Gabriel da Silva

List of Publications by Year
in descending order

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144 papers	5,489 citations	61984 43 h-index	106344 65 g-index
162 all docs	162 docs citations	162 times ranked	5172 citing authors

#	Article	IF	Citations
1	Toxic Chemical Formation during Vaping of Ethyl Ester Flavor Additives: A Chemical Kinetic Modeling Study. Chemical Research in Toxicology, 2022, 35, 522-528.	3.3	2
2	PAH Growth in Flames and Space: Formation of the Phenalenyl Radical. Journal of Physical Chemistry A, 2022, 126, 101-108.	2.5	8
3	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.	2.8	0
4	Isotope-specific reactions of acetonitrile (CH3CN) with trapped, translationally cold CCl+. Journal of Chemical Physics, 2021, 154, 074305.	3.0	13
5	Thermal Decomposition Kinetics of the Indenyl Radical: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 2782-2790.	2.5	5
6	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.	5.2	4
7	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
8	Thermal decomposition and isomerization of furfural and 2-pyrone: a theoretical kinetic study. Physical Chemistry Chemical Physics, 2021, 23, 2046-2054.	2.8	7
9	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.	2.8	8
10	Decomposition kinetics of perfluorinated sulfonic acids. Chemosphere, 2020, 238, 124615.	8.2	55
11	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.	2.8	9
12	Selfâ€catalyzed ketoâ€enol tautomerization of malonic acid. International Journal of Quantum Chemistry, 2020, 120, e26114.	2.0	0
13	Thermal decomposition kinetics of glyphosate (GP) and its metabolite aminomethylphosphonic acid (AMPA). Environmental Sciences: Processes and Impacts, 2020, 22, 152-160.	3.5	7
14	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.	1.9	2
15	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.	2.5	17
16	Pyrolysis of Triclosan and Its Chlorinated Derivatives. Journal of Physical Chemistry A, 2020, 124, 8050-8056.	2.5	0
17	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.	2.5	2
18	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.	1.6	6

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19	Electronic Spectrum and Photodissociation Chemistry of the 1-Butyn-3-yl Cation, H₃CCHCCH⁺. Journal of Physical Chemistry A, 2020, 124, 2366-2371.	2.5	3
20	Near-infrared reversible photoswitching of an isolated azobenzene-stilbene dye. Chemical Physics Letters, 2020, 741, 137065.	2.6	3
21	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
22	Barrierless Reactions of Three Benzonitrile Radical Cations with Ethylene. Australian Journal of Chemistry, 2020, 73, 705.	0.9	5
23	Reactions of Thiiranium and Sulfonium Ions with Alkenes in the Gas Phase. Journal of Organic Chemistry, 2019, 84, 10076-10087.	3.2	9
24	Product detection study of the gas-phase oxidation of methylphenyl radicals using synchrotron photoionisation mass spectrometry. Physical Chemistry Chemical Physics, 2019, 21, 17939-17949.	2.8	8
25	Molecular Weight Growth in the Gas-Phase Reactions of Dehydroanilinium Radical Cations with Propene. Journal of Physical Chemistry A, 2019, 123, 8881-8892.	2.5	4
26	Multiphoton dissociation dynamics of the indenyl radical at 248 nm and 193 nm. Journal of Chemical Physics, 2019, 151, 174303.	3.0	3
27	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.	2.5	9
28	Atmospheric Oxidation of Piperazine Initiated by OH: A Theoretical Kinetics Investigation. ACS Earth and Space Chemistry, 2019, 3, 2510-2516.	2.7	10
29	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.	1.6	9
30	Ultrafast photoisomerisation of an isolated retinoid. Physical Chemistry Chemical Physics, 2019, 21, 10567-10579.	2.8	12
31	Photoinitiated Intramolecular Proton Transfer in Deprotonated para-Coumaric Acid. Journal of Physical Chemistry A, 2019, 123, 4419-4430.	2.5	18
32	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.	2.8	1
33	Insights into the mechanochromism of spiropyran elastomers. Polymer Chemistry, 2019, 10, 1650-1659.	3.9	33
34	Unveiling New Isomers and Rearrangement Routes on the C₇H₈⁺ Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 823-830.	2.5	5
35	Photoswitching an Isolated Donorâ€“Acceptor Stenhouse Adduct. Journal of Physical Chemistry Letters, 2018, 9, 665-671.	4.6	46
36	Interconversion of Methyltropyl and Xylyl Radicals: A Pathway Unavailable to the Benzylâ€“Tropyl Rearrangement. Journal of Physical Chemistry A, 2018, 122, 1261-1269.	2.5	13

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37	Double Molecular Photoswitch Driven by Light and Collisions. Physical Review Letters, 2018, 120, 223002.	7.8	24
38	Improved rate coefficient expressions for the reaction of methyl bromide with OH and Cl radicals. Chemical Physics Letters, 2018, 706, 371-374.	2.6	0
39	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.	2.7	8
40	Bonding of Aqueous Citrate with Zn²⁺ and ZnO Nanoclusters: A Theoretical Study. ChemistrySelect, 2017, 2, 2055-2064.	1.5	6
41	Electronic spectrum and photodissociation chemistry of the linear methyl propargyl cation H2C4H3+. Journal of Chemical Physics, 2017, 146, 044307.	3.0	4
42	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.	2.5	29
43	Seleniranium Ions Undergo Ï€-Ligand Exchange via an Associative Mechanism in the Gas Phase. Journal of Organic Chemistry, 2017, 82, 6289-6297.	3.2	10
44	Modeling End-Gas Autoignition of Ethanol/Gasoline Surrogate Blends in the Cooperative Fuel Research Engine. Energy & Fuels, 2017, 31, 2378-2389.	5.1	40
45	Photoelectron Spectrum and Energetics of the meta-Xylylene Diradical. Journal of the American Chemical Society, 2017, 139, 14348-14351.	13.7	34
46	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.	2.0	7
47	Highly efficient gas-phase reactivity of protonated pyridine radicals with propene. Physical Chemistry Chemical Physics, 2017, 19, 31072-31084.	2.8	9
48	Gas-Phase Mechanisms of the Reactions of Reduced Organic Nitrogen Compounds with OH Radicals. Environmental Science & Technology, 2016, 50, 11723-11734.	10.0	41
49	Gas Phase Oxidation of Nicotine by OH Radicals: Kinetics, Mechanisms, and Formation of HNCO. Environmental Science and Technology Letters, 2016, 3, 327-331.	8.7	49
50	Decomposition of Pyruvic Acid on the Ground-State Potential Energy Surface. Journal of Physical Chemistry A, 2016, 120, 276-283.	2.5	26
51	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
52	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.	3.3	104
53	Radical Formation in the Gasâ€Phase Ozonolysis of Deprotonated Cysteine. Angewandte Chemie - International Edition, 2015, 54, 12947-12951.	13.8	9
54	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

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55	Carbonic anhydrase promoted absorption of CO₂ into potassium carbonate solutions. , 2015, 5, 108-114.		30
56	Are the three hydroxyphenyl radical isomers created equal? â€“ The role of the phenoxy radical â€“. Physical Chemistry Chemical Physics, 2015, 17, 30076-30083.	2.8	35
57	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
58	The autoignition of Liquefied Petroleum Gas (LPG) in spark-ignition engines. Proceedings of the Combustion Institute, 2015, 35, 2933-2940.	3.9	35
59	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
60	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.	13.8	12
61	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.	4.6	113
62	Demonstration of a Concentrated Potassium Carbonate Process for CO₂ Capture. Energy & Fuels, 2014, 28, 299-306.	5.1	58
63	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
64	Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical. Physical Chemistry Chemical Physics, 2014, 16, 24954-24964.	2.8	9
65	Atmospheric Chemistry of Enols: A Theoretical Study of the Vinyl Alcohol + OH + O₂ Reaction Mechanism. Environmental Science & Technology, 2014, 48, 6694-6701.	10.0	55
66	Use of Vanadium(V) Oxide as a Catalyst for CO₂ Hydration in Potassium Carbonate Systems. Industrial & Engineering Chemistry Research, 2014, 53, 3029-3039.	3.7	31
67	Direct versus Water-Mediated Protodecarboxylation of Acetic Acid Catalyzed by Group 10 Carboxylates, [(phen)M(O₂CCH₃)]⁺. Organometallics, 2014, 33, 5185-5197.	2.3	28
68	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
69	The octane numbers of ethanol blended with gasoline and its surrogates. Fuel, 2014, 115, 727-739.	6.4	238
70	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.	2.8	5
71	Hydroxyl radical formation in the gas phase oxidation of distonic 2-methylphenyl radical cations. Physical Chemistry Chemical Physics, 2013, 15, 20577.	2.8	16
72	G3X-K theory: A composite theoretical method for thermochemical kinetics. Chemical Physics Letters, 2013, 558, 109-113.	2.6	46

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73	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.	5.2	271
74	The Research and Motor octane numbers of Liquefied Petroleum Gas (LPG). Fuel, 2013, 108, 797-811.	6.4	80
75	On the Separation of Timescales in Chemically Activated Reactions. International Journal of Chemical Kinetics, 2013, 45, 387-396.	1.6	16
76	Formation of Nitrosamines and Alkyldiazohydroxides in the Gas Phase: The CH₃NH + NO Reaction Revisited. Environmental Science & Technology, 2013, 47, 7766-7772.	10.0	33
77	Amino Acids as Carbon Capture Solvents: Chemical Kinetics and Mechanism of the Glycine + CO₂ Reaction. Energy & Fuels, 2013, 27, 3898-3904.	5.1	101
78	Photoisomerization Action Spectroscopy of the Carbocyanine Dye DTC⁺ in the Gas Phase. Journal of Physical Chemistry A, 2013, 117, 13319-13325.	2.5	20
79	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.	4.6	56
80	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.	2.3	43
81	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
82	A detailed chemical kinetic model for pyrolysis of the lignin model compound chroman. AIMS Environmental Science, 2013, 1, 12-25.	1.4	9
83	A kinetic and process modeling study of CO2 capture with MEA-promoted potassium carbonate solutions. Chemical Engineering Journal, 2012, 210, 271-279.	12.7	82
84	Who Wins: Pesci, Peters, or Deacon? Intrinsic Reactivity Orders for Organocuprate Formation via Ligand Decomposition. Organometallics, 2012, 31, 1801-1807.	2.3	49
85	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
86	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.	2.6	80
87	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.	4.6	29
88	Reaction mechanism for the free-edge oxidation of soot by O2. Combustion and Flame, 2012, 159, 3423-3436.	5.2	93
89	Atmospheric Chemistry of 2-Aminoethanol (MEA): Reaction of the NH₂^{â€¢}CHCH₂OH Radical with O₂. Journal of Physical Chemistry A, 2012, 116, 10980-10986.	2.5	34
90	Kinetics of the benzyl + O(3P) reaction: a quantum chemical/statistical reaction rate theory study. Physical Chemistry Chemical Physics, 2012, 14, 16143.	2.8	12

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91	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.	2.5	61
92	Goldâ€Mediated Cï£¿I Bond Activation of Iodobenzene. Angewandte Chemie - International Edition, 2012, 51, 3812-3817.	13.8	90
93	Carbon dioxide absorption into unpromoted and borate-catalyzed potassium carbonate solutions. Chemical Engineering Journal, 2012, 181-182, 694-701.	12.7	66
94	Chemically activated reactions on the C7H5 energy surface: propargyl + diacetylene, i-C5H3 + acetylene, and n-C5H3 + acetylene. Physical Chemistry Chemical Physics, 2011, 13, 8940.	2.8	34
95	Reactions of simple and peptidic alpha-carboxylate radical anions with dioxygen in the gas phase. Physical Chemistry Chemical Physics, 2011, 13, 16314.	2.8	45
96	Reaction of the i-C₄H₅ (CH₂CCHCH₂) Radical with O₂. Journal of Physical Chemistry A, 2011, 115, 1018-1026.	2.5	14
97	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	2.8	17
98	Kinetics and Mechanism of the Glyoxal + HO₂Reaction: Conversion of HO₂to OH by Carbonyls. Journal of Physical Chemistry A, 2011, 115, 291-297.	2.5	23
99	Borate-Catalyzed Carbon Dioxide Hydration via the Carbonic Anhydrase Mechanism. Environmental Science & Technology, 2011, 45, 4802-4807.	10.0	77
100	Pyrolysis of fulvenallene (C7H6) and fulvenallenyl (C7H5): Theoretical kinetics and experimental product detection. Chemical Physics Letters, 2011, 517, 144-148.	2.6	40
101	Carboxylic Acid Catalyzed Ketoâ€Enol Tautomerizations in the Gas Phase. Angewandte Chemie - International Edition, 2010, 49, 7523-7525.	13.8	104
102	On the reactivity of methylbenzenes. Combustion and Flame, 2010, 157, 2175-2183.	5.2	37
103	Unimolecular Î²-Hydroxyperoxy Radical Decomposition with OH Recycling in the Photochemical Oxidation of Isoprene. Environmental Science & Technology, 2010, 44, 250-256.	10.0	122
104	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. Journal of Physical Chemistry A, 2010, 114, 6235-6249.	2.5	33
105	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
106	Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions. Journal of Physical Chemistry A, 2010, 114, 2275-2283.	2.5	57
107	Quantum Chemical Study of the Acrolein (CH₂CHCHO) + OH + O₂ Reactions. Journal of Physical Chemistry A, 2010, 114, 8302-8311.	2.5	63
108	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.	2.8	44

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109	Kinetic modeling of the benzyl+HO2 reaction. Proceedings of the Combustion Institute, 2009, 32, 287-294.	3.9	59
110	Thermal decomposition of pyrazole to vinylcarbene+N2: A first principles/RRKM study. Chemical Physics Letters, 2009, 474, 13-17.	2.6	26
111	Role of the Î±-hydroxyethylperoxy radical in the reactions of acetaldehyde and vinyl alcohol with HO2. Chemical Physics Letters, 2009, 483, 25-29.	2.6	43
112	Indene Formation from Alkylated Aromatics: Kinetics and Products of the Fulvenallene + Acetylene Reaction. Journal of Physical Chemistry A, 2009, 113, 8971-8978.	2.5	33
113	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.	2.5	78
114	Decomposition of Methylbenzyl Radicals in the Pyrolysis and Oxidation of Xylenes. Journal of Physical Chemistry A, 2009, 113, 10264-10278.	2.5	55
115	Benzoxyl Radical Decomposition Kinetics: Formation of Benzaldehyde + H, Phenyl + CH₂O, and Benzene + HCO. Journal of Physical Chemistry A, 2009, 113, 6979-6986.	2.5	50
116	Thermal Decomposition of the Benzyl Radical to Fulvenallene (C₇H₆) + H. Journal of Physical Chemistry A, 2009, 113, 6111-6120.	2.5	100
117	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.	5.3	85
118	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
119	Ethanol Oxidation: Kinetics of the Î±-Hydroxyethyl Radical + O₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 8923-8933.	2.5	118
120	Retro-[3 + 2]-Cycloaddition Reactions in the Decomposition of Five-Membered Nitrogen-Containing Heterocycles. Journal of Organic Chemistry, 2008, 73, 1343-1353.	3.2	40
121	Variational Analysis of the Phenyl + O₂ and Phenoxy + O Reactions. Journal of Physical Chemistry A, 2008, 112, 3566-3575.	2.5	82
122	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.	2.5	30
123	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.	2.5	77
124	Ab Initio Study of Bonding between Nucleophilic Species and the Nitroso Group. Journal of Physical Chemistry A, 2007, 111, 1300-1306.	2.5	5
125	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.	3.1	36
126	Elementary reaction step model of the Nâ€nitrosation of ammonia. International Journal of Chemical Kinetics, 2007, 39, 645-656.	1.6	18

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127	Nucleophilic reactivity of aniline derivatives towards the nitroso group. Journal of Physical Organic Chemistry, 2007, 20, 167-179.	1.9	15
128	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	2.5	14
129	Ab Initio Procedure for Aqueous-Phase pKa Calculation:â€‰ The Acidity of Nitrous Acid. Journal of Physical Chemistry A, 2006, 110, 11371-11376.	2.5	97
130	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.	2.5	93
131	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.	2.5	88
132	An experimental and theoretical study of the nitrosation of ammonia and thiourea. Chemical Engineering Science, 2006, 61, 3186-3197.	3.8	21
133	Bond dissociation energy of the phenol OH bond from ab initio calculations. Chemical Physics Letters, 2006, 424, 42-45.	2.6	66
134	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
135	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. ChemPhysChem, 2006, 7, 1119-1126.	2.1	53
136	Water-in-oil emulsion foaming by thiourea nitrosation: Reaction and mass transfer. AICHE Journal, 2006, 52, 1558-1565.	3.6	14
137	Effect of Added Nucleophilic Species on the Rate of Primary Amino Acid Nitrosation. Journal of the American Chemical Society, 2005, 127, 3664-3665.	13.7	29
138	Relative importance of diffusion and reaction control during the bacterial and ferric sulphate leaching of zinc sulphide. Hydrometallurgy, 2004, 73, 313-324.	4.3	46
139	Kinetics and mechanism of the bacterial and ferric sulphate oxidation of galena. Hydrometallurgy, 2004, 75, 99-110.	4.3	41
140	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.	3.7	8
141	Electrochemical passivation of sphalerite during bacterial oxidation in the presence of galena. Minerals Engineering, 2003, 16, 199-203.	4.3	46
142	Nucleophilic Catalysis of Nitrosation: Relationship between Nitrosating Agent Equilibrium Constant and Catalyst Nucleophilicity. Journal of Chemical Research, 2002, 2002, 589-590.	1.3	14
143	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
144	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