Predicting Thermochemistry of Polycyclic Aromatic Hydrocarbons â^' Bond-Centered Group Additivity. Journal of the American Chemical Society, 2004, 126, 12685-12700.	6.6	87
53	High-temperature oxidation chemistry of n-butanol â€“ experiments in low-pressure premixed flames and detailed kinetic modeling. Physical Chemistry Chemical Physics, 2011, 13, 20262.	1.3	86
54	Direct Kinetic Measurements of Reactions between the Simplest Criegee Intermediate CH₂OO and Alkenes. Journal of Physical Chemistry A, 2014, 118, 1997-2006.	1.1	86

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55	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. Combustion and Flame, 2016, 168, 310-330.	2.8	85
56	Theoretical assignment of the visible spectrum of singlet methylene. Journal of Chemical Physics, 1991, 94, 118-132.	1.2	84
57	Unimolecular Reaction Pathways of a Î³-Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. Journal of the American Chemical Society, 2018, 140, 1035-1048.	6.6	82
58	Vibration-rotation coordinates and kinetic energy operators for polyatomic molecules. Molecular Physics, 1991, 73, 1183-1208.	0.8	81
59	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. Combustion and Flame, 2015, 162, 3115-3129.	2.8	80
60	Global Dynamic Optimization for Parameter Estimation in Chemical Kinetics. Journal of Physical Chemistry A, 2006, 110, 971-976.	1.1	79
61	Computer Construction of Detailed Chemical Kinetic Models for Gas-Phase Reactors. Industrial & Engineering Chemistry Research, 2001, 40, 5362-5370.	1.8	78
62	Transfer learning for solvation free energies: From quantum chemistry to experiments. Chemical Engineering Journal, 2021, 418, 129307.	6.6	77
63	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	2.4	75
64	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. Chemical Science, 2021, 12, 2198-2208.	3.7	75
65	Kinetic anharmonic coupling in the trihalomethanes: A mechanism for rapid intramolecular redistribution of CH stretch vibrational energy. Journal of Chemical Physics, 1987, 86, 6000-6011.	1.2	74
66	Structural Properties and Reactivity Trends of Molybdenum Oxide Catalysts Supported on Zirconia for the Hydrodeoxygenation of Anisole. ACS Sustainable Chemistry and Engineering, 2017, 5, 5293-5301.	3.2	74
67	A perturbation theory guide to openâ€shell complexes: OHâ€“Ar(Xâ€‰2Î). Journal of Chemical Physics, 1992, 96, 2573-2584.	1.2	73
68	A priori rate constants for kinetic modeling. Theoretical Chemistry Accounts, 2002, 108, 187-213.	0.5	73
69	Oxygenate, oxyalkyl and alkoxycarbonyl thermochemistry and rates for hydrogen abstraction from oxygenates. Physical Chemistry Chemical Physics, 2003, 5, 3402-3417.	1.3	72
70	Computed Rate Coefficients and Product Yields for c-C₅H₅ + CH₃ â†' Products. Journal of Physical Chemistry A, 2009, 113, 8871-8882.	1.1	72
71	Rate coefficients and kinetic isotope effects of the X + CH4 â†' CH3 + HX (X = H, D, Mu) reactions from ring polymer molecular dynamics. Journal of Chemical Physics, 2013, 138, 094307.	1.2	72
72	Direct Determination of the Simplest Criegee Intermediate (CH₂OO) Self Reaction Rate. Journal of Physical Chemistry Letters, 2014, 5, 2224-2228.	2.1	72

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73	Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach. Journal of Physical Chemistry A, 2019, 123, 5826-5835.	1.1	72
74	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. Industrial & Engineering Chemistry Research, 2010, 49, 10399-10420.	1.8	71
75	Communication: Full dimensional quantum rate coefficients and kinetic isotope effects from ring polymer molecular dynamics for a seven-atom reaction OH + CH4 â†' CH3 + H2O. Journal of Chemical Physics, 2013, 138, 221103.	1.2	71
76	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. Scientific Data, 2020, 7, 137.	2.4	71
77	Global solution of semi-infinite programs. Mathematical Programming, 2005, 103, 283-307.	1.6	70
78	Toward a Comprehensive Model of the Synthesis of TiO₂ Particles from TiCl₄. Industrial & Engineering Chemistry Research, 2007, 46, 6147-6156.	1.8	70
79	Ring Polymer Molecular Dynamics Calculations of Thermal Rate Constants for the O(³P) + CH₄ â†' OH + CH₃ Reaction: Contributions of Quantum Effects. Journal of Physical Chemistry Letters, 2013, 4, 48-52.	2.1	68
80	Chemically activated formation of organic acids in reactions of the Criegee intermediate with aldehydes and ketones. Physical Chemistry Chemical Physics, 2013, 15, 16841.	1.3	68
81	First-Principles Thermochemistry for the Production of TiO2from TiCl4. Journal of Physical Chemistry A, 2007, 111, 3560-3565.	1.1	66
82	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. Combustion and Flame, 2013, 160, 1907-1929.	2.8	65
83	Kinetic model for polycrystalline Pd/PdOx in oxidation/reduction cycles. Applied Catalysis A: General, 2003, 244, 323-340.	2.2	64
84	The Electrostatic Origin of Abraham's Solute Polarity Parameter. Journal of Physical Chemistry B, 2005, 109, 7564-7573.	1.2	64
85	Stress Test for Quantum Dynamics Approximations: Deep Tunneling in the Muonium Exchange Reaction D + HMu â†' DMu + H. Journal of Physical Chemistry Letters, 2014, 5, 4219-4224.	2.1	64
86	Detailed Kinetic Modeling of Iron Nanoparticle Synthesis from the Decomposition of Fe(CO)5. Journal of Physical Chemistry C, 2007, 111, 5677-5688.	1.5	63
87	The role of catalyst in supercritical water desulfurization. Applied Catalysis B: Environmental, 2014, 147, 144-155.	10.8	63
88	Reaction Rate Predictions Via Group Additivity. Part 3:â€‰ Effect of Substituents with CH2 as the Mediator. Journal of Physical Chemistry A, 2002, 106, 5474-5489.	1.1	62
89	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. Proceedings of the Combustion Institute, 2019, 37, 363-371.	2.4	62
90	Coupling of CH stretching and bending vibrations in trihalomethanes. Journal of Chemical Physics, 1987, 86, 5994-5999.	1.2	61

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91	Elementary Reaction Mechanism for Benzene Oxidation in Supercritical Waterâ€. Journal of Physical Chemistry A, 2000, 104, 10576-10586.	1.1	61
92	On upgrading the numerics in combustion chemistry codes. Combustion and Flame, 2002, 128, 270-291.	2.8	60
93	Predicting solvation energies for kinetic modeling. Annual Reports on the Progress of Chemistry Section C, 2010, 106, 211.	4.4	59
94	Group Contribution and Machine Learning Approaches to Predict Abraham Solute Parameters, Solvation Free Energy, and Solvation Enthalpy. Journal of Chemical Information and Modeling, 2022, 62, 433-446.	2.5	59
95	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. Combustion and Flame, 2018, 187, 247-256.	2.8	58
96	Theoretical Kinetics Study of the O(³P) + CH₄/CD₄ Hydrogen Abstraction Reaction: The Role of Anharmonicity, Recrossing Effects, and Quantum Mechanical Tunneling. Journal of Physical Chemistry A, 2014, 118, 3243-3252.	1.1	57
97	Combining experiment and theory to elucidate the role of supercritical water in sulfide decomposition. Physical Chemistry Chemical Physics, 2014, 16, 9220-9228.	1.3	56
98	Minimizing E-factor in the continuous-flow synthesis of diazepam and atropine. Bioorganic and Medicinal Chemistry, 2017, 25, 6233-6241.	1.4	56
99	Steam methane reforming on a Ni-based bimetallic catalyst: density functional theory and experimental studies of the catalytic consequence of surface alloying of Ni with Ag. Catalysis Science and Technology, 2017, 7, 1713-1725.	2.1	55
100	A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi. Combustion and Flame, 2014, 161, 711-724.	2.8	54
101	Iterative experimental design based on active machine learning reduces the experimental burden associated with reaction screening. Reaction Chemistry and Engineering, 2020, 5, 1963-1972.	1.9	54
102	Quantum Rate Coefficients and Kinetic Isotope Effect for the Reaction Cl + CH₄ â†' HCl + CH₃ from Ring Polymer Molecular Dynamics. Journal of Physical Chemistry A, 2014, 118, 1989-1996.	1.1	53
103	Accelerating multi-dimensional combustion simulations using GPU and hybrid explicit/implicit ODE integration. Combustion and Flame, 2012, 159, 2388-2397.	2.8	52
104	Experimental and modeling study of the mutual oxidation of N-pentane and nitrogen dioxide at low and high temperatures in a jet stirred reactor. Energy, 2018, 165, 727-738.	4.5	52
105	Economic and Environmental Benefits of Higher-Octane Gasoline. Environmental Science & Technology, 2014, 48, 6561-6568.	4.6	51
106	Bondâ€breaking without barriers. II. Vibrationally excited products. Journal of Chemical Physics, 1991, 94, 1961-1969.	1.2	50
107	A study of the ground electronic state of the isomers of CHNO. Molecular Physics, 1993, 78, 319-343.	0.8	50
108	Exchange-correlation functionals from ab initio electron densities. Chemical Physics Letters, 1997, 273, 183-194.	1.2	50

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109	Ab initio prediction of fundamental, overtone and combination band infrared intensities. Chemical Physics Letters, 1990, 169, 127-137.	1.2	49
110	Interval Methods for Semi-Infinite Programs. Computational Optimization and Applications, 2005, 30, 63-93.	0.9	49
111	A detailed kinetic model for combustion synthesis of titania from TiCl4. Combustion and Flame, 2009, 156, 1764-1770.	2.8	49
112	Oxidative Desulfurization of Middle-Distillate Fuels Using Activated Carbon and Power Ultrasound. Energy & Fuels, 2012, 26, 5164-5176.	2.5	49
113	Ring-polymer molecular dynamics: Rate coefficient calculations for energetically symmetric (near) Tj ETQq1 1 0.784314 rgBT /Overloc Physics, 2014, 141, 244103.	1.2	49
114	Ab initio screening of metal sorbents for elemental mercury capture in syngas streams. Chemical Engineering Science, 2010, 65, 3025-3033.	1.9	48
115	Design and implementation of a next-generation software interface for on-the-fly quantum and force field calculations in automated reaction mechanism generation. Computers and Chemical Engineering, 2013, 52, 35-45.	2.0	48
116	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. Energy & Fuels, 2014, 28, 4976-4985.	2.5	48
117	Transition to electric vehicles in China: Implications for private motorization rate and battery market. Energy Policy, 2020, 144, 111654.	4.2	48
118	Machine Learning of Reaction Properties via Learned Representations of the Condensed Graph of Reaction. Journal of Chemical Information and Modeling, 2022, 62, 2101-2110.	2.5	48
119	Rigorous valid ranges for optimally reduced kinetic models. Combustion and Flame, 2006, 146, 348-365.	2.8	47
120	Kinetic Modeling of Jet Propellant-10 Pyrolysis. Energy & Fuels, 2015, 29, 413-427.	2.5	46
121	Understanding Unimolecular Dissociations with Loose Transition States: Photofragmentation Dynamics of Ketene at the Singlet Threshold. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1988, 92, 389-396.	0.9	45
122	Perspective on Mechanism Development and Structureâ€Activity Relationships for Gasâ€Phase Atmospheric Chemistry. International Journal of Chemical Kinetics, 2018, 50, 435-469.	1.0	45
123	Predictive Kinetics: A New Approach for the 21st Century. Advances in Chemical Engineering, 2007, , 1-313.	0.5	44
124	Redesigning combustion modeling algorithms for the Graphics Processing Unit (GPU): Chemical kinetic rate evaluation and ordinary differential equation integration. Combustion and Flame, 2011, 158, 836-847.	2.8	44
125	The predictive capability of an automatically generated combustion chemistry mechanism: Chemical structures of premixed iso-butanol flames. Combustion and Flame, 2013, 160, 2343-2351.	2.8	44
126	Modeling of 1,3-hexadiene, 2,4-hexadiene and 1,4-hexadiene-doped methane flames: Flame modeling, benzene and styrene formation. Combustion and Flame, 2010, 157, 1331-1345.	2.8	43

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127	Detailed chemical kinetic modeling of JPâ€10 (exoâ€tetrahydrodicyclopentadiene) highâ€temperature oxidation: Exploring the role of biradical species in initial decomposition steps. International Journal of Chemical Kinetics, 2012, 44, 179-193.	1.0	43
128	A consistent-splitting approach to computing stiff steady-state reacting flows with adaptive chemistry. Combustion Theory and Modelling, 2003, 7, 383-399.	1.0	42
129	Ab Initio Aqueous Thermochemistry:â€‰ Application to the Oxidation of Hydroxylamine in Nitric Acid Solution. Journal of Physical Chemistry B, 2007, 111, 11968-11983.	1.2	42
130	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. Journal of Physical Chemistry A, 2019, 123, 2142-2152.	1.1	42
131	Thermodynamic Properties of Ketenes:Â Group Additivity Values from Quantum Chemical Calculations. Journal of Physical Chemistry A, 2002, 106, 7937-7949.	1.1	41
132	Structure of Polymer-Stabilized Magnetic Fluids:Â Small-Angle Neutron Scattering and Mean-Field Lattice Modeling. Langmuir, 2004, 20, 5223-5234.	1.6	38
133	Order out of Randomness: Self-Organization Processes in Astrophysics. Space Science Reviews, 2018, 214, 1.	3.7	38
134	Kinetic analysis and reaction mechanism for anisole conversion over zirconia-supported molybdenum oxide. Journal of Catalysis, 2019, 376, 248-257.	3.1	38
135	Prediction of the Knock Limit and Viable Operating Range for a Homogeneous-Charge Compression-Ignition (HCCI) Engine. , 2003, , .		37
136	Reaction of Phenyl Radical with Propylene as a Possible Source of Indene and Other Polycyclic Aromatic Hydrocarbons: An Ab Initio/RRKM-ME Study. Journal of Physical Chemistry A, 2012, 116, 4176-4191.	1.1	37
137	Balanced Splitting and Rebalanced Splitting. SIAM Journal on Numerical Analysis, 2013, 51, 3084-3105.	1.1	37
138	Temperature and Molecular Size Dependence of the High-Pressure Limit. Journal of Physical Chemistry A, 2003, 107, 6206-6211.	1.1	36
139	Temperature- and Pressure-Dependent Kinetics of CH₂OO + CH₃COCH₃and CH₂OO + CH₃CHO: Direct Measurements and Theoretical Analysis. International Journal of Chemical Kinetics, 2016, 48, 474-488.	1.0	36
140	Using adaptive proper orthogonal decomposition to solve the reactionâ€“diffusion equation. Applied Numerical Mathematics, 2009, 59, 272-279.	1.2	35
141	Which Ab Initio Wave Function Methods Are Adequate for Quantitative Calculations of the Energies of Biradicals? The Performance of Coupled-Cluster and Multi-Reference Methods Along a Single-Bond Dissociation Coordinate. Journal of Chemical Theory and Computation, 2013, 9, 418-431.	2.3	35
142	Modeling study of the anti-knock tendency of substituted phenols as additives: an application of the reaction mechanism generator (RMG). Physical Chemistry Chemical Physics, 2018, 20, 10637-10649.	1.3	35
143	Generating transition states of isomerization reactions with deep learning. Physical Chemistry Chemical Physics, 2020, 22, 23618-23626.	1.3	35
144	Missing Thermochemical Groups for Large Unsaturated Hydrocarbons:Â Contrasting Predictions of G2 and CBS-Q. Journal of Physical Chemistry A, 2002, 106, 11141-11149.	1.1	34

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145	Response of Different Types of Sulfur Compounds to Oxidative Desulfurization of Jet Fuel. Energy & Fuels, 2014, 28, 2977-2983.	2.5	34
146	Optimal automatic reaction and species elimination in kinetic mechanisms. Combustion and Flame, 2008, 155, 118-132.	2.8	33
147	The Underlying Physics and Chemistry behind Fuel Sensitivity. SAE International Journal of Fuels and Lubricants, 0, 3, 256-265.	0.2	33
148	Thermochemical production of hydrogen from hydrogen sulfide with iodine thermochemical cycles. International Journal of Hydrogen Energy, 2018, 43, 12939-12947.	3.8	33
149	Application of Computational Kinetic Mechanism Generation to Model the Autocatalytic Pyrolysis of Methane. Industrial & Engineering Chemistry Research, 2003, 42, 1000-1010.	1.8	32
150	NOx-Mediated Homogeneous Pathways for the Synthesis of Formaldehyde from CH4â^'O2Mixtures. Industrial & Engineering Chemistry Research, 2006, 45, 2677-2688.	1.8	32
151	Co-oxidation of methylphosphonic acid and ethanol in supercritical water. Journal of Supercritical Fluids, 2006, 39, 239-245.	1.6	32
152	Modeling of aromatics formation in fuel-rich methane oxy-combustion with an automatically generated pressure-dependent mechanism. Physical Chemistry Chemical Physics, 2019, 21, 813-832.	1.3	32
153	New vibrational bands of CH2 (). Journal of Molecular Spectroscopy, 1989, 138, 614-629.	0.4	31
154	Predictive chemical kinetics: Density functional and hartree-fock calculations on free-radial reaction transition states. International Journal of Quantum Chemistry, 1994, 52, 837-847.	1.0	31
155	Predicting Infrared Spectra with Message Passing Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 2594-2609.	2.5	31
156	Predicting Solubility Limits of Organic Solutes for a Wide Range of Solvents and Temperatures. Journal of the American Chemical Society, 2022, 144, 10785-10797.	6.6	31
157	An Extended Group Additivity Method for Polycyclic Thermochemistry Estimation. International Journal of Chemical Kinetics, 2018, 50, 294-303.	1.0	30
158	An Integrated Assessment of Emissions, Air Quality, and Public Health Impacts of Chinaâ€™s Transition to Electric Vehicles. Environmental Science & Technology, 2022, 56, 6836-6846.	4.6	30
159	A priori falloff analysis for OH + NO2. International Journal of Chemical Kinetics, 2000, 32, 245-262.	1.0	29
160	Measurements and Automated Mechanism Generation Modeling of OH Production in Photolytically Initiated Oxidation of the Neopentyl Radicalâ€–. Journal of Physical Chemistry A, 2007, 111, 3891-3900.	1.1	29
161	Computational Investigation on Hydrodeoxygenation (HDO) of Acetone to Propylene on Î±-MoO₃ (010) Surface. Journal of Physical Chemistry C, 2017, 121, 17848-17855.	1.5	29
162	Investigating the technoâ€•economic tradeâ€•offs of hydrogen source using a response surface model of dropâ€•in biofuel production via bioâ€•oil upgrading. Biofuels, Bioproducts and Biorefining, 2012, 6, 503-520.	1.9	28

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163	A Signature of Roaming Dynamics in the Thermal Decomposition of Ethyl Nitrite: Chirped-Pulse Rotational Spectroscopy and Kinetic Modeling. Journal of Physical Chemistry Letters, 2014, 5, 3641-3648.	2.1	28
164	Experimental study of catalyst nanoparticle and single walled carbon nanotube formation in a controlled premixed combustion. Journal of Materials Chemistry, 2008, 18, 1561.	6.7	27
165	Temperature-Dependent Kinetics of the Vinyl Radical (C₂H₃) Self-Reaction. Journal of Physical Chemistry A, 2009, 113, 1278-1286.	1.1	27
166	An Extensible Framework for Capturing Solvent Effects in Computer Generated Kinetic Models. Journal of Physical Chemistry B, 2013, 117, 2955-2970.	1.2	27
167	The engine reformer: Syngas production in an engine for compact gasâ€toâ€liquids synthesis. Canadian Journal of Chemical Engineering, 2016, 94, 623-635.	0.9	27
168	Moving from postdictive to predictive kinetics in reaction engineering. AICHE Journal, 2020, 66, e17059.	1.8	27
169	Hydrogen abstraction rates via density functional theory. Chemical Physics Letters, 1999, 312, 262-268.	1.2	26
170	Obtaining accurate solutions using reduced chemical kinetic models: a new model reduction method for models rigorously validated over ranges. Combustion Theory and Modelling, 2007, 11, 127-146.	1.0	26
171	Influence of the double bond position on the oxidation of decene isomers at high pressures and temperatures. Proceedings of the Combustion Institute, 2015, 35, 333-340.	2.4	26
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