William H Green

List of Publications by Year
in descending order

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297	16,892	13332	25230
papers	citations	70 h-index	113 g-index

306	306	306	12360
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	Detailed Reaction Mechanism for 350â€“400 Â°C Pyrolysis of an Alkane, Aromatic, and Long-Chain Alkylaromatic Mixture. Energy & Fuels, 2022, 36, 1635-1646.	2.5	9
4	Multi-fidelity prediction of molecular optical peaks with deep learning. Chemical Science, 2022, 13, 1152-1162.	3.7	24
5	Detailed Kinetic Modeling for the Pyrolysis of a Jet A Surrogate. Energy & Fuels, 2022, 36, 1304-1315.	2.5	11
6	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
7	Automatically generated model for light alkene combustion. Combustion and Flame, 2022, 241, 112080.	2.8	23
8	Influence of Template Size, Canonicalization, and Exclusivity for Retrosynthesis and Reaction Prediction Applications. Journal of Chemical Information and Modeling, 2022, 62, 16-26.	2.5	8
9	Kinetic Modeling of API Oxidation: (2) Imipramine Stress Testing. Molecular Pharmaceutics, 2022, 19, 1526-1539.	2.3	6
10	Similarity based enzymatic retrosynthesis. Chemical Science, 2022, 13, 6039-6053.	3.7	10
11	Fast Predictions of Reaction Barrier Heights: Toward Coupled-Cluster Accuracy. Journal of Physical Chemistry A, 2022, 126, 3976-3986.	1.1	26
12	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
13	High accuracy barrier heights, enthalpies, and rate coefficients for chemical reactions. Scientific Data, 2022, 9, .	2.4	19
14	Predicting polycyclic aromatic hydrocarbon formation with an automatically generated mechanism for acetylene pyrolysis. International Journal of Chemical Kinetics, 2021, 53, 27-42.	1.0	11
15	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
16	Reaction Mechanism Generator v3.0: Advances in Automatic Mechanism Generation. Journal of Chemical Information and Modeling, 2021, 61, 2686-2696.	2.5	116
17	Predicting Infrared Spectra with Message Passing Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 2594-2609.	2.5	31
18	Oxidation and pyrolysis of methyl propyl ether. International Journal of Chemical Kinetics, 2021, 53, 915-938.	1.0	15

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19	Kinetic Modeling of API Oxidation: (1) The AIBN/H₂O/CH₃OH Radical â€œSoupâ€• Molecular Pharmaceutics, 2021, 18, 3037-3049.	2.3	12
20	Transfer learning for solvation free energies: From quantum chemistry to experiments. Chemical Engineering Journal, 2021, 418, 129307.	6.6	77
21	Screening for New Pathways in Atmospheric Oxidation Chemistry with Automated Mechanism Generation. Journal of Physical Chemistry A, 2021, 125, 6772-6788.	1.1	7
22	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. Journal of Chemical Information and Modeling, 2021, 61, 4949-4961.	2.5	7
23	C₁₄H₁₀ polycyclic aromatic hydrocarbon formation by acetylene addition to naphthalenyl radicals observed. Physical Chemistry Chemical Physics, 2021, 23, 14325-14339.	1.3	5
24	Learning to Optimize Molecular Geometries Using Reinforcement Learning. Journal of Chemical Theory and Computation, 2021, 17, 818-825.	2.3	19
25	Effects of surface species and homogeneous reactions on rates and selectivity in ethane oxidation on oxide catalysts. AICHE Journal, 2021, 67, e17483.	1.8	5
26	Chemistry of Simple Organic Peroxy Radicals under Atmospheric through Combustion Conditions: Role of Temperature, Pressure, and NO_x Level. Journal of Physical Chemistry A, 2021, 125, 10303-10314.	1.1	7
27	Moving from postdictive to predictive kinetics in reaction engineering. AICHE Journal, 2020, 66, e17059.	1.8	27
28	Pressure-dependent kinetics of peroxy radicals formed in isobutanol combustion. Physical Chemistry Chemical Physics, 2020, 22, 19802-19815.	1.3	4
29	Theoretical study on the HACA chemistry of naphthalenyl radicals and acetylene: The formation of C₁₂H₈, C₁₄H₈, and C₁₄H₁₀ species. International Journal of Chemical Kinetics, 2020, 52, 752-768.	1.0	10
30	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
31	Temperatureâ€dependent vaporâ€“liquid equilibria and solvation free energy estimation from minimal data. AICHE Journal, 2020, 66, e16976.	1.8	16
32	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. Scientific Data, 2020, 7, 137.	2.4	71
33	Deep Learning of Activation Energies. Journal of Physical Chemistry Letters, 2020, 11, 2992-2997.	2.1	102
34	Intramolecular 13C isotope distributions of butane from natural gases. Chemical Geology, 2020, 541, 119571.	1.4	15
35	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. Journal of Medicinal Chemistry, 2020, 63, 8667-8682.	2.9	118
36	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

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37	Direct Measurement of Radical-Catalyzed C₆H₆ Formation from Acetylene and Validation of Theoretical Rate Coefficients for C₂H₃ + C₂H₂ and C₄H₅ + C₂H₂ Reactions. Journal of Physical Chemistry A, 2020, 124, 2871-2884.	1.1	10
38	Recharging systems and business operations to improve the economics of electrified taxi fleets. Sustainable Cities and Society, 2020, 57, 102119.	5.1	10
39	Transition to electric vehicles in China: Implications for private motorization rate and battery market. Energy Policy, 2020, 144, 111654.	4.2	48
40	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. Frontiers in Chemical Engineering, 2020, 2, .	1.3	16
41	Thermochemistry Prediction and Automatic Reaction Mechanism Generation for Oxygenated Sulfur Systems: A Case Study of Dimethyl Sulfide Oxidation. ChemSystemsChem, 2020, 2, e1900051.	1.1	11
42	Direct Kinetics and Product Measurement of Phenyl Radical + Ethylene. Journal of Physical Chemistry A, 2020, 124, 2352-2365.	1.1	4
43	Uncertainty analysis of correlated parameters in automated reaction mechanism generation. International Journal of Chemical Kinetics, 2020, 52, 266-282.	1.0	14
44	Formation of Two-Ring Aromatics in Hexylbenzene Pyrolysis. Energy & Fuels, 2020, 34, 1365-1377.	2.5	5
45	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. Reaction Chemistry and Engineering, 2020, 5, 367-376.	1.9	5
46	Revealing the critical role of radical-involved pathways in high temperature cyclopentanone pyrolysis. Combustion and Flame, 2020, 216, 280-292.	2.8	14
47	Generating transition states of isomerization reactions with deep learning. Physical Chemistry Chemical Physics, 2020, 22, 23618-23626.	1.3	35
48	Methyl propyl ether combustion. , 2020, , .		0
49	Development of a high temperature pyrolysis mechanism for cyclopentanone, a potential biofuel derived from biomass. , 2020, , .		0
50	Capturing aromaticity in automatic mechanism generation software. Proceedings of the Combustion Institute, 2019, 37, 575-581.	2.4	9
51	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
52	An experimental, theoretical, and modeling study of the ignition behavior of cyclopentanone. Proceedings of the Combustion Institute, 2019, 37, 657-665.	2.4	18
53	A robotic platform for flow synthesis of organic compounds informed by AI planning. Science, 2019, 365, .	6.0	548
54	Automated chemical resonance generation and structure filtration for kinetic modeling. International Journal of Chemical Kinetics, 2019, 51, 760-776.	1.0	4

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55	Kinetic analysis and reaction mechanism for anisole conversion over zirconia-supported molybdenum oxide. Journal of Catalysis, 2019, 376, 248-257.	3.1	38
56	Scalability strategies for automated reaction mechanism generation. Computers and Chemical Engineering, 2019, 131, 106578.	2.0	4
57	Detailed kinetic model for hexyl sulfide pyrolysis and its desulfurization by supercritical water. Physical Chemistry Chemical Physics, 2019, 21, 10311-10324.	1.3	12
58	Reaction Pathways, Thermodynamics, and Kinetics of Cyclopentanone Oxidation Intermediates: A Theoretical Approach. Journal of Physical Chemistry A, 2019, 123, 9644-9657.	1.1	6
59	A graph-convolutional neural network model for the prediction of chemical reactivity. Chemical Science, 2019, 10, 370-377.	3.7	430
60	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
61	Learning only buys you so much: Practical limits on battery price reduction. Applied Energy, 2019, 239, 218-224.	5.1	115
62	Numerical investigation of strained extinction at engine-relevant pressures: Pressure dependence and sensitivity to chemical and physical parameters for methane-based flames. Combustion and Flame, 2019, 202, 318-333.	2.8	15
63	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
64	Automatic generation of reaction mechanisms. Computer Aided Chemical Engineering, 2019, , 259-294.	0.3	14
65	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
66	Large Intermediates in Hydrazine Decomposition: A Theoretical Study of the N₃H₅ and N₄H₆ Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 4679-4692.	1.1	14
67	H2 Generation from H2O and H2S through an Iodine Cycle. ACS Sustainable Chemistry and Engineering, 2019, 7, 7369-7377.	3.2	4
68	Thermochemistry and Kinetics of Intermolecular Addition of Radicals to Toluene and Alkylaromatics. Journal of Physical Chemistry A, 2019, 123, 3176-3184.	1.1	8
69	Cooperative Co 0 /Co II Sites Stabilized by a Perovskite Matrix Enable Selective Câ˜O and Câ˜C bond Hydrogenolysis of Oxygenated Arenes. ChemSusChem, 2019, 12, 2171-2175.	3.6	17
70	Computer-generated isotope model achieves experimental accuracy of filiation for position-specific isotope analysis. Chemical Geology, 2019, 514, 1-9.	1.4	9
71	Thermochemistry and Group Additivity Values for Fused Two-Ring Species and Radicals. Journal of Physical Chemistry A, 2019, 123, 3418-3428.	1.1	11
72	Correct Symmetry Treatment for X + X Reactions Prevents Large Errors in Predicted Isotope Enrichment. Journal of Physical Chemistry A, 2019, 123, 2320-2324.	1.1	4

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73	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. Journal of Physical Chemistry A, 2019, 123, 2142-2152.	1.1	42
74	From benzene to naphthalene: direct measurement of reactions and intermediates of phenyl radicals and acetylene. Physical Chemistry Chemical Physics, 2019, 21, 22248-22258.	1.3	21
75	An apparatus-independent extinction strain rate in counterflow flames. Proceedings of the Combustion Institute, 2019, 37, 1979-1987.	2.4	11
76	Reaction pathways of cyclopentanone oxidation intermediates. , 2019, , .		0
77	A Decision Tree Based Machine Learning Algorithm for Rate Estimation. , 2019, , .		1
78	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. Energy & Fuels, 2018, 32, 3920-3934.	2.5	26
79	Chemistry of Alkylaromatics Reconsidered. Energy & Fuels, 2018, 32, 5489-5500.	2.5	14
80	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
81	Phenyl radical + propene: a prototypical reaction surface for aromatic-catalyzed 1,2-hydrogen-migration and subsequent resonance-stabilized radical formation. Physical Chemistry Chemical Physics, 2018, 20, 13191-13214.	1.3	17
82	Automated Reaction Mechanism Generation Including Nitrogen as a Heteroatom. International Journal of Chemical Kinetics, 2018, 50, 243-258.	1.0	23
83	An Extended Group Additivity Method for Polycyclic Thermochemistry Estimation. International Journal of Chemical Kinetics, 2018, 50, 294-303.	1.0	30
84	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
85	SCScore: Synthetic Complexity Learned from a Reaction Corpus. Journal of Chemical Information and Modeling, 2018, 58, 252-261.	2.5	176
86	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
87	Machine Learning in Computer-Aided Synthesis Planning. Accounts of Chemical Research, 2018, 51, 1281-1289.	7.6	430
88	An experimental and modeling study of vacuum residue upgrading in supercritical water. AICHE Journal, 2018, 64, 1732-1743.	1.8	26
89	Order out of Randomness: Self-Organization Processes in Astrophysics. Space Science Reviews, 2018, 214, 1.	3.7	38
90	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. Combustion and Flame, 2018, 187, 247-256.	2.8	58

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91	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. ACS Central Science, 2018, 4, 1465-1476.	5.3	245
92	Incorporating Multiple Uncertainties into Projections of Chinese Private Car Sales and Stock. Transportation Research Record, 2018, 2672, 182-193.	1.0	18
93	Kinetics of Intramolecular Phenyl Migration and Fused Ring Formation in Hexylbenzene Radicals. Journal of Physical Chemistry A, 2018, 122, 9778-9791.	1.1	4
94	A Fragment-Based Mechanistic Kinetic Modeling Framework for Complex Systems. Industrial & Engineering Chemistry Research, 2018, 57, 14022-14030.	1.8	10
95	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
96	Ember: An open-source, transient solver for 1D reacting flow using large kinetic models, applied to strained extinction. Combustion and Flame, 2018, 195, 105-116.	2.8	14
97	Thermochemical production of hydrogen from hydrogen sulfide with iodine thermochemical cycles. International Journal of Hydrogen Energy, 2018, 43, 12939-12947.	3.8	33
98	A combined photoionization time-of-flight mass spectrometry and laser absorption spectrometry flash photolysis apparatus for simultaneous determination of reaction rates and product branching. Review of Scientific Instruments, 2018, 89, 074102.	0.6	11
99	Modeling Study of High Temperature Pyrolysis of Natural Gas. Industrial & Engineering Chemistry Research, 2018, 57, 7404-7420.	1.8	14
100	Automated Generation of Chemical Mechanisms for Predicting Extinction Strain Rates with Applications in Flame Stabilization and Combustion Instabilitie. , 2017, , .		4
101	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
102	Minimizing E-factor in the continuous-flow synthesis of diazepam and atropine. Bioorganic and Medicinal Chemistry, 2017, 25, 6233-6241.	1.4	56
103	On-the-fly pruning for rate-based reaction mechanism generation. Computers and Chemical Engineering, 2017, 100, 1-8.	2.0	12
104	Prediction of Organic Reaction Outcomes Using Machine Learning. ACS Central Science, 2017, 3, 434-443.	5.3	477
105	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
106	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 1757-1772.	2.5	317
107	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
108	Computer-Assisted Retrosynthesis Based on Molecular Similarity. ACS Central Science, 2017, 3, 1237-1245.	5.3	200

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109	Combustion of Synthetic Jet Fuel: Chemical Kinetic Modeling and Uncertainty Analysis. Journal of Propulsion and Power, 2017, 33, 350-359.	1.3	3
110	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
111	Microâ€syngas technology options for GtL. Canadian Journal of Chemical Engineering, 2016, 94, 613-622.	0.9	19
112	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
113	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. Combustion and Flame, 2016, 168, 310-330.	2.8	85
114	The Effect of Alcohol and Carbonyl Functional Groups on the Competition between Unimolecular Decomposition and Isomerization in C₄ and C₅ Alkoxy Radicals. International Journal of Chemical Kinetics, 2016, 48, 544-555.	1.0	1
115	Automatic mechanism generation for pyrolysis of di-tert-butyl sulfide. Physical Chemistry Chemical Physics, 2016, 18, 21651-21658.	1.3	23
116	Methanol formation from the treatment of glycerol in supercritical water and with ethylsulfide. Journal of Supercritical Fluids, 2016, 117, 80-88.	1.6	9
117	Reaction Mechanism Generator: Automatic construction of chemical kinetic mechanisms. Computer Physics Communications, 2016, 203, 212-225.	3.0	515
118	Natural Gas and Cellulosic Biomass: A Clean Fuel Combination? Determining the Natural Gas Blending Wall in Biofuel Production. Environmental Science & Technology, 2015, 49, 8183-8192.	4.6	14
119	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
120	Continuous Thermal Oxidation of Alkenes with Nitrous Oxide in a Packed Bed Reactor. Industrial & Engineering Chemistry Research, 2015, 54, 4166-4173.	1.8	18
121	Kinetic Modeling of Jet Propellant-10 Pyrolysis. Energy & Fuels, 2015, 29, 413-427.	2.5	46
122	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
123	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
124	Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene. Journal of Physical Chemistry A, 2015, 119, 7325-7338.	1.1	20
125	Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. Chemical Engineering Journal, 2015, 278, 385-393.	6.6	25
126	A kinetic and thermochemical database for organic sulfur and oxygen compounds. Physical Chemistry Chemical Physics, 2015, 17, 13625-13639.	1.3	16

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127	Supercritical Water Treatment of Crude Oil and Hexylbenzene: An Experimental and Mechanistic Study on Alkylbenzene Decomposition. Energy & Fuels, 2015, 29, 5290-5302.	2.5	22
128	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	2.8	122
129	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
130	Upgrading and desulfurization of heavy oils by supercritical water. Journal of Supercritical Fluids, 2015, 96, 114-123.	1.6	109
131	System and Market Analysis of Methanol Production Using Compact Engine Reformers. , 2014, , .		2
132	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
133	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
134	Cleavage of Side Chains on Thiophenic Compounds by Supercritical Water Treatment of Crude Oil Quantified by Two-Dimensional Gas Chromatography with Sulfur Chemiluminescence Detection. Energy & Fuels, 2014, 28, 6589-6595.	2.5	22
135	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
136	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
137	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
138	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
139	Analysis of Adsorbent-Based Warm CO₂ Capture Technology for Integrated Gasification Combined Cycle (IGCC) Power Plants. Industrial & Engineering Chemistry Research, 2014, 53, 11145-11158.	1.8	22
140	Direct Determination of the Simplest Criegee Intermediate (CH₂OO) Self Reaction Rate. Journal of Physical Chemistry Letters, 2014, 5, 2224-2228.	2.1	72
141	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
142	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. Energy & Fuels, 2014, 28, 4976-4985.	2.5	48
143	Response of Different Types of Sulfur Compounds to Oxidative Desulfurization of Jet Fuel. Energy & Fuels, 2014, 28, 2977-2983.	2.5	34
144	Economic and Environmental Benefits of Higher-Octane Gasoline. Environmental Science & Technology, 2014, 48, 6561-6568.	4.6	51

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145	The role of catalyst in supercritical water desulfurization. Applied Catalysis B: Environmental, 2014, 147, 144-155.	10.8	63
146	Ring-polymer molecular dynamics: Rate coefficient calculations for energetically symmetric (near) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Physics, 2014, 141, 244103.	1.2	49
147	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
148	Dehydration of Isobutanol and the Elimination of Water from Fuel Alcohols. Journal of Physical Chemistry A, 2013, 117, 6724-6736.	1.1	16
149	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
150	Supercritical Water Desulfurization of Organic Sulfides Is Consistent with Free-Radical Kinetics. Energy & Fuels, 2013, 27, 6108-6117.	2.5	90
151	RPMDrate: Bimolecular chemical reaction rates from ring polymer molecular dynamics. Computer Physics Communications, 2013, 184, 833-840.	3.0	101
152	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
153	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
154	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
155	Experimental Investigation of Sorbent for Warm CO₂ Capture by Pressure Swing Adsorption. Industrial & Engineering Chemistry Research, 2013, 52, 9665-9673.	1.8	25
156	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
157	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
158	An Extensible Framework for Capturing Solvent Effects in Computer Generated Kinetic Models. Journal of Physical Chemistry B, 2013, 117, 2955-2970.	1.2	27
159	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. Combustion and Flame, 2013, 160, 1907-1929.	2.8	65
160	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
161	Editorial: New Editor, Craig A. Taatjes. International Journal of Chemical Kinetics, 2013, 45, 477-477.	1.0	0
162	Balanced Splitting and Rebalanced Splitting. SIAM Journal on Numerical Analysis, 2013, 51, 3084-3105.	1.1	37

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163	Automatic Generation of Detailed Mechanisms. Green Energy and Technology, 2013, , 59-92.	0.4	18
164	Oxidative Desulfurization of Middle-Distillate Fuels Using Activated Carbon and Power Ultrasound. Energy & Fuels, 2012, 26, 5164-5176.	2.5	49
165	Crossed beam reaction of phenyl and D5-phenyl radicals with propene and deuterated counterpartsâ€"competing atomic hydrogen and methyl loss pathways. Physical Chemistry Chemical Physics, 2012, 14, 720-729.	1.3	23
166	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
167	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
168	Screening of binary alloys for warm temperature capture of elemental mercury using density functional theory. Chemical Engineering Science, 2012, 80, 128-133.	1.9	6
169	Automatic estimation of pressure-dependent rate coefficients. Physical Chemistry Chemical Physics, 2012, 14, 1131-1155.	1.3	96
170	Analysis of Hydroxide Sorbents for CO₂ Capture from Warm Syngas. Industrial & Engineering Chemistry Research, 2012, 51, 13473-13481.	1.8	15
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