

Gabriel da Silva

List of Publications by Year in descending order

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61984

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162
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162
times ranked

5172
citing authors

#	ARTICLE	IF	CITATIONS
1	Biochar production from waste rubber-wood-sawdust and its potential use in C sequestration: Chemical and physical characterization. <i>Industrial Crops and Products</i> , 2013, 44, 18-24.	5.2	271
2	The octane numbers of ethanol blended with gasoline and its surrogates. <i>Fuel</i> , 2014, 115, 727-739.	6.4	238
3	Unimolecular $\dot{\text{I}}^2$ -Hydroxyperoxy Radical Decomposition with OH Recycling in the Photochemical Oxidation of Isoprene. <i>Environmental Science & Technology</i> , 2010, 44, 250-256.	10.0	122
4	Ethanol Oxidation: Kinetics of the $\dot{\text{I}}^\pm$ -Hydroxyethyl Radical + O_2 Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8923-8933.	2.5	118
5	A kinetic study of CO ₂ capture with potassium carbonate solutions promoted with various amino acids: Glycine, sarcosine and proline. <i>International Journal of Greenhouse Gas Control</i> , 2014, 20, 212-222.	4.6	113
6	Carboxylic Acid Catalyzed Keto-Enol Tautomerizations in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 7523-7525.	13.8	104
7	Modeling the IR Spectra of Aqueous Metal Carboxylate Complexes: Correlation between Bonding Geometry and Stretching Mode Wavenumber Shifts. <i>Chemistry - A European Journal</i> , 2015, 21, 6801-6805.	3.3	104
8	Amino Acids as Carbon Capture Solvents: Chemical Kinetics and Mechanism of the Glycine + CO_2 Reaction. <i>Energy & Fuels</i> , 2013, 27, 3898-3904.	5.1	101
9	Thermal Decomposition of the Benzyl Radical to Fulvenallene (C_7H_6) + H. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6111-6120.	2.5	100
10	Ab Initio Procedure for Aqueous-Phase pKa Calculation: The Acidity of Nitrous Acid. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11371-11376.	2.5	97
11	Enthalpies of Formation, Bond Dissociation Energies, and Molecular Structures of then-Aldehydes (Acetaldehyde, Propanal, Butanal, Pentanal, Hexanal, and Heptanal) and Their Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 13058-13067.	2.5	93
12	Reaction mechanism for the free-edge oxidation of soot by O ₂ . <i>Combustion and Flame</i> , 2012, 159, 3423-3436.	5.2	93
13	Gold-Mediated C-Cl Bond Activation of Iodobenzene. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3812-3817.	13.8	90
14	Thermodynamic Properties (Enthalpy, Bond Energy, Entropy, and Heat Capacity) and Internal Rotor Potentials of Vinyl Alcohol, Methyl Vinyl Ether, and Their Corresponding Radicals. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7925-7934.	2.5	88
15	Oxidation of the Benzyl Radical: Mechanism, Thermochemistry, and Kinetics for the Reactions of Benzyl Hydroperoxide. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3185-3194.	5.3	85
16	The Effect of Charge Cooling on the RON of Ethanol/Gasoline Blends. <i>SAE International Journal of Fuels and Lubricants</i> , 0, 6, 34-43.	0.2	83
17	Variational Analysis of the Phenyl + O_2 and Phenoxy + O Reactions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 3566-3575.	2.5	82
18	A kinetic and process modeling study of CO ₂ capture with MEA-promoted potassium carbonate solutions. <i>Chemical Engineering Journal</i> , 2012, 210, 271-279.	12.7	82

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19	First Principles ρ -K _a Calculations on Carboxylic Acids Using the SMD Solvation Model: Effect of Thermodynamic Cycle, Model Chemistry, and Explicit Solvent Molecules. Journal of Physical Chemistry B, 2012, 116, 11999-12006.	2.6	80
20	The Research and Motor octane numbers of Liquefied Petroleum Gas (LPG). Fuel, 2013, 108, 797-811.	6.4	80
21	The C ₇ H ₅ Fulvenallenyl Radical as a Combustion Intermediate: Potential New Pathways to Two- and Three-Ring PAHs. Journal of Physical Chemistry A, 2009, 113, 12045-12048.	2.5	78
22	Toluene Combustion: Reaction Paths, Thermochemical Properties, and Kinetic Analysis for the Methylphenyl Radical + O ₂ Reaction. Journal of Physical Chemistry A, 2007, 111, 8663-8676.	2.5	77
23	Borate-Catalyzed Carbon Dioxide Hydration via the Carbonic Anhydrase Mechanism. Environmental Science & Technology, 2011, 45, 4802-4807.	10.0	77
24	Bond dissociation energy of the phenol OH bond from ab initio calculations. Chemical Physics Letters, 2006, 424, 42-45.	2.6	66
25	Carbon dioxide absorption into unpromoted and borate-catalyzed potassium carbonate solutions. Chemical Engineering Journal, 2012, 181-182, 694-701.	12.7	66
26	Experimental and Theoretical Understanding of the Gas Phase Oxidation of Atmospheric Amides with OH Radicals: Kinetics, Products, and Mechanisms. Journal of Physical Chemistry A, 2015, 119, 4298-4308.	2.5	65
27	Quantum Chemical Study of the Acrolein (CH ₂ CHCHO) + OH + O ₂ Reactions. Journal of Physical Chemistry A, 2010, 114, 8302-8311.	2.5	63
28	Reaction of Methacrolein with the Hydroxyl Radical in Air: Incorporation of Secondary O ₂ Addition into the MACR + OH Master Equation. Journal of Physical Chemistry A, 2012, 116, 5317-5324.	2.5	61
29	Kinetic modeling of the benzyl+HO ₂ reaction. Proceedings of the Combustion Institute, 2009, 32, 287-294.	3.9	59
30	Quantum Chemical Study of the Structure and Thermochemistry of the Five-Membered Nitrogen-Containing Heterocycles and Their Anions and Radicals. Journal of Physical Chemistry A, 2006, 110, 13979-13988.	2.5	58
31	Demonstration of a Concentrated Potassium Carbonate Process for CO ₂ Capture. Energy & Fuels, 2014, 28, 299-306.	5.1	58
32	Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions. Journal of Physical Chemistry A, 2010, 114, 2275-2283.	2.5	57
33	Isomer-Specific Product Detection of Gas-Phase Xylyl Radical Rearrangement and Decomposition Using VUV Synchrotron Photoionization. Journal of Physical Chemistry A, 2014, 118, 3593-3604.	2.5	57
34	Gas-phase reactions of aryl radicals with 2-butyne: experimental and theoretical investigation employing the N-methyl-pyridinium-4-yl radical cation. Physical Chemistry Chemical Physics, 2012, 14, 2417.	2.8	56
35	Direct Observation of <i>para</i> -Xylylene as the Decomposition Product of the <i>meta</i> -Xylyl Radical Using VUV Synchrotron Radiation. Journal of Physical Chemistry Letters, 2013, 4, 2546-2550.	4.6	56
36	Decomposition of Methylbenzyl Radicals in the Pyrolysis and Oxidation of Xylenes. Journal of Physical Chemistry A, 2009, 113, 10264-10278.	2.5	55

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37	Atmospheric Chemistry of Enols: A Theoretical Study of the Vinyl Alcohol + OH + O ₂ Reaction Mechanism. <i>Environmental Science & Technology</i> , 2014, 48, 6694-6701.	10.0	55
38	Decomposition kinetics of perfluorinated sulfonic acids. <i>Chemosphere</i> , 2020, 238, 124615.	8.2	55
39	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. <i>ChemPhysChem</i> , 2006, 7, 1119-1126.	2.1	53
40	Benzoyl Radical Decomposition Kinetics: Formation of Benzaldehyde + H, Phenyl + CH ₂ O, and Benzene + HCO. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6979-6986.	2.5	50
41	Who Wins: Pesci, Peters, or Deacon? Intrinsic Reactivity Orders for Organocuprate Formation via Ligand Decomposition. <i>Organometallics</i> , 2012, 31, 1801-1807.	2.3	49
42	Gas Phase Oxidation of Nicotine by OH Radicals: Kinetics, Mechanisms, and Formation of HNCO. <i>Environmental Science and Technology Letters</i> , 2016, 3, 327-331.	8.7	49
43	Electrochemical passivation of sphalerite during bacterial oxidation in the presence of galena. <i>Minerals Engineering</i> , 2003, 16, 199-203.	4.3	46
44	Relative importance of diffusion and reaction control during the bacterial and ferric sulphate leaching of zinc sulphide. <i>Hydrometallurgy</i> , 2004, 73, 313-324.	4.3	46
45	G3X-K theory: A composite theoretical method for thermochemical kinetics. <i>Chemical Physics Letters</i> , 2013, 558, 109-113.	2.6	46
46	Photoswitching an Isolated Donor-Acceptor Stenhouse Adduct. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 665-671.	4.6	46
47	Reactions of simple and peptidic alpha-carboxylate radical anions with dioxygen in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16314.	2.8	45
48	Hydroxyl radical regeneration in the photochemical oxidation of glyoxal: kinetics and mechanism of the HC(O)CO + O ₂ reaction. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6698.	2.8	44
49	Role of the $\dot{\text{C}}\text{H}_2$ -hydroxyethylperoxy radical in the reactions of acetaldehyde and vinyl alcohol with HO ₂ . <i>Chemical Physics Letters</i> , 2009, 483, 25-29.	2.6	43
50	Role of the Metal, Ligand, and Alkyl/Aryl Group in the Hydrolysis Reactions of Group 10 Organometallic Cations [(L)M(R)] ⁺ . <i>Organometallics</i> , 2013, 32, 6931-6944.	2.3	43
51	Kinetics and mechanism of the bacterial and ferric sulphate oxidation of galena. <i>Hydrometallurgy</i> , 2004, 75, 99-110.	4.3	41
52	Gas-Phase Mechanisms of the Reactions of Reduced Organic Nitrogen Compounds with OH Radicals. <i>Environmental Science & Technology</i> , 2016, 50, 11723-11734.	10.0	41
53	Retro-[3 + 2]-Cycloaddition Reactions in the Decomposition of Five-Membered Nitrogen-Containing Heterocycles. <i>Journal of Organic Chemistry</i> , 2008, 73, 1343-1353.	3.2	40
54	Pyrolysis of fulvenallene (C ₇ H ₆) and fulvenallenyl (C ₇ H ₅): Theoretical kinetics and experimental product detection. <i>Chemical Physics Letters</i> , 2011, 517, 144-148.	2.6	40

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55	Modeling End-Gas Autoignition of Ethanol/Gasoline Surrogate Blends in the Cooperative Fuel Research Engine. <i>Energy & Fuels</i> , 2017, 31, 2378-2389.	5.1	40
56	On the reactivity of methylbenzenes. <i>Combustion and Flame</i> , 2010, 157, 2175-2183.	5.2	37
57	Theoretical Study of the Oxidation Catalyst N-Hydroxyphthalimide (NHPI): ΔH° Thermochemical Properties, Internal Rotor Potential, and Gas- and Liquid-Phase Bond Dissociation Energies. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5760-5765.	3.1	36
58	Are the three hydroxyphenyl radical isomers created equal? ΔH° The role of the phenoxy radical ΔH° . <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30076-30083.	2.8	35
59	The autoignition of Liquefied Petroleum Gas (LPG) in spark-ignition engines. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 2933-2940.	3.9	35
60	Chemically activated reactions on the C ₇ H ₅ energy surface: propargyl + diacetylene, i-C ₅ H ₃ + acetylene, and n-C ₅ H ₃ + acetylene. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 8940.	2.8	34
61	Atmospheric Chemistry of 2-Aminoethanol (MEA): Reaction of the NH ₂ CHCH ₂ OH Radical with O ₂ . <i>Journal of Physical Chemistry A</i> , 2012, 116, 10980-10986.	2.5	34
62	Photoelectron Spectrum and Energetics of the <i>meta</i> -Xylylene Diradical. <i>Journal of the American Chemical Society</i> , 2017, 139, 14348-14351.	13.7	34
63	Indene Formation from Alkylated Aromatics: Kinetics and Products of the Fulvenallene + Acetylene Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8971-8978.	2.5	33
64	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6235-6249.	2.5	33
65	Formation of Nitrosamines and Alkyldiazohydroxides in the Gas Phase: The CH ₃ NH + NO Reaction Revisited. <i>Environmental Science & Technology</i> , 2013, 47, 7766-7772.	10.0	33
66	Insights into the mechanochromism of spiropyran elastomers. <i>Polymer Chemistry</i> , 2019, 10, 1650-1659.	3.9	33
67	Use of Vanadium(V) Oxide as a Catalyst for CO ₂ Hydration in Potassium Carbonate Systems. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 3029-3039.	3.7	31
68	Quantum Chemical Study of the Thermal Decomposition of <i>o</i> -Quinone Methide (6-Methylene-2,4-cyclohexadien-1-one). <i>Journal of Physical Chemistry A</i> , 2007, 111, 7987-7994.	2.5	30
69	Carbonic anhydrase promoted absorption of CO ₂ into potassium carbonate solutions. , 2015, 5, 108-114.		30
70	Effect of Added Nucleophilic Species on the Rate of Primary Amino Acid Nitrosation. <i>Journal of the American Chemical Society</i> , 2005, 127, 3664-3665.	13.7	29
71	Concerted HO ₂ Elimination from β -Aminoalkylperoxyl Free Radicals: Experimental and Theoretical Evidence from the Gas-Phase NH ₂ CHCH ₂ CO ₂ + O ₂ Reaction. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 805-811.	4.6	29
72	Mystery of 1-Vinylpropargyl Formation from Acetylene Addition to the Propargyl Radical: An Open-and-Shut Case. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2086-2095.	2.5	29

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73	Hydroxyl Radical Initiated Oxidation of s-Triazine: Hydrogen Abstraction Is Faster than Hydroxyl Addition. Journal of Physical Chemistry A, 2009, 113, 8596-8606.	2.5	28
74	Direct versus Water-Mediated Protodecarboxylation of Acetic Acid Catalyzed by Group 10 Carboxylates, [(phen)M(O ₂ CCH ₃)] ⁺ . Organometallics, 2014, 33, 5185-5197.	2.3	28
75	Modeling Solvation of Magnesium Centers by Ether Ligands: Gas-Phase Synthesis and Hydrolysis of the Organomagnesium Cations [CH ₃ Mg(3 <i>X</i> -crown- <i>X</i>)] ⁺ (<i>X</i> = Tj ETQq1 20.7843147gBT /Ov	2.5	28
76	Thermal decomposition of pyrazole to vinylcarbene+N ₂ : A first principles/RRKM study. Chemical Physics Letters, 2009, 474, 13-17.	2.6	26
77	Oxidation of Carboxylic Acids Regenerates Hydroxyl Radicals in the Unpolluted and Nighttime Troposphere. Journal of Physical Chemistry A, 2010, 114, 6861-6869.	2.5	26
78	Decomposition of Pyruvic Acid on the Ground-State Potential Energy Surface. Journal of Physical Chemistry A, 2016, 120, 276-283.	2.5	26
79	Formation and stability of gas-phase o-benzoquinone from oxidation of ortho-hydroxyphenyl: a combined neutral and distonic radical study. Physical Chemistry Chemical Physics, 2016, 18, 4320-4332.	2.8	24
80	Double Molecular Photoswitch Driven by Light and Collisions. Physical Review Letters, 2018, 120, 223002.	7.8	24
81	Kinetics and Mechanism of the Glyoxal + HO ₂ Reaction: Conversion of HO ₂ to OH by Carbonyls. Journal of Physical Chemistry A, 2011, 115, 291-297.	2.5	23
82	Reaction of Benzene with Atomic Carbon: Pathways to Fulvenallene and the Fulvenallenyl Radical in Extraterrestrial Atmospheres and the Interstellar Medium. Journal of Physical Chemistry A, 2014, 118, 3967-3972.	2.5	23
83	An experimental and theoretical study of the nitrosation of ammonia and thiourea. Chemical Engineering Science, 2006, 61, 3186-3197.	3.8	21
84	Photoisomerization Action Spectroscopy of the Carbocyanine Dye DTC ⁺ in the Gas Phase. Journal of Physical Chemistry A, 2013, 117, 13319-13325.	2.5	20
85	A Theoretical Study of the Photoisomerization of Glycolaldehyde and Subsequent OH Radical-Initiated Oxidation of 1,2-Ethenediol. Journal of Physical Chemistry A, 2015, 119, 9812-9820.	2.5	20
86	Elementary reaction step model of the NaCN nitrosation of ammonia. International Journal of Chemical Kinetics, 2007, 39, 645-656.	1.6	18
87	Design and Analysis of a Modified CFR Engine for the Octane Rating of Liquefied Petroleum Gases (LPG). SAE International Journal of Fuels and Lubricants, 0, 7, 283-300.	0.2	18
88	Photoinitiated Intramolecular Proton Transfer in Deprotonated <i>para</i> -Coumaric Acid. Journal of Physical Chemistry A, 2019, 123, 4419-4430.	2.5	18
89	Does "Dry Hit" vaping of vitamin E acetate contribute to EVALI? Simulating toxic ketene formation during e-cigarette use. PLoS ONE, 2020, 15, e0238140.	2.5	17
90	Hydroxyl radical formation in the gas phase oxidation of distonic 2-methylphenyl radical cations. Physical Chemistry Chemical Physics, 2013, 15, 20577.	2.8	16

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91	On the Separation of Timescales in Chemically Activated Reactions. International Journal of Chemical Kinetics, 2013, 45, 387-396.	1.6	16
92	Nucleophilic reactivity of aniline derivatives towards the nitroso group. Journal of Physical Organic Chemistry, 2007, 20, 167-179.	1.9	15
93	Nucleophilic Catalysis of Nitrosation: Relationship between Nitrosating Agent Equilibrium Constant and Catalyst Nucleophilicity. Journal of Chemical Research, 2002, 2002, 589-590.	1.3	14
94	Water-in-oil emulsion foaming by thiourea nitrosation: Reaction and mass transfer. AIChE Journal, 2006, 52, 1558-1565.	3.6	14
95	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	2.5	14
96	Reaction of the C_4H_5 ($\text{CH}_2\text{CCHCH}_2$) Radical with O_2 . Journal of Physical Chemistry A, 2011, 115, 1018-1026.	2.5	14
97	Modeling the antisymmetric and symmetric stretching vibrational modes of aqueous carboxylate anions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 134, 535-542.	3.9	14
98	Interconversion of Methyltropylium and Xylyl Radicals: A Pathway Unavailable to the Benzyl-Tropylium Rearrangement. Journal of Physical Chemistry A, 2018, 122, 1261-1269.	2.5	13
99	Isotope-specific reactions of acetonitrile (CH_3CN) with trapped, translationally cold CCl^+ . Journal of Chemical Physics, 2021, 154, 074305.	3.0	13
100	Reactivity Trends in the Gas-Phase Addition of Acetylene to the N^+ -Protonated Aryl Radical Cations of Pyridine, Aniline, and Benzonitrile. Journal of the American Society for Mass Spectrometry, 2021, 32, 537-547.	2.8	13
101	Kinetics of the benzyl + $\text{O}(^3\text{P})$ reaction: a quantum chemical/statistical reaction rate theory study. Physical Chemistry Chemical Physics, 2012, 14, 16143.	2.8	12
102	Molecular Salt Effects in the Gas Phase: Tuning the Kinetic Basicity of $[\text{HCCl}_2\text{Li}]^+$ and $[\text{HCCMgCl}_2]^+$ by LiCl and MgCl_2 . Angewandte Chemie - International Edition, 2014, 53, 10979-10983.	13.8	12
103	Ultrafast photoisomerisation of an isolated retinoid. Physical Chemistry Chemical Physics, 2019, 21, 10567-10579.	2.8	12
104	Gas phase reactions of iodide and bromide anions with ozone: evidence for stepwise and reversible reactions. Physical Chemistry Chemical Physics, 2020, 22, 9982-9989.	2.8	12
105	Seleniranium Ions Undergo π -Ligand Exchange via an Associative Mechanism in the Gas Phase. Journal of Organic Chemistry, 2017, 82, 6289-6297.	3.2	10
106	Atmospheric Oxidation of Piperazine Initiated by OH: A Theoretical Kinetics Investigation. ACS Earth and Space Chemistry, 2019, 3, 2510-2516.	2.7	10
107	Reaction of Aromatic Peroxyl Radicals with Alkynes: A Mass Spectrometric and Computational Study Using the Distonic Radical Ion Approach. Chemistry - an Asian Journal, 2013, 8, 450-464.	3.3	9
108	Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical. Physical Chemistry Chemical Physics, 2014, 16, 24954-24964.	2.8	9

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109	Radical Formation in the Gas-Phase Ozonolysis of Deprotonated Cysteine. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12947-12951.	13.8	9
110	Highly efficient gas-phase reactivity of protonated pyridine radicals with propene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31072-31084.	2.8	9
111	Reactions of Thiiranium and Sulfonium Ions with Alkenes in the Gas Phase. <i>Journal of Organic Chemistry</i> , 2019, 84, 10076-10087.	3.2	9
112	Experimental and DFT Studies on the Identity Exchange Reactions between Phenyl Chalcogen Iridium Ions and Alkenes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8200-8207.	2.5	9
113	Nitramine and nitrosamine formation is a minor pathway in the atmospheric oxidation of methylamine: A theoretical kinetic study of the $\text{CH}_3\text{NH} + \text{O}_2$ reaction. <i>International Journal of Chemical Kinetics</i> , 2019, 51, 723-728.	1.6	9
114	Reactions of a distonic peroxy radical anion influenced by SOMO \rightarrow HOMO conversion: an example of anion-directed channel switching. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 2130-2141.	2.8	9
115	A detailed chemical kinetic model for pyrolysis of the lignin model compound chroman. <i>AIMS Environmental Science</i> , 2013, 1, 12-25.	1.4	9
116	Integrated Kinetic and Thermodynamic Model Describing the Nitrosation of Aniline and Its Derivatives under Reaction- and Encounter-Controlled Conditions. <i>Industrial & Engineering Chemistry Research</i> , 2004, 43, 2296-2301.	3.7	8
117	Photoisomerization of Methyl Vinyl Ketone and Methacrolein in the Troposphere: A Theoretical Investigation of Ground-State Reaction Pathways. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 753-763.	2.7	8
118	Product detection study of the gas-phase oxidation of methylphenyl radicals using synchrotron photoionisation mass spectrometry. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17939-17949.	2.8	8
119	Experimental and theoretical investigations into the mechanisms of haliranium ion π -ligand exchange reactions with cyclic alkenes in the gas phase. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25572-25589.	2.8	8
120	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. <i>Journal of Physical Chemistry A</i> , 2022, 126, 101-108.	2.5	8
121	The gas phase aldose \rightarrow ketone isomerization mechanism: Direct interconversion of the model hydroxycarbonyls 2 \rightarrow hydroxypropanal and hydroxyacetone. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25434.	2.0	7
122	Thermal decomposition kinetics of glyphosate (GP) and its metabolite aminomethylphosphonic acid (AMPA). <i>Environmental Sciences: Processes and Impacts</i> , 2020, 22, 152-160.	3.5	7
123	Thermal decomposition and isomerization of furfural and 2-pyrone: a theoretical kinetic study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2046-2054.	2.8	7
124	Bonding of Aqueous Citrate with Zn^{2+} and ZnO Nanoclusters: A Theoretical Study. <i>ChemistrySelect</i> , 2017, 2, 2055-2064.	1.5	6
125	A detailed chemical kinetic model for the supercritical water oxidation of methylamine: The importance of imine formation. <i>International Journal of Chemical Kinetics</i> , 2020, 52, 701-711.	1.6	6
126	Ab Initio Study of Bonding between Nucleophilic Species and the Nitroso Group. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1300-1306.	2.5	5

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127	Using Distonic Radical Ions to Probe the Chemistry of Key Combustion Intermediates: The Case of the Benzoyl Radical Anion. <i>Journal of the American Society for Mass Spectrometry</i> , 2013, 24, 493-501.	2.8	5
128	Unveiling New Isomers and Rearrangement Routes on the $C_7H_8^{+}$ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2019, 123, 823-830.	2.5	5
129	Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2782-2790.	2.5	5
130	Barrierless Reactions of Three Benzonitrile Radical Cations with Ethylene. <i>Australian Journal of Chemistry</i> , 2020, 73, 705.	0.9	5
131	Electronic spectrum and photodissociation chemistry of the linear methyl propargyl cation $H_2C_4H_3^+$. <i>Journal of Chemical Physics</i> , 2017, 146, 044307.	3.0	4
132	Molecular Weight Growth in the Gas-Phase Reactions of Dehydroanilinium Radical Cations with Propene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8881-8892.	2.5	4
133	Kinetics of C_5H_4 isomer $\hat{A}+\hat{A}H$ reactions and incorporation of C_5H ($x\hat{A}=3 \hat{A} \hat{A} \hat{A} \hat{A} \hat{A}$) chemistry into a detailed chemical kinetic model. <i>Combustion and Flame</i> , 2021, 227, 227-237.	5.2	4
134	Multiphoton dissociation dynamics of the indenyl radical at 248 nm and 193 nm. <i>Journal of Chemical Physics</i> , 2019, 151, 174303.	3.0	3
135	Electronic Spectrum and Photodissociation Chemistry of the 1-Butyn-3-yl Cation, $H_3CCHCHCH^+$. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2366-2371.	2.5	3
136	Near-infrared reversible photoswitching of an isolated azobenzene-stilbene dye. <i>Chemical Physics Letters</i> , 2020, 741, 137065.	2.6	3
137	Evidence that $\hat{E} \hat{A} \hat{A}$ ligand exchange reactions of chalcogen iranium ions proceed via $H\hat{A}^{1/4}ckel$ pseudocoarctate transition states. <i>Journal of Physical Organic Chemistry</i> , 2020, 33, e4111.	1.9	2
138	Auto-Oxidation of a Volatile Silicon Compound: A Theoretical Study of the Atmospheric Chemistry of Tetramethylsilane. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6544-6551.	2.5	2
139	Toxic Chemical Formation during Vaping of Ethyl Ester Flavor Additives: A Chemical Kinetic Modeling Study. <i>Chemical Research in Toxicology</i> , 2022, 35, 522-528.	3.3	2
140	Mechanistic study of the reaction of CH_2F_2 with Cl atoms in the absence and presence of CH_4 or C_2H_6 : decomposition of CHF_2OH and fate of the CHF_2O radical. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9376-9383.	2.8	1
141	Improved rate coefficient expressions for the reaction of methyl bromide with OH and Cl radicals. <i>Chemical Physics Letters</i> , 2018, 706, 371-374.	2.6	0
142	Self-catalyzed keto-enol tautomerization of malonic acid. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26114.	2.0	0
143	Pyrolysis of Triclosan and Its Chlorinated Derivatives. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8050-8056.	2.5	0
144	Five vs. six membered-ring PAH products from reaction of <i>o</i> -methylphenyl radical and two C_3H_4 isomers. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14913-14924.	2.8	0