Gabriel da Silva

List of Publications by Year
in descending order

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144 papers	5,489 citations	61857 43 h-index	106150 65 g-index
162 all docs	162 docs citations	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. Industrial Crops and Products, 2013, 44, 18-24.	2.5	271
2	The octane numbers of ethanol blended with gasoline and its surrogates. Fuel, 2014, 115, 727-739.	3.4	238
3	Unimolecular Î²-Hydroxyperoxy Radical Decomposition with OH Recycling in the Photochemical Oxidation of Isoprene. Environmental Science & Technology, 2010, 44, 250-256.	4.6	122
4	Ethanol Oxidation: Kinetics of the Î±-Hydroxyethyl Radical + O₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 8923-8933.	1.1	118
5	A kinetic study of CO2 capture with potassium carbonate solutions promoted with various amino acids: Glycine, sarcosine and proline. International Journal of Greenhouse Gas Control, 2014, 20, 212-222.	2.3	113
6	Carboxylic Acid Catalyzed Ketoâ€Enol Tautomerizations in the Gas Phase. Angewandte Chemie - International Edition, 2010, 49, 7523-7525.	7.2	104
7	Modeling the IR Spectra of Aqueous Metal Carboxylate Complexes: Correlation between Bonding Geometry and Stretching Mode Wavenumber Shifts. Chemistry - A European Journal, 2015, 21, 6801-6805.	1.7	104
8	Amino Acids as Carbon Capture Solvents: Chemical Kinetics and Mechanism of the Glycine + CO₂ Reaction. Energy & Fuels, 2013, 27, 3898-3904.	2.5	101
9	Thermal Decomposition of the Benzyl Radical to Fulvenallene (C₇H₆) + H. Journal of Physical Chemistry A, 2009, 113, 6111-6120.	1.1	100
10	Ab Initio Procedure for Aqueous-Phase pKa Calculation:â€‰ The Acidity of Nitrous Acid. Journal of Physical Chemistry A, 2006, 110, 11371-11376.	1.1	97
11	Enthalpies of Formation, Bond Dissociation Energies, and Molecular Structures of then-Aldehydes (Acetaldehyde, Propanal, Butanal, Pentanal, Hexanal, and Heptanal) and Their Radicals. Journal of Physical Chemistry A, 2006, 110, 13058-13067.	1.1	93
12	Reaction mechanism for the free-edge oxidation of soot by O2. Combustion and Flame, 2012, 159, 3423-3436.	2.8	93
13	Goldâ€Mediated Cï£¿I Bond Activation of Iodobenzene. Angewandte Chemie - International Edition, 2012, 51, 3812-3817.	7.2	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. Journal of Physical Chemistry A, 2006, 110, 7925-7934.	1.1	88
15	Oxidation of the Benzyl Radical: Mechanism, Thermochemistry, and Kinetics for the Reactions of Benzyl Hydroperoxide. Journal of Chemical Theory and Computation, 2009, 5, 3185-3194.	2.3	85
16	The Effect of Charge Cooling on the RON of Ethanol/Gasoline Blends. SAE International Journal of Fuels and Lubricants, 0, 6, 34-43.	0.2	83
17	Variational Analysis of the Phenyl + O₂ and Phenoxy + O Reactions. Journal of Physical Chemistry A, 2008, 112, 3566-3575.	1.1	82
18	A kinetic and process modeling study of CO2 capture with MEA-promoted potassium carbonate solutions. Chemical Engineering Journal, 2012, 210, 271-279.	6.6	82

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19	First Principles pK_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.	1.2	80
20	The Research and Motor octane numbers of Liquefied Petroleum Gas (LPG). Fuel, 2013, 108, 797-811.	3.4	80
21	The C₇H₅ Fulvenallenyl Radical as a Combustion Intermediate: Potential New Pathways to Two- and Three-Ring PAHs. Journal of Physical Chemistry A, 2009, 113, 12045-12048.	1.1	78
22	Toluene Combustion:â€‰ Reaction Paths, Thermochemical Properties, and Kinetic Analysis for the Methylphenyl Radical + O₂ Reaction. Journal of Physical Chemistry A, 2007, 111, 8663-8676.	1.1	77
23	Borate-Catalyzed Carbon Dioxide Hydration via the Carbonic Anhydrase Mechanism. Environmental Science & Technology, 2011, 45, 4802-4807.	4.6	77
24	Bond dissociation energy of the phenol OH bond from ab initio calculations. Chemical Physics Letters, 2006, 424, 42-45.	1.2	66
25	Carbon dioxide absorption into unpromoted and borate-catalyzed potassium carbonate solutions. Chemical Engineering Journal, 2012, 181-182, 694-701.	6.6	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.	1.1	65
27	Quantum Chemical Study of the Acrolein (CH₂CHCHO) + OH + O₂ Reactions. Journal of Physical Chemistry A, 2010, 114, 8302-8311.	1.1	63
28	Reaction of Methacrolein with the Hydroxyl Radical in Air: Incorporation of Secondary O₂ Addition into the MACR + OH Master Equation. Journal of Physical Chemistry A, 2012, 116, 5317-5324.	1.1	61
29	Kinetic modeling of the benzyl+HO2 reaction. Proceedings of the Combustion Institute, 2009, 32, 287-294.	2.4	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.	1.1	58
31	Demonstration of a Concentrated Potassium Carbonate Process for CO₂ Capture. Energy & Fuels, 2014, 28, 299-306.	2.5	58
32	Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions. Journal of Physical Chemistry A, 2010, 114, 2275-2283.	1.1	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.	1.1	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.	1.3	56
35	Direct Observation of para-Xylylene as the Decomposition Product of the meta-Xylyl Radical Using VUV Synchrotron Radiation. Journal of Physical Chemistry Letters, 2013, 4, 2546-2550.	2.1	56
36	Decomposition of Methylbenzyl Radicals in the Pyrolysis and Oxidation of Xylenes. Journal of Physical Chemistry A, 2009, 113, 10264-10278.	1.1	55

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37	Atmospheric Chemistry of Enols: A Theoretical Study of the Vinyl Alcohol + OH + O₂ Reaction Mechanism. Environmental Science & Technology, 2014, 48, 6694-6701.	4.6	55
38	Decomposition kinetics of perfluorinated sulfonic acids. Chemosphere, 2020, 238, 124615.	4.2	55
39	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. ChemPhysChem, 2006, 7, 1119-1126.	1.0	53
40	Benzoxyl Radical Decomposition Kinetics: Formation of Benzaldehyde + H, Phenyl + CH₂O, and Benzene + HCO. Journal of Physical Chemistry A, 2009, 113, 6979-6986.	1.1	50
41	Who Wins: Pesci, Peters, or Deacon? Intrinsic Reactivity Orders for Organocuprate Formation via Ligand Decomposition. Organometallics, 2012, 31, 1801-1807.	1.1	49
42	Gas Phase Oxidation of Nicotine by OH Radicals: Kinetics, Mechanisms, and Formation of HNCO. Environmental Science and Technology Letters, 2016, 3, 327-331.	3.9	49
43	Electrochemical passivation of sphalerite during bacterial oxidation in the presence of galena. Minerals Engineering, 2003, 16, 199-203.	1.8	46
44	Relative importance of diffusion and reaction control during the bacterial and ferric sulphate leaching of zinc sulphide. Hydrometallurgy, 2004, 73, 313-324.	1.8	46
45	G3X-K theory: A composite theoretical method for thermochemical kinetics. Chemical Physics Letters, 2013, 558, 109-113.	1.2	46
46	Photoswitching an Isolated Donorâ€“Acceptor Stenhouse Adduct. Journal of Physical Chemistry Letters, 2018, 9, 665-671.	2.1	46
47	Reactions of simple and peptidic alpha-carboxylate radical anions with dioxygen in the gas phase. Physical Chemistry Chemical Physics, 2011, 13, 16314.	1.3	45
48	Hydroxyl radical regeneration in the photochemical oxidation of glyoxal: kinetics and mechanism of the HC(O)CO + O2 reaction. Physical Chemistry Chemical Physics, 2010, 12, 6698.	1.3	44
49	Role of the Î±-hydroxyethylperoxy radical in the reactions of acetaldehyde and vinyl alcohol with HO2. Chemical Physics Letters, 2009, 483, 25-29.	1.2	43
50	Role of the Metal, Ligand, and Alkyl/Aryl Group in the Hydrolysis Reactions of Group 10 Organometallic Cations [(L)M(R)]⁺. Organometallics, 2013, 32, 6931-6944.	1.1	43
51	Kinetics and mechanism of the bacterial and ferric sulphate oxidation of galena. Hydrometallurgy, 2004, 75, 99-110.	1.8	41
52	Gas-Phase Mechanisms of the Reactions of Reduced Organic Nitrogen Compounds with OH Radicals. Environmental Science & Technology, 2016, 50, 11723-11734.	4.6	41
53	Retro-[3 + 2]-Cycloaddition Reactions in the Decomposition of Five-Membered Nitrogen-Containing Heterocycles. Journal of Organic Chemistry, 2008, 73, 1343-1353.	1.7	40
54	Pyrolysis of fulvenallene (C7H6) and fulvenallenyl (C7H5): Theoretical kinetics and experimental product detection. Chemical Physics Letters, 2011, 517, 144-148.	1.2	40

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55	Modeling End-Gas Autoignition of Ethanol/Gasoline Surrogate Blends in the Cooperative Fuel Research Engine. Energy & Fuels, 2017, 31, 2378-2389.	2.5	40
56	On the reactivity of methylbenzenes. Combustion and Flame, 2010, 157, 2175-2183.	2.8	37
57	Theoretical Study of the Oxidation CatalystN-Hydroxyphthalimide (NHPI):â€‰ Thermochemical Properties, Internal Rotor Potential, and Gas- and Liquid-Phase Bond Dissociation Energies. Journal of Physical Chemistry C, 2007, 111, 5760-5765.	1.5	36
58	Are the three hydroxyphenyl radical isomers created equal? â€“ The role of the phenoxy radical â€“. Physical Chemistry Chemical Physics, 2015, 17, 30076-30083.	1.3	35
59	The autoignition of Liquefied Petroleum Gas (LPG) in spark-ignition engines. Proceedings of the Combustion Institute, 2015, 35, 2933-2940.	2.4	35
60	Chemically activated reactions on the C7H5 energy surface: propargyl + diacetylene, i-C5H3 + acetylene, and n-C5H3 + acetylene. Physical Chemistry Chemical Physics, 2011, 13, 8940.	1.3	34
61	Atmospheric Chemistry of 2-Aminoethanol (MEA): Reaction of the NH₂^{â€¢}CHCH₂OH Radical with O₂. Journal of Physical Chemistry A, 2012, 116, 10980-10986.	1.1	34
62	Photoelectron Spectrum and Energetics of the meta-Xylylene Diradical. Journal of the American Chemical Society, 2017, 139, 14348-14351.	6.6	34
63	Indene Formation from Alkylated Aromatics: Kinetics and Products of the Fulvenallene + Acetylene Reaction. Journal of Physical Chemistry A, 2009, 113, 8971-8978.	1.1	33
64	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. Journal of Physical Chemistry A, 2010, 114, 6235-6249.	1.1	33
65	Formation of Nitrosamines and Alkyldiazohydroxides in the Gas Phase: The CH₃NH + NO Reaction Revisited. Environmental Science & Technology, 2013, 47, 7766-7772.	4.6	33
66	Insights into the mechanochromism of spiropyran elastomers. Polymer Chemistry, 2019, 10, 1650-1659.	1.9	33
67	Use of Vanadium(V) Oxide as a Catalyst for CO₂ Hydration in Potassium Carbonate Systems. Industrial & Engineering Chemistry Research, 2014, 53, 3029-3039.	1.8	31
68	Quantum Chemical Study of the Thermal Decomposition of o-Quinone Methide (6-Methylene-2,4-cyclohexadien-1-one). Journal of Physical Chemistry A, 2007, 111, 7987-7994.	1.1	30
69	Carbonic anhydrase promoted absorption of CO₂ into potassium carbonate solutions. , 2015, 5, 108-114.		30
70	Effect of Added Nucleophilic Species on the Rate of Primary Amino Acid Nitrosation. Journal of the American Chemical Society, 2005, 127, 3664-3665.	6.6	29
71	Concerted HO₂ Elimination from Î±-Aminoalkylperoxyl Free Radicals: Experimental and Theoretical Evidence from the Gas-Phase NH₂^{â€¢}CHCO₂^{â€“} + O₂ Reaction. Journal of Physical Chemistry Letters, 2012, 3, 805-811.	2.1	29
72	Mystery of 1-Vinylpropargyl Formation from Acetylene Addition to the Propargyl Radical: An Open-and-Shut Case. Journal of Physical Chemistry A, 2017, 121, 2086-2095.	1.1	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.	1.1	28
74	Direct versus Water-Mediated Protodecarboxylation of Acetic Acid Catalyzed by Group 10 Carboxylates, [(phen)M(O₂CCH₃)]⁺. Organometallics, 2014, 33, 5185-5197.	1.1	28
75	Modeling Solvation of Magnesium Centers by Ether Ligands: Gas-Phase Synthesis and Hydrolysis of the Organomagnesium Cations [CH₃Mg(3X-crown-X)]⁺(X=) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	27
76	Thermal decomposition of pyrazole to vinylcarbene+N2: A first principles/RRKM study. Chemical Physics Letters, 2009, 474, 13-17.	1.2	26
77	Oxidation of Carboxylic Acids Regenerates Hydroxyl Radicals in the Unpolluted and Nighttime Troposphere. Journal of Physical Chemistry A, 2010, 114, 6861-6869.	1.1	26
78	Decomposition of Pyruvic Acid on the Ground-State Potential Energy Surface. Journal of Physical Chemistry A, 2016, 120, 276-283.	1.1	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.	1.3	24
80	Double Molecular Photoswitch Driven by Light and Collisions. Physical Review Letters, 2018, 120, 223002.	2.9	24
81	Kinetics and Mechanism of the Glyoxal + HO₂Reaction: Conversion of HO₂to OH by Carbonyls. Journal of Physical Chemistry A, 2011, 115, 291-297.	1.1	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.	1.1	23
83	An experimental and theoretical study of the nitrosation of ammonia and thiourea. Chemical Engineering Science, 2006, 61, 3186-3197.	1.9	21
84	Photoisomerization Action Spectroscopy of the Carbocyanine Dye DTC⁺ in the Gas Phase. Journal of Physical Chemistry A, 2013, 117, 13319-13325.	1.1	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.	1.1	20
86	Elementary reaction step model of the Nâ€•nitrosation of ammonia. International Journal of Chemical Kinetics, 2007, 39, 645-656.	1.0	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 para-Coumaric Acid. Journal of Physical Chemistry A, 2019, 123, 4419-4430.	1.1	18
89	Does â€¯Dry Hitâ€™ vaping of vitamin E acetate contribute to EVALI? Simulating toxic ketene formation during e-cigarette use. PLoS ONE, 2020, 15, e0238140.	1.1	17
90	Hydroxyl radical formation in the gas phase oxidation of distonic 2-methylphenyl radical cations. Physical Chemistry Chemical Physics, 2013, 15, 20577.	1.3	16

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91	On the Separation of Timescales in Chemically Activated Reactions. International Journal of Chemical Kinetics, 2013, 45, 387-396.	1.0	16
92	Nucleophilic reactivity of aniline derivatives towards the nitroso group. Journal of Physical Organic Chemistry, 2007, 20, 167-179.	0.9	15
93	Nucleophilic Catalysis of Nitrosation: Relationship between Nitrosating Agent Equilibrium Constant and Catalyst Nucleophilicity. Journal of Chemical Research, 2002, 2002, 589-590.	0.6	14
94	Water-in-oil emulsion foaming by thiourea nitrosation: Reaction and mass transfer. AICHE Journal, 2006, 52, 1558-1565.	1.8	14
95	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	1.1	14
96	Reaction of the i-C₄H₅ (CH₂CCHCH₂) Radical with O₂. Journal of Physical Chemistry A, 2011, 115, 1018-1026.	1.1	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.	2.0	14
98	Interconversion of Methyltropyl and Xylyl Radicals: A Pathway Unavailable to the Benzylâ€“Tropyl Rearrangement. Journal of Physical Chemistry A, 2018, 122, 1261-1269.	1.1	13
99	Isotope-specific reactions of acetonitrile (CH3CN) with trapped, translationally cold CCl+. Journal of Chemical Physics, 2021, 154, 074305.	1.2	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.	1.2	13
101	Kinetics of the benzyl + O(3P) reaction: a quantum chemical/statistical reaction rate theory study. Physical Chemistry Chemical Physics, 2012, 14, 16143.	1.3	12
102	Molecular Salt Effects in the Gas Phase: Tuning the Kinetic Basicity of [HCCLiCl]^{â^'} and [HCCMgCl₂]^{â^'} by LiCl and MgCl₂. Angewandte Chemie - International Edition, 2014, 53, 10979-10983.	7.2	12
103	Ultrafast photoisomerisation of an isolated retinoid. Physical Chemistry Chemical Physics, 2019, 21, 10567-10579.	1.3	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.	1.3	12
105	Seleniranium Ions Undergo Ï€-Ligand Exchange via an Associative Mechanism in the Gas Phase. Journal of Organic Chemistry, 2017, 82, 6289-6297.	1.7	10
106	Atmospheric Oxidation of Piperazine Initiated by OH: A Theoretical Kinetics Investigation. ACS Earth and Space Chemistry, 2019, 3, 2510-2516.	1.2	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.	1.7	9
108	Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical. Physical Chemistry Chemical Physics, 2014, 16, 24954-24964.	1.3	9

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109	Radical Formation in the Gasâ€Phase Ozonolysis of Deprotonated Cysteine. Angewandte Chemie - International Edition, 2015, 54, 12947-12951.	7.2	9
110	Highly efficient gas-phase reactivity of protonated pyridine radicals with propene. Physical Chemistry Chemical Physics, 2017, 19, 31072-31084.	1.3	9
111	Reactions of Thiiranium and Sulfonium Ions with Alkenes in the Gas Phase. Journal of Organic Chemistry, 2019, 84, 10076-10087.	1.7	9
112	Experimental and DFT Studies on the Identity Exchange Reactions between Phenyl Chalcogen Iranium Ions and Alkenes. Journal of Physical Chemistry A, 2019, 123, 8200-8207.	1.1	9
113	Nitramine and nitrosamine formation is a minor pathway in the atmospheric oxidation of methylamine: A theoretical kinetic study of the CH 3 NH + O 2 reaction. International Journal of Chemical Kinetics, 2019, 51, 723-728.	1.0	9
114	Reactions of a distonic peroxyl radical anion influenced by SOMOâ€“HOMO conversion: an example of anion-directed channel switching. Physical Chemistry Chemical Physics, 2020, 22, 2130-2141.	1.3	9
115	A detailed chemical kinetic model for pyrolysis of the lignin model compound chroman. AIMS Environmental Science, 2013, 1, 12-25.	0.7	9
116	Integrated Kinetic and Thermodynamic Model Describing the Nitrosation of Aniline and Its Derivatives under Reaction- and Encounter-Controlled Conditions. Industrial & Engineering Chemistry Research, 2004, 43, 2296-2301.	1.8	8
117	Photoisomerization of Methyl Vinyl Ketone and Methacrolein in the Troposphere: A Theoretical Investigation of Ground-State Reaction Pathways. ACS Earth and Space Chemistry, 2018, 2, 753-763.	1.2	8
118	Product detection study of the gas-phase oxidation of methylphenyl radicals using synchrotron photoionisation mass spectrometry. Physical Chemistry Chemical Physics, 2019, 21, 17939-17949.	1.3	8
119	Experimental and theoretical investigations into the mechanisms of haliranium ion Ï€-ligand exchange reactions with cyclic alkenes in the gas phase. Physical Chemistry Chemical Physics, 2021, 23, 25572-25589.	1.3	8
120	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108.	1.1	8
121	The gas phase aldoseâ€ketone isomerization mechanism: Direct interconversion of the model hydroxycarbonyls 2â€hydroxypropanal and hydroxyacetone. International Journal of Quantum Chemistry, 2017, 117, e25434.	1.0	7
122	Thermal decomposition kinetics of glyphosate (GP) and its metabolite aminomethylphosphonic acid (AMPA). Environmental Sciences: Processes and Impacts, 2020, 22, 152-160.	1.7	7
123	Thermal decomposition and isomerization of furfural and 2-pyrone: a theoretical kinetic study. Physical Chemistry Chemical Physics, 2021, 23, 2046-2054.	1.3	7
124	Bonding of Aqueous Citrate with Zn²⁺ and ZnO Nanoclusters: A Theoretical Study. ChemistrySelect, 2017, 2, 2055-2064.	0.7	6
125	A detailed chemical kinetic model for the supercritical water oxidation of methylamine: The importance of imine formation. International Journal of Chemical Kinetics, 2020, 52, 701-711.	1.0	6
126	Ab Initio Study of Bonding between Nucleophilic Species and the Nitroso Group. Journal of Physical Chemistry A, 2007, 111, 1300-1306.	1.1	5

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127	Using Distonic Radical Ions to Probe the Chemistry of Key Combustion Intermediates: The Case of the Benzoxyl Radical Anion. Journal of the American Society for Mass Spectrometry, 2013, 24, 493-501.	1.2	5
128	Unveiling New Isomers and Rearrangement Routes on the C₇H₈⁺ Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 823-830.	1.1	5
129	Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 2782-2790.	1.1	5
130	Barrierless Reactions of Three Benzonitrile Radical Cations with Ethylene. Australian Journal of Chemistry, 2020, 73, 705.	0.5	5
131	Electronic spectrum and photodissociation chemistry of the linear methyl propargyl cation H2C4H3+. Journal of Chemical Physics, 2017, 146, 044307.	1.2	4
132	Molecular Weight Growth in the Gas-Phase Reactions of Dehydroanilinium Radical Cations with Propene. Journal of Physical Chemistry A, 2019, 123, 8881-8892.	1.1	4
133	Kinetics of C5H4 isomerÂ+ÂH reactions and incorporation of C5H (xÂ=Â3 â€“ 5) chemistry into a detailed chemical kinetic model. Combustion and Flame, 2021, 227, 227-237.	2.8	4
134	Multiphoton dissociation dynamics of the indenyl radical at 248 nm and 193 nm. Journal of Chemical Physics, 2019, 151, 174303.	1.2	3
135	Electronic Spectrum and Photodissociation Chemistry of the 1-Butyn-3-yl Cation, H₃CCHCCH⁺. Journal of Physical Chemistry A, 2020, 124, 2366-2371.	1.1	3
136	Near-infrared reversible photoswitching of an isolated azobenzene-stilbene dye. Chemical Physics Letters, 2020, 741, 137065.	1.2	3
137	Evidence that Ï€â€ligand exchange reactions of chalcogen iranium ions proceed via HÃ¼ckel pseudocoarctate transition states. Journal of Physical Organic Chemistry, 2020, 33, e4111.	0.9	2
138	Auto-Oxidation of a Volatile Silicon Compound: A Theoretical Study of the Atmospheric Chemistry of Tetramethylsilane. Journal of Physical Chemistry A, 2020, 124, 6544-6551.	1.1	2
139	Toxic Chemical Formation during Vaping of Ethyl Ester Flavor Additives: A Chemical Kinetic Modeling Study. Chemical Research in Toxicology, 2022, 35, 522-528.	1.7	2
140	Mechanistic study of the reaction of CH2F2 with Cl atoms in the absence and presence of CH4 or C2H6: decomposition of CHF2OH and fate of the CHF2O radical. Physical Chemistry Chemical Physics, 2019, 21, 9376-9383.	1.3	1
141	Improved rate coefficient expressions for the reaction of methyl bromide with OH and Cl radicals. Chemical Physics Letters, 2018, 706, 371-374.	1.2	0
142	Selfâ€catalyzed ketoâ€enol tautomerization of malonic acid. International Journal of Quantum Chemistry, 2020, 120, e26114.	1.0	0
143	Pyrolysis of Triclosan and Its Chlorinated Derivatives. Journal of Physical Chemistry A, 2020, 124, 8050-8056.	1.1	0
144	Five vs. six membered-ring PAH products from reaction of o-methylphenyl radical and two C₃H₄ isomers. Physical Chemistry Chemical Physics, 2021, 23, 14913-14924.	1.3	0