

William H Green

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

282
papers

12,637
citations

62
h-index

97
g-index

306
ext. papers

14,800
ext. citations

4.7
avg, IF

6.9
L-index

#	Paper	IF	Citations
282	Reaction Mechanism Generator: Automatic construction of chemical kinetic mechanisms. <i>Computer Physics Communications</i> , 2016 , 203, 212-225	4.2	335
281	Prediction of Organic Reaction Outcomes Using Machine Learning. <i>ACS Central Science</i> , 2017 , 3, 434-443	16.8	325
280	A robotic platform for flow synthesis of organic compounds informed by AI planning. <i>Science</i> , 2019 , 365,	33.3	271
279	Machine Learning in Computer-Aided Synthesis Planning. <i>Accounts of Chemical Research</i> , 2018 , 51, 1281-1289	14.9	255
278	A graph-convolutional neural network model for the prediction of chemical reactivity. <i>Chemical Science</i> , 2019 , 10, 370-377	9.4	237
277	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. <i>Combustion and Flame</i> , 2011 , 158, 16-41	5.3	210
276	Detailed modeling of PAH and soot formation in a laminar premixed benzene/oxygen/argon low-pressure flame. <i>Proceedings of the Combustion Institute</i> , 2005 , 30, 1397-1405	5.9	207
275	High-gradient magnetic separation of coated magnetic nanoparticles. <i>AIChE Journal</i> , 2004 , 50, 2835-2848	4.6	201
274	Intramolecular hydrogen migration in alkylperoxy and hydroperoxyalkylperoxy radicals: accurate treatment of hindered rotors. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 5689-701	2.8	196
273	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 1757-1772	6.1	191
272	Role of O ₂ + QOOH in low-temperature ignition of propane. 1. Temperature and pressure dependent rate coefficients. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3325-46	2.8	188
271	Computational Investigation of Thermochemistry and Kinetics of Steam Methane Reforming on Ni(111) under Realistic Conditions. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 4898-4908	3.8	186
270	Rate-Based Construction of Kinetic Models for Complex Systems. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 3731-3740	2.8	173
269	Reactivity and stability investigation of supported molybdenum oxide catalysts for the hydrodeoxygenation (HDO) of m-cresol. <i>Journal of Catalysis</i> , 2015 , 331, 86-97	7.3	159
268	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. <i>Journal of the American Chemical Society</i> , 1995 , 117, 2929-2930	16.4	143
267	Transition States and Rate Constants for Unimolecular Reactions. <i>Annual Review of Physical Chemistry</i> , 1992 , 43, 591-626	15.7	139
266	Database of small molecule thermochemistry for combustion. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 9033-57	2.8	133

265	Using Machine Learning To Predict Suitable Conditions for Organic Reactions. <i>ACS Central Science</i> , 2018 , 4, 1465-1476	16.8	131
264	Optimally-reduced kinetic models: reaction elimination in large-scale kinetic mechanisms. <i>Combustion and Flame</i> , 2003 , 135, 191-208	5.3	129
263	Reaction Rate Prediction via Group Additivity Part 1: H Abstraction from Alkanes by H and CH ₃ . <i>Journal of Physical Chemistry A</i> , 2001 , 105, 6910-6925	2.8	129
262	New pathways for formation of acids and carbonyl products in low-temperature oxidation: the Korcek decomposition of α -keto hydroperoxides. <i>Journal of the American Chemical Society</i> , 2013 , 135, 11100-14	16.4	124
261	Bond breaking without barriers: Photofragmentation of ketene at the singlet threshold. <i>Journal of Chemical Physics</i> , 1988 , 89, 314-328	3.9	123
260	Anharmonic corrections to vibrational transition intensities. <i>The Journal of Physical Chemistry</i> , 1990 , 94, 5608-5616		119
259	Formation of polycyclic aromatic hydrocarbons and their radicals in a nearly sooting premixed benzene flame. <i>Proceedings of the Combustion Institute</i> , 2000 , 28, 2609-2618	5.9	118
258	Water-Based Magnetic Fluids as Extractants for Synthetic Organic Compounds. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 4739-4749	3.9	117
257	Capturing pressure-dependence in automated mechanism generation: Reactions through cycloalkyl intermediates. <i>International Journal of Chemical Kinetics</i> , 2003 , 35, 95-119	1.4	116
256	Electronic Structures and Geometries of C ₆₀ Anions via Density Functional Calculations. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 14892-14898		115
255	Computer-Assisted Retrosynthesis Based on Molecular Similarity. <i>ACS Central Science</i> , 2017 , 3, 1237-1245	6.8	112
254	Anharmonic vibrational properties of CH ₂ F ₂ : A comparison of theory and experiment. <i>Journal of Chemical Physics</i> , 1991 , 95, 8323-8336	3.9	110
253	Upper bound on the yield for oxidative coupling of methane. <i>Journal of Catalysis</i> , 2003 , 218, 321-333	7.3	109
252	Understanding low-temperature first-stage ignition delay: Propane. <i>Combustion and Flame</i> , 2015 , 162, 3658-3673	5.3	101
251	Reaction Rate Prediction via Group Additivity, Part 2: H-Abstraction from Alkenes, Alkynes, Alcohols, Aldehydes, and Acids by H Atoms. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 8969-8984	2.8	98
250	Automatic reaction network generation using RMG for steam cracking of n-hexane. <i>AIChE Journal</i> , 2006 , 52, 718-730	3.6	97
249	Thermodynamic Properties and Kinetic Parameters for Cyclic Ether Formation from Hydroperoxyalkyl Radicals. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 4908-4920	2.8	95
248	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH ₃ . <i>Journal of Chemical Physics</i> , 1990 , 93, 4965-4981	3.9	94

247	Detailed Kinetic Study of the Growth of Small Polycyclic Aromatic Hydrocarbons. 1. 1-Naphthyl + Ethyne <i>Journal of Physical Chemistry A</i> , 2001 , 105, 1561-1573	2.8	92
246	SCScore: Synthetic Complexity Learned from a Reaction Corpus. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 252-261	6.1	90
245	Automated Discovery of Elementary Chemical Reaction Steps Using Freezing String and Berny Optimization Methods. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4248-59	6.4	86
244	Upgrading and desulfurization of heavy oils by supercritical water. <i>Journal of Supercritical Fluids</i> , 2015 , 96, 114-123	4.2	86
243	RPMDrate: Bimolecular chemical reaction rates from ring polymer molecular dynamics. <i>Computer Physics Communications</i> , 2013 , 184, 833-840	4.2	84
242	High-temperature oxidation chemistry of n-butanol--experiments in low-pressure premixed flames and detailed kinetic modeling. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20262-74	3.6	83
241	Mechanism Generation with Integrated Pressure Dependence: A New Model for Methane Pyrolysis. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 8552-8565	2.8	79
240	Accurate and efficient method for predicting thermochemistry of polycyclic aromatic hydrocarbons - bond-centered group additivity. <i>Journal of the American Chemical Society</i> , 2004 , 126, 12685-700	16.4	78
239	An adaptive chemistry approach to modeling complex kinetics in reacting flows. <i>Combustion and Flame</i> , 2003 , 133, 451-465	5.3	78
238	Theoretical assignment of the visible spectrum of singlet methylene. <i>Journal of Chemical Physics</i> , 1991 , 94, 118-132	3.9	77
237	Automatic estimation of pressure-dependent rate coefficients. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 1131-55	3.6	76
236	Vibration-rotation coordinates and kinetic energy operators for polyatomic molecules. <i>Molecular Physics</i> , 1991 , 73, 1183-1208	1.7	76
235	Global dynamic optimization for parameter estimation in chemical kinetics. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 971-6	2.8	74
234	Direct kinetic measurements of reactions between the simplest Criegee intermediate CH ₂ OO and alkenes. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 1997-2006	2.8	73
233	Computational Investigation of the Thermochemistry and Kinetics of Steam Methane Reforming Over a Multi-Faceted Nickel Catalyst. <i>Topics in Catalysis</i> , 2011 , 54, 828-844	2.3	73
232	Computer Construction of Detailed Chemical Kinetic Models for Gas-Phase Reactors. <i>Industrial & Engineering Chemistry Research</i> , 2001 , 40, 5362-5370	3.9	73
231	Kinetic anharmonic coupling in the trihalomethanes: A mechanism for rapid intramolecular redistribution of CH stretch vibrational energy. <i>Journal of Chemical Physics</i> , 1987 , 86, 6000-6011	3.9	72
230	Supercritical Water Desulfurization of Organic Sulfides Is Consistent with Free-Radical Kinetics. <i>Energy & Fuels</i> , 2013 , 27, 6108-6117	4.1	71

229	A priori rate constants for kinetic modeling. <i>Theoretical Chemistry Accounts</i> , 2002 , 108, 187-213	1.9	71
228	A perturbation theory guide to open-shell complexes: $\text{OH}\ddot{\text{A}}\text{r}(\text{X} 2\dot{\text{I}})$. <i>Journal of Chemical Physics</i> , 1992 , 96, 2573-2584	3.9	70
227	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 10399-10420	3.9	68
226	Oxygenate, oxyalkyl and alkoxy carbonyl thermochemistry and rates for hydrogen abstraction from oxygenates. <i>Physical Chemistry Chemical Physics</i> , 2003 , 5, 3402-3417	3.6	67
225	Rate coefficients and kinetic isotope effects of the $\text{X} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{HX}$ ($\text{X} = \text{H}, \text{D}, \text{Mu}$) reactions from ring polymer molecular dynamics. <i>Journal of Chemical Physics</i> , 2013 , 138, 094307	3.9	66
224	Theoretical rate coefficients for allyl+HO ₂ and allyloxy decomposition. <i>Proceedings of the Combustion Institute</i> , 2011 , 33, 273-282	5.9	64
223	Toward a Comprehensive Model of the Synthesis of TiO ₂ Particles from TiCl ₄ . <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 6147-6156	3.9	64
222	Direct Determination of the Simplest Criegee Intermediate (CH ₂ OO) Self Reaction Rate. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2224-8	6.4	63
221	Ring Polymer Molecular Dynamics Calculations of Thermal Rate Constants for the O((3)P) + CH ₄ → OH + CH ₃ Reaction: Contributions of Quantum Effects. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 48-52	6.4	63
220	Communication: full dimensional quantum rate coefficients and kinetic isotope effects from ring polymer molecular dynamics for a seven-atom reaction $\text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O}$. <i>Journal of Chemical Physics</i> , 2013 , 138, 221103	3.9	62
219	First-principles thermochemistry for the production of TiO ₂ from TiCl ₄ . <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3560-5	2.8	62
218	Kinetic model for polycrystalline Pd/PdOx in oxidation/reduction cycles. <i>Applied Catalysis A: General</i> , 2003 , 244, 323-340	5.1	62
217	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. <i>Combustion and Flame</i> , 2013 , 160, 1907-1929	5.3	61
216	Global solution of semi-infinite programs. <i>Mathematical Programming</i> , 2005 , 103, 283-307	2.1	61
215	Computed rate coefficients and product yields for $\text{c-C}_5\text{H}_5 + \text{CH}_3 \rightarrow \text{products}$. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 8871-82	2.8	60
214	A detailed combined experimental and theoretical study on dimethyl ether/propane blended oxidation. <i>Combustion and Flame</i> , 2016 , 168, 310-330	5.3	60
213	Reaction Rate Predictions Via Group Additivity. Part 3: Effect of Substituents with CH ₂ as the Mediator. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 5474-5489	2.8	58
212	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. <i>Combustion and Flame</i> , 2015 , 162, 3115-3129	5.3	57

211	Detailed Kinetic Modeling of Iron Nanoparticle Synthesis from the Decomposition of Fe(CO) ₅ . <i>Journal of Physical Chemistry C</i> , 2007 , 111, 5677-5688	3.8	56
210	The electrostatic origin of Abraham's solute polarity parameter. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 7564-73	3.4	56
209	Coupling of CH stretching and bending vibrations in trihalomethanes. <i>Journal of Chemical Physics</i> , 1987 , 86, 5994-5999	3.9	56
208	Structural Properties and Reactivity Trends of Molybdenum Oxide Catalysts Supported on Zirconia for the Hydrodeoxygenation of Anisole. <i>ACS Sustainable Chemistry and Engineering</i> , 2017 , 5, 5293-5301	8.3	55
207	Elementary Reaction Mechanism for Benzene Oxidation in Supercritical Water. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 10576-10586	2.8	55
206	Learning only buys you so much: Practical limits on battery price reduction. <i>Applied Energy</i> , 2019 , 239, 218-224	10.7	54
205	Stress Test for Quantum Dynamics Approximations: Deep Tunneling in the Muonium Exchange Reaction D + HMu → DMu + H. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 4219-24	6.4	54
204	On upgrading the numerics in combustion chemistry codes. <i>Combustion and Flame</i> , 2002 , 128, 270-291	5.3	54
203	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 8667-8682	8.3	53
202	The role of catalyst in supercritical water desulfurization. <i>Applied Catalysis B: Environmental</i> , 2014 , 147, 144-155	21.8	51
201	Unimolecular Reaction Pathways of a Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. <i>Journal of the American Chemical Society</i> , 2018 , 140, 1035-1048	16.4	50
200	Evaluating Scalable Uncertainty Estimation Methods for Deep Learning-Based Molecular Property Prediction. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 2697-2717	6.1	49
199	A study of the ground electronic state of the isomers of CHNO. <i>Molecular Physics</i> , 1993 , 78, 319-343	1.7	49
198	Combining experiment and theory to elucidate the role of supercritical water in sulfide decomposition. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9220-8	3.6	48
197	Quantum rate coefficients and kinetic isotope effect for the reaction Cl + CH ₄ → HCl + CH ₃ from ring polymer molecular dynamics. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 1989-96	2.8	47
196	Ab initio prediction of fundamental, overtone and combination band infrared intensities. <i>Chemical Physics Letters</i> , 1990 , 169, 127-137	2.5	47
195	Theoretical kinetics study of the O(¹ P) + CH ₂ CD ₂ hydrogen abstraction reaction: the role of anharmonicity, recrossing effects, and quantum mechanical tunneling. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 3243-52	2.8	46
194	Oxidative Desulfurization of Middle-Distillate Fuels Using Activated Carbon and Power Ultrasound. <i>Energy & Fuels</i> , 2012 , 26, 5164-5176	4.1	46

193	Ab initio screening of metal sorbents for elemental mercury capture in syngas streams. <i>Chemical Engineering Science</i> , 2010 , 65, 3025-3033	4.4	46
192	Exchange-correlation functionals from ab initio electron densities. <i>Chemical Physics Letters</i> , 1997 , 273, 183-194	2.5	46
191	Bond-breaking without barriers. II. Vibrationally excited products. <i>Journal of Chemical Physics</i> , 1991 , 94, 1961-1969	3.9	46
190	A coordinated investigation of the combustion chemistry of diisopropyl ketone, a prototype for biofuels produced by endophytic fungi. <i>Combustion and Flame</i> , 2014 , 161, 711-724	5.3	45
189	A detailed kinetic model for combustion synthesis of titania from TiCl ₄ . <i>Combustion and Flame</i> , 2009 , 156, 1764-1770	5.3	45
188	Interval Methods for Semi-Infinite Programs. <i>Computational Optimization and Applications</i> , 2005 , 30, 63-93	1.4	45
187	Economic and environmental benefits of higher-octane gasoline. <i>Environmental Science & Technology</i> , 2014 , 48, 6561-8	10.3	44
186	Chemically activated formation of organic acids in reactions of the Criegee intermediate with aldehydes and ketones. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 16841-52	3.6	44
185	Predicting solvation energies for kinetic modeling. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2010 , 106, 211		44
184	Rigorous valid ranges for optimally reduced kinetic models. <i>Combustion and Flame</i> , 2006 , 146, 348-365	5.3	44
183	RDChiral: An RDKit Wrapper for Handling Stereochemistry in Retrosynthetic Template Extraction and Application. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 2529-2537	6.1	43
182	Ring-polymer molecular dynamics: rate coefficient calculations for energetically symmetric (near thermoneutral) insertion reactions (X + H ₂) → HX + H(X = C(1D), S(1D)). <i>Journal of Chemical Physics</i> , 2014 , 141, 244103	3.9	43
181	Accelerating multi-dimensional combustion simulations using GPU and hybrid explicit/implicit ODE integration. <i>Combustion and Flame</i> , 2012 , 159, 2388-2397	5.3	43
180	Understanding Unimolecular Dissociations with Loose Transition States: Photofragmentation Dynamics of Ketene at the Singlet Threshold. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1988 , 92, 389-396		43
179	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. <i>Combustion and Flame</i> , 2018 , 187, 247-256	5.3	42
178	The predictive capability of an automatically generated combustion chemistry mechanism: Chemical structures of premixed iso-butanol flames. <i>Combustion and Flame</i> , 2013 , 160, 2343-2351	5.3	42
177	Design and implementation of a next-generation software interface for on-the-fly quantum and force field calculations in automated reaction mechanism generation. <i>Computers and Chemical Engineering</i> , 2013 , 52, 35-45	4	42
176	Minimizing E-factor in the continuous-flow synthesis of diazepam and atropine. <i>Bioorganic and Medicinal Chemistry</i> , 2017 , 25, 6233-6241	3.4	41

175	A consistent-splitting approach to computing stiff steady-state reacting flows with adaptive chemistry. <i>Combustion Theory and Modelling</i> , 2003 , 7, 383-399	1.5	41
174	Accurate Thermochemistry with Small Data Sets: A Bond Additivity Correction and Transfer Learning Approach. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 5826-5835	2.8	40
173	Ab initio aqueous thermochemistry: application to the oxidation of hydroxylamine in nitric acid solution. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 11968-83	3.4	40
172	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. <i>Catalysis Science and Technology</i> , 2017 , 7, 1713-1725	5.5	39
171	Redesigning combustion modeling algorithms for the Graphics Processing Unit (GPU): Chemical kinetic rate evaluation and ordinary differential equation integration. <i>Combustion and Flame</i> , 2011 , 158, 836-847	5.3	39
170	Detailed chemical kinetic modeling of JP-10 (exo-tetrahydrodicyclopentadiene) high-temperature oxidation: Exploring the role of biradical species in initial decomposition steps. <i>International Journal of Chemical Kinetics</i> , 2012 , 44, 179-193	1.4	38
169	Modeling of 1,3-hexadiene, 2,4-hexadiene and 1,4-hexadiene-doped methane flames: Flame modeling, benzene and styrene formation. <i>Combustion and Flame</i> , 2010 , 157, 1331-1345	5.3	38
168	Predictive Kinetics: A New Approach for the 21st Century. <i>Advances in Chemical Engineering</i> , 2007 , 1-313	0.6	38
167	Thermodynamic Properties of Ketenes: Group Additivity Values from Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 7937-7949	2.8	38
166	Deep Learning of Activation Energies. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2992-2997	6.4	37
165	Automated computational thermochemistry for butane oxidation: A prelude to predictive automated combustion kinetics. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 363-371	5.9	37
164	Kinetic Modeling of Jet Propellant-10 Pyrolysis. <i>Energy & Fuels</i> , 2015 , 29, 413-427	4.1	37
163	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. <i>Energy & Fuels</i> , 2014 , 28, 4976-4985	4.1	36
162	Reaction of phenyl radical with propylene as a possible source of indene and other polycyclic aromatic hydrocarbons: an ab initio/RRKM-ME study. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 4176-91	2.8	35
161	Perspective on Mechanism Development and Structure-Activity Relationships for Gas-Phase Atmospheric Chemistry. <i>International Journal of Chemical Kinetics</i> , 2018 , 50, 435-469	1.4	34
160	Structure of polymer-stabilized magnetic fluids: small-angle neutron scattering and mean-field lattice modeling. <i>Langmuir</i> , 2004 , 20, 5223-34	4	34
159	Prediction of the Knock Limit and Viable Operating Range for a Homogeneous-Charge Compression-Ignition (HCCI) Engine 2003 ,		33
158	Reaction Mechanism Generator v3.0: Advances in Automatic Mechanism Generation. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2686-2696	6.1	32

157	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. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 418-31	6.4	31
156	Optimal automatic reaction and species elimination in kinetic mechanisms. <i>Combustion and Flame</i> , 2008 , 155, 118-132	5.3	31
155	Missing Thermochemical Groups for Large Unsaturated Hydrocarbons: Contrasting Predictions of G2 and CBS-Q. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 11141-11149	2.8	31
154	The Underlying Physics and Chemistry behind Fuel Sensitivity. <i>SAE International Journal of Fuels and Lubricants</i> , 2010 , 3, 256-265	1.8	30
153	Response of Different Types of Sulfur Compounds to Oxidative Desulfurization of Jet Fuel. <i>Energy & Fuels</i> , 2014 , 28, 2977-2983	4.1	29
152	Using adaptive proper orthogonal decomposition to solve the reaction-diffusion equation. <i>Applied Numerical Mathematics</i> , 2009 , 59, 272-279	2.5	29
151	Application of Computational Kinetic Mechanism Generation to Model the Autocatalytic Pyrolysis of Methane. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 1000-1010	3.9	29
150	Temperature and Molecular Size Dependence of the High-Pressure Limit. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 6206-6211	2.8	29
149	Experimental and modeling study of the mutual oxidation of N-pentane and nitrogen dioxide at low and high temperatures in a jet stirred reactor. <i>Energy</i> , 2018 , 165, 727-738	7.9	29
148	A priori falloff analysis for OH + NO ₂ . <i>International Journal of Chemical Kinetics</i> , 2000 , 32, 245-262	1.4	28
147	Predictive chemical kinetics: Density functional and hartree-fock calculations on free-radial reaction transition states. <i>International Journal of Quantum Chemistry</i> , 1994 , 52, 837-847	2.1	28
146	New vibrational bands of CH ₂ (ν_2). <i>Journal of Molecular Spectroscopy</i> , 1989 , 138, 614-629	1.3	28
145	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. <i>Scientific Data</i> , 2020 , 7, 137	8.2	27
144	Measurements and automated mechanism generation modeling of OH production in photolytically initiated oxidation of the neopentyl radical. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3891-900	2.8	27
143	NO _x -Mediated Homogeneous Pathways for the Synthesis of Formaldehyde from CH ₄ /O ₂ Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 2677-2688	3.9	27
142	Self-Evolving Machine: A Continuously Improving Model for Molecular Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 2142-2152	2.8	27
141	An Extended Group Additivity Method for Polycyclic Thermochemistry Estimation. <i>International Journal of Chemical Kinetics</i> , 2018 , 50, 294-303	1.4	26
140	A Signature of Roaming Dynamics in the Thermal Decomposition of Ethyl Nitrite: Chirped-Pulse Rotational Spectroscopy and Kinetic Modeling. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3641-8	6.4	26

139	Investigating the techno-economic trade-offs of hydrogen source using a response surface model of drop-in biofuel production via bio-oil upgrading. <i>Biofuels, Bioproducts and Biorefining</i> , 2012 , 6, 503-520	5.3	26
138	Temperature-dependent kinetics of the vinyl radical (C ₂ H ₃) self-reaction. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 1278-86	2.8	26
137	Modeling study of the anti-knock tendency of substituted phenols as additives: an application of the reaction mechanism generator (RMG). <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10637-10649	3.6	25
136	Order out of Randomness: Self-Organization Processes in Astrophysics. <i>Space Science Reviews</i> , 2018 , 214, 1	7.5	25
135	Kinetic analysis and reaction mechanism for anisole conversion over zirconia-supported molybdenum oxide. <i>Journal of Catalysis</i> , 2019 , 376, 248-257	7.3	25
134	Obtaining accurate solutions using reduced chemical kinetic models: a new model reduction method for models rigorously validated over ranges. <i>Combustion Theory and Modelling</i> , 2007 , 11, 127-146	1.5	25
133	Influence of the double bond position on the oxidation of decene isomers at high pressures and temperatures. <i>Proceedings of the Combustion Institute</i> , 2015 , 35, 333-340	5.9	24
132	Screening of metal oxides and metal sulfides as sorbents for elemental mercury at elevated temperatures. <i>Fuel</i> , 2012 , 97, 783-795	7.1	24
131	Experimental study of catalyst nanoparticle and single walled carbon nanotube formation in a controlled premixed combustion. <i>Journal of Materials Chemistry</i> , 2008 , 18, 1561		24
130	Thermochemical production of hydrogen from hydrogen sulfide with iodine thermochemical cycles. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 12939-12947	6.7	24
129	Modeling of aromatics formation in fuel-rich methane oxy-combustion with an automatically generated pressure-dependent mechanism. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 813-832	3.6	23
128	An extensible framework for capturing solvent effects in computer generated kinetic models. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 2955-70	3.4	23
127	Crossed beam reaction of phenyl and D ₅ -phenyl radicals with propene and deuterated counterparts--competing atomic hydrogen and methyl loss pathways. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 720-9	3.6	23
126	Balanced Splitting and Rebalanced Splitting. <i>SIAM Journal on Numerical Analysis</i> , 2013 , 51, 3084-3105	2.4	23
125	Co-oxidation of methylphosphonic acid and ethanol in supercritical water. <i>Journal of Supercritical Fluids</i> , 2006 , 39, 239-245	4.2	23
124	Rate-based screening of pressure-dependent reaction networks. <i>Computer Physics Communications</i> , 2001 , 138, 237-249	4.2	23
123	Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. <i>Chemical Engineering Journal</i> , 2015 , 278, 385-393	14.7	22
122	Analysis of Membrane and Adsorbent Processes for Warm Syngas Cleanup in Integrated Gasification Combined-Cycle Power with CO ₂ Capture and Sequestration. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 11313-11336	3.9	22

121	PREDICTION OF PERFORMANCE MAPS FOR HOMOGENEOUS-CHARGE COMPRESSION-IGNITION ENGINES. <i>Combustion Science and Technology</i> , 2004 , 176, 1243-1282	1.5	22
120	Temperature- and Pressure-Dependent Kinetics of CH ₂ OO + CH ₃ COCH ₃ and CH ₂ OO + CH ₃ CHO: Direct Measurements and Theoretical Analysis. <i>International Journal of Chemical Kinetics</i> , 2016 , 48, 474-488	1.4	22
119	Experimental Investigation of Sorbent for Warm CO ₂ Capture by Pressure Swing Adsorption. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 9665-9673	3.9	21
118	Computational Investigation on Hydrodeoxygenation (HDO) of Acetone to Propylene on γ -MoO ₃ (010) Surface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 17848-17855	3.8	21
117	Hydrogen abstraction rates via density functional theory. <i>Chemical Physics Letters</i> , 1999 , 312, 262-268	2.5	21
116	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. <i>Chemical Science</i> , 2020 , 12, 2198-2208	9.4	21
115	An experimental and modeling study of vacuum residue upgrading in supercritical water. <i>AICHE Journal</i> , 2018 , 64, 1732-1743	3.6	20
114	Analysis of Adsorbent-Based Warm CO ₂ Capture Technology for Integrated Gasification Combined Cycle (IGCC) Power Plants. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 11145-11158	3.9	20
113	Pressure and temperature dependence of the reaction of vinyl radical with ethylene. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 6843-51	2.8	20
112	Transition to electric vehicles in China: Implications for private motorization rate and battery market. <i>Energy Policy</i> , 2020 , 144, 111654	7.2	19
111	Automatic mechanism generation for pyrolysis of di-tert-butyl sulfide. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 21651-8	3.6	19
110	Iterative experimental design based on active machine learning reduces the experimental burden associated with reaction screening. <i>Reaction Chemistry and Engineering</i> , 2020 , 5, 1963-1972	4.9	19
109	Supercritical Water Treatment of Crude Oil and Hexylbenzene: An Experimental and Mechanistic Study on Alkylbenzene Decomposition. <i>Energy & Fuels</i> , 2015 , 29, 5290-5302	4.1	18
108	Predicted reaction rates of H(x)N(y)O(z) intermediates in the oxidation of hydroxylamine by aqueous nitric acid. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 7577-93	2.8	18
107	Predicting chemical kinetics with computational chemistry: is QOOH->HOQO important in fuel ignition?. <i>Molecular Physics</i> , 2004 , 102, 371-380	1.7	18
106	Valid parameter range analyses for chemical reaction kinetic models. <i>Chemical Engineering Science</i> , 2002 , 57, 4475-4491	4.4	18
105	The engine reformer: Syngas production in an engine for compact gas-to-liquids synthesis. <i>Canadian Journal of Chemical Engineering</i> , 2016 , 94, 623-635	2.3	18
104	Kinetics and Products of Vinyl + 1,3-Butadiene, a Potential Route to Benzene. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 7325-38	2.8	17

103	Cleavage of Side Chains on Thiophenic Compounds by Supercritical Water Treatment of Crude Oil Quantified by Two-Dimensional Gas Chromatography with Sulfur Chemiluminescence Detection. <i>Energy & Fuels</i> , 2014 , 28, 6589-6595	4.1	17
102	Thermochemical properties and group values for nitrogen-containing molecules. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 9144-52	2.8	17
101	A theoretical and experimental kinetic study of phenyl radical addition to butadiene. <i>Proceedings of the Combustion Institute</i> , 2005 , 30, 1049-1056	5.9	17
100	Transient vibrational spectroscopy of. <i>Journal of Molecular Spectroscopy</i> , 1989 , 138, 596-601	1.3	17
99	Modelling gas-phase synthesis of single-walled carbon nanotubes on iron catalyst particles. <i>Carbon</i> , 2008 , 46, 422-433	10.4	16
98	Elementary reaction rate model for MPA oxidation in supercritical water. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 4310	3.6	16
97	Micro-syngas technology options for GtL. <i>Canadian Journal of Chemical Engineering</i> , 2016 , 94, 613-622	2.3	16
96	Transfer learning for solvation free energies: From quantum chemistry to experiments. <i>Chemical Engineering Journal</i> , 2021 , 418, 129307	14.7	16
95	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. <i>Energy & Fuels</i> , 2018 , 32, 3920-3934	4.1	15
94	Co-oxidation of ammonia and ethanol in supercritical water, part 2: Modeling demonstrates the importance of H ₂ NNO _x . <i>International Journal of Chemical Kinetics</i> , 2008 , 40, 653-662	1.4	15
93	Ab initio modeling of organophosphorus combustion chemistry. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 4296	3.6	15
92	Analysis of an elementary reaction mechanism for benzene oxidation in supercritical water. <i>Proceedings of the Combustion Institute</i> , 2000 , 28, 1529-1536	5.9	15
91	A kinetic and thermochemical database for organic sulfur and oxygen compounds. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 13625-39	3.6	14
90	Phenyl radical + propene: a prototypical reaction surface for aromatic-catalyzed 1,2-hydrogen-migration and subsequent resonance-stabilized radical formation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 13191-13214	3.6	14
89	Automated Reaction Mechanism Generation Including Nitrogen as a Heteroatom. <i>International Journal of Chemical Kinetics</i> , 2018 , 50, 243-258	1.4	14
88	Dehydration of isobutanol and the elimination of water from fuel alcohols. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 6724-36	2.8	14
87	Kinetic modeling to estimate fundamental yield bounds for selective propylene oxidation over bifunctional catalysts. <i>Applied Catalysis A: General</i> , 2006 , 303, 177-191	5.1	14
86	Effects of large-amplitude torsions on partition functions: beyond the conventional separability assumption. <i>Molecular Physics</i> , 2005 , 103, 1027-1034	1.7	14

85	Automatic Generation of Detailed Mechanisms. <i>Green Energy and Technology</i> , 2013 , 59-92	0.6	14
84	An experimental, theoretical, and modeling study of the ignition behavior of cyclopentanone. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 657-665	5.9	13
83	Accurate and efficient method for predicting thermochemistry of furans and ortho-arynes: expansion of the bond-centered group additivity method. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 6971-7	2.8	13
82	Direct Measurement of the Fast, Reversible Addition of Oxygen to Cyclohexadienyl Radicals in Nonpolar Solvents. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 7193-7203	2.8	13
81	A Collaborative Informatics Infrastructure for Multi-Scale Science. <i>Cluster Computing</i> , 2005 , 8, 243-253	2.1	13
80	Natural Gas and Cellulosic Biomass: A Clean Fuel Combination? Determining the Natural Gas Blending Wall in Biofuel Production. <i>Environmental Science & Technology</i> , 2015 , 49, 8183-92	10.3	12
79	Continuous Thermal Oxidation of Alkenes with Nitrous Oxide in a Packed Bed Reactor. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 4166-4173	3.9	12
78	MODELING OXIDATION AND HYDROLYSIS REACTIONS IN SUPERCRITICAL WATER—FREE RADICAL ELEMENTARY REACTION NETWORKS AND THEIR APPLICATIONS. <i>Combustion Science and Technology</i> , 2006 , 178, 363-398	1.5	12
77	Generating transition states of isomerization reactions with deep learning. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 23618-23626	3.6	12
76	A combined photoionization time-of-flight mass spectrometry and laser absorption spectrometry flash photolysis apparatus for simultaneous determination of reaction rates and product branching. <i>Review of Scientific Instruments</i> , 2018 , 89, 074102	1.7	11
75	Pressure and temperature dependence of the reaction of vinyl radical with alkenes II: Measured rates and predicted product distributions for vinyl+propene. <i>Proceedings of the Combustion Institute</i> , 2009 , 32, 139-148	5.9	11
74	Moving from postdictive to predictive kinetics in reaction engineering. <i>AIChE Journal</i> , 2020 , 66, e17059	3.6	11
73	On-the-fly pruning for rate-based reaction mechanism generation. <i>Computers and Chemical Engineering</i> , 2017 , 100, 1-8	4	10
72	Numerical investigation of strained extinction at engine-relevant pressures: Pressure dependence and sensitivity to chemical and physical parameters for methane-based flames. <i>Combustion and Flame</i> , 2019 , 202, 318-333	5.3	10
71	Chemistry of Alkylaromatics Reconsidered. <i>Energy & Fuels</i> , 2018 , 32, 5489-5500	4.1	10
70	Analysis of Hydroxide Sorbents for CO ₂ Capture from Warm Syngas. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 13473-13481	3.9	10
69	From benzene to naphthalene: direct measurement of reactions and intermediates of phenyl radicals and acetylene. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22248-22258	3.6	10
68	Ember: An open-source, transient solver for 1D reacting flow using large kinetic models, applied to strained extinction. <i>Combustion and Flame</i> , 2018 , 195, 105-116	5.3	10

67	Detailed kinetic model for hexyl sulfide pyrolysis and its desulfurization by supercritical water. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 10311-10324	3.6	9
66	Cooperative Co /Co Sites Stabilized by a Perovskite Matrix Enable Selective C-O and C-C bond Hydrogenolysis of Oxygenated Arenes. <i>ChemSusChem</i> , 2019 , 12, 2171-2175	8.3	9
65	Thermochemistry and Group Additivity Values for Fused Two-Ring Species and Radicals. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 3418-3428	2.8	9
64	Uncertainty analysis of correlated parameters in automated reaction mechanism generation. <i>International Journal of Chemical Kinetics</i> , 2020 , 52, 266-282	1.4	9
63	Modeling Study of High Temperature Pyrolysis of Natural Gas. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 7404-7420	3.9	9
62	Incorporating Multiple Uncertainties into Projections of Chinese Private Car Sales and Stock. <i>Transportation Research Record</i> , 2018 , 2672, 182-193	1.7	9
61	Learning to Optimize Molecular Geometries Using Reinforcement Learning. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 818-825	6.4	9
60	Automatic generation of reaction mechanisms. <i>Computer Aided Chemical Engineering</i> , 2019 , 259-294	0.6	8
59	Intramolecular ¹³ C isotope distributions of butane from natural gases. <i>Chemical Geology</i> , 2020 , 541, 119571	4.2	8
58	Revealing the critical role of radical-involved pathways in high temperature cyclopentanone pyrolysis. <i>Combustion and Flame</i> , 2020 , 216, 280-292	5.3	8
57	Methanol formation from the treatment of glycerol in supercritical water and with ethylsulfide. <i>Journal of Supercritical Fluids</i> , 2016 , 117, 80-88	4.2	8
56	Capturing aromaticity in automatic mechanism generation software. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 575-581	5.9	8
55	An Exact-Steady-state Adaptive Chemistry method for combustion simulations: Combining the efficiency of reduced models and the accuracy of the full model. <i>Combustion and Flame</i> , 2012 , 159, 2352-2362	5.3	8
54	Pressure and temperature dependence of the reaction of vinyl radical with alkenes III: measured rates and predicted product distributions for vinyl + butene. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13357-71	2.8	8
53	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. <i>Frontiers in Chemical Engineering</i> , 2020 , 2,	1	7
52	Detailed chemical kinetic simulations of homogeneous charge compression ignition engine transients. <i>International Journal of Engine Research</i> , 2008 , 9, 149-164	2.7	7
51	A collaborative informatics infrastructure for multi-scale science		7
50	Effects of Variations in Market Gasoline Properties on HCCI Load Limits 2007 ,		6

49	A crossed molecular beam study of $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$: The effect of ozone rotational energy. <i>Journal of Chemical Physics</i> , 1984 , 80, 3644-3650	3.9	6
48	Group Contribution and Machine Learning Approaches to Predict Abraham Solute Parameters, Solvation Free Energy, and Solvation Enthalpy.. <i>Journal of Chemical Information and Modeling</i> , 2022 ,	6.1	6
47	Theoretical study on the HACA chemistry of naphthalenyl radicals and acetylene: The formation of C_{12}H_8 , C_{14}H_8 , and $\text{C}_{14}\text{H}_{10}$ species. <i>International Journal of Chemical Kinetics</i> , 2020 , 52, 752-768	1.4	6
46	Predicting polycyclic aromatic hydrocarbon formation with an automatically generated mechanism for acetylene pyrolysis. <i>International Journal of Chemical Kinetics</i> , 2021 , 53, 27-42	1.4	6
45	A Fragment-Based Mechanistic Kinetic Modeling Framework for Complex Systems. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 14022-14030	3.9	6
44	Computer-generated isotope model achieves experimental accuracy of filiation for position-specific isotope analysis. <i>Chemical Geology</i> , 2019 , 514, 1-9	4.2	5
43	Temperature-dependent vapor/liquid equilibria and solvation free energy estimation from minimal data. <i>AIChE Journal</i> , 2020 , 66, e16976	3.6	5
42	Direct Measurement of Radical-Catalyzed CH Formation from Acetylene and Validation of Theoretical Rate Coefficients for $\text{CH} + \text{CH}$ and $\text{CH} + \text{CH}$ Reactions. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 2871-2884	2.8	5
41	Recharging systems and business operations to improve the economics of electrified taxi fleets. <i>Sustainable Cities and Society</i> , 2020 , 57, 102119	10.1	5
40	Thermochemistry Prediction and Automatic Reaction Mechanism Generation for Oxygenated Sulfur Systems: A Case Study of Dimethyl Sulfide Oxidation. <i>ChemSystemsChem</i> , 2020 , 2, e1900051	3.1	5
39	Screening of binary alloys for warm temperature capture of elemental mercury using density functional theory. <i>Chemical Engineering Science</i> , 2012 , 80, 128-133	4.4	5
38	The high-resolution spectroscopy of dissociating molecules. <i>Philosophical Transactions of the Royal Society: Physical and Engineering Sciences</i> , 1990 , 332, 297-307		5
37	Kinetic Modeling of API Oxidation: (1) The AIBN/HO/CHOH Radical "Soup". <i>Molecular Pharmaceutics</i> , 2021 , 18, 3037-3049	5.6	5
36	An apparatus-independent extinction strain rate in counterflow flames. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 1979-1987	5.9	5
35	Automated Generation of Chemical Mechanisms for Predicting Extinction Strain Rates with Applications in Flame Stabilization and Combustion Instabilities 2017 ,		4
34	Reaction Pathways, Thermodynamics, and Kinetics of Cyclopentanone Oxidation Intermediates: A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9644-9657	2.8	4
33	Large Intermediates in Hydrazine Decomposition: A Theoretical Study of the NH and NH Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 4679-4692	2.8	4
32	H_2 Generation from H_2O and H_2S through an Iodine Cycle. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 7369-7377	8.3	4

31	Thermochemistry and Kinetics of Intermolecular Addition of Radicals to Toluene and Alkylaromatics. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 3176-3184	2.8	4
30	Automated chemical resonance generation and structure filtration for kinetic modeling. <i>International Journal of Chemical Kinetics</i> , 2019 , 51, 760-776	1.4	4
29	Predicting Infrared Spectra with Message Passing Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2594-2609	6.1	4
28	Automatically generated model for light alkene combustion. <i>Combustion and Flame</i> , 2022 , 241, 112080	5.3	4
27	Combining retrosynthesis and mixed-integer optimization for minimizing the chemical inventory needed to realize a WHO essential medicines list. <i>Reaction Chemistry and Engineering</i> , 2020 , 5, 367-376	4.9	3
26	Scalability strategies for automated reaction mechanism generation. <i>Computers and Chemical Engineering</i> , 2019 , 131, 106578	4	3
25	Combustion of Synthetic Jet Fuel: Chemical Kinetic Modeling and Uncertainty Analysis. <i>Journal of Propulsion and Power</i> , 2017 , 33, 350-359	1.8	3
24	Learnings from exchange-correlation potentials. <i>Chemical Physics Letters</i> , 1998 , 290, 465-472	2.5	3
23	Development of the RIOT web service and information technologies to enable mechanism reduction for HCCI simulations. <i>Journal of Physics: Conference Series</i> , 2005 , 16, 107-112	0.3	3
22	Pressure-dependent kinetics of peroxy radicals formed in isobutanol combustion. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 19802-19815	3.6	3
21	Oxidation and pyrolysis of methyl propyl ether. <i>International Journal of Chemical Kinetics</i> , 2021 , 53, 915-938		3
20	Correct Symmetry Treatment for X + X Reactions Prevents Large Errors in Predicted Isotope Enrichment. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 2320-2324	2.8	3
19	Kinetics of Intramolecular Phenyl Migration and Fused Ring Formation in Hexylbenzene Radicals. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 9778-9791	2.8	3
18	Direct Kinetics and Product Measurement of Phenyl Radical + Ethylene. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 2352-2365	2.8	2
17	Formation of Two-Ring Aromatics in Hexylbenzene Pyrolysis. <i>Energy & Fuels</i> , 2020 , 34, 1365-1377	4.1	2
16	Reply to comment on Automatic estimation of pressure-dependent rate coefficients (J. W. Allen, C. F. Goldsmith, and W. H. Green, <i>Phys. Chem. Chem. Phys.</i> , 2011, 14, 1131-1155). <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 8434	3.6	2
15	Primary Reference Fuel Behavior in a HCCI Engine near the Low-Load Limit. <i>SAE International Journal of Fuels and Lubricants</i> , 2008 , 1, 1098-1109	1.8	2
14	Forecasting veterinary school admission probabilities for undergraduate student profiles. <i>Journal of Veterinary Medical Education</i> , 2006 , 33, 441-6	1.3	2

13	Multi-fidelity prediction of molecular optical peaks with deep learning.. <i>Chemical Science</i> , 2022 , 13, 11529-1162	2
12	Detailed Kinetic Modeling for the Pyrolysis of a Jet A Surrogate. <i>Energy & Fuels</i> , 2022 , 36, 1304-1315	2.1
11	Transition to Electric Vehicles in China: Implications for Total Cost of Ownership and Cost to Society1,	2
10	Adaptive chemistry 2001 , 1209-1212	2
9	Screening for New Pathways in Atmospheric Oxidation Chemistry with Automated Mechanism Generation. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 6772-6788	2.8
8	CH polycyclic aromatic hydrocarbon formation by acetylene addition to naphthalenyl radicals observed. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14325-14339	3.6
7	System and Market Analysis of Methanol Production Using Compact Engine Reformers 2014 ,	1
6	Detailed Reaction Mechanism for 350-700 °C Pyrolysis of an Alkane, Aromatic, and Long-Chain Alkylaromatic Mixture. <i>Energy & Fuels</i> , 2022 , 36, 1635-1646	4.1
5	The Effect of Alcohol and Carbonyl Functional Groups on the Competition between Unimolecular Decomposition and Isomerization in C4 and C5 Alkoxy Radicals. <i>International Journal of Chemical Kinetics</i> , 2016 , 48, 544-555	1.4
4	EHreact: Extended Hasse Diagrams for the Extraction and Scoring of Enzymatic Reaction Templates. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4949-4961	6.1
3	Chemistry of Simple Organic Peroxy Radicals under Atmospheric through Combustion Conditions: Role of Temperature, Pressure, and NO Level. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 10303-10314	2.8
2	Effects of surface species and homogeneous reactions on rates and selectivity in ethane oxidation on oxide catalysts. <i>AIChE Journal</i> , 2021 , 67, e17483	3.6
1	Reduced models for adaptive chemistry simulation of reacting flows 2003 , 1422-1425	0