

Joseph Bozzelli

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9489939/publications.pdf>

Version: 2024-02-01

209
papers

7,184
citations

47006

47
h-index

79698

73
g-index

212
all docs

212
docs citations

212
times ranked

3773
citing authors

#	ARTICLE	IF	CITATIONS
1	THERM: Thermodynamic property estimation for gas phase radicals and molecules. International Journal of Chemical Kinetics, 1991, 23, 767-778.	1.6	460
2	O + NNH: A possible new route for NOX formation in flames. International Journal of Chemical Kinetics, 1995, 27, 1097-1109.	1.6	222
3	Hydrogen Atom Bond Increments for Calculation of Thermodynamic Properties of Hydrocarbon Radical Species. The Journal of Physical Chemistry, 1995, 99, 14514-14527.	2.9	160
4	Hydrocarbon radical reactions with oxygen: comparison of allyl, formyl, and vinyl to ethyl. The Journal of Physical Chemistry, 1993, 97, 4427-4441.	2.9	145
5	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels: Ethyl Propanoate and Methyl Butanoate. Journal of Physical Chemistry A, 2007, 111, 3727-3739.	2.5	145
6	Impact of SO2 and NO on CO oxidation under post-flame conditions. International Journal of Chemical Kinetics, 1996, 28, 773-790.	1.6	140
7	Detailed Kinetics and Thermochemistry of C2H5 + O2: Reaction Kinetics of the Chemically-Activated and Stabilized CH3CH2OO. Journal of Physical Chemistry A, 2002, 106, 7276-7293.	2.5	140
8	Ethanol Oxidation: Kinetics of the 1-Hydroxyethyl Radical + O2 Reaction. Journal of Physical Chemistry A, 2009, 113, 8923-8933.	2.5	118
9	Chemical activation analysis of the reaction of ethyl radical with oxygen. The Journal of Physical Chemistry, 1990, 94, 3313-3317.	2.9	107
10	Enthalpies of Formation and Group Additivity of Alkyl Peroxides and Trioxides. Journal of Physical Chemistry A, 1997, 101, 9505-9510.	2.5	105
11	Ab Initio Study of 1-Chlorinated Ethyl Hydroperoxides CH3CH2OOH, CH3CHClOOH, and CH3CCl2OOH: Conformational Analysis, Internal Rotation Barriers, Vibrational Frequencies, and Thermodynamic Properties. The Journal of Physical Chemistry, 1996, 100, 8240-8249.	2.9	104
12	Thermal Decomposition of the Benzyl Radical to Fulvenallene (C7H6) + H. Journal of Physical Chemistry A, 2009, 113, 6111-6120.	2.5	100
13	Detailed Kinetic Study of the Growth of Small Polycyclic Aromatic Hydrocarbons. 1. 1-Naphthyl + Ethyne. Journal of Physical Chemistry A, 2001, 105, 1561-1573.	2.5	97
14	Enthalpies of Formation, Bond Dissociation Energies, and Molecular Structures of Alkyl Aldehydes (Acetaldehyde, Propanal, Butanal, Pentanal, Hexanal, and Heptanal) and Their Radicals. Journal of Physical Chemistry A, 2006, 110, 13058-13067.	2.5	93
15	Thermochemical and Kinetic Analysis of the H, OH, HO2, O, and O2 Association Reactions with Cyclopentadienyl Radical. Journal of Physical Chemistry A, 1998, 102, 3537-3555.	2.5	91
16	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
17	Oxidation of the Benzyl Radical: Mechanism, Thermochemistry, and Kinetics for the Reactions of Benzyl Hydroperoxide. Journal of Chemical Theory and Computation, 2009, 9, 3185-3194.	5.3	85
18	CHEMFACT: A Computer Code to Estimate Rate Constants for Chemically-Activated Reactions. Combustion Science and Technology, 1991, 80, 63-85.	2.3	84

#	ARTICLE	IF	CITATIONS
19	Thermal reactions of CH ₂ Cl ₂ in H ₂ /O ₂ mixtures: Implications for chlorine inhibition of CO conversion to CO ₂ . Combustion and Flame, 1992, 88, 265-295.	5.2	82
20	Variational Analysis of the Phenyl + O ₂ and Phenoxy + O Reactions. Journal of Physical Chemistry A, 2008, 112, 3566-3575.	2.5	82
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	Kinetics and Thermochemistry for the Gas-Phase Keto-Enol Tautomerism of Phenol at 2,4-Cyclohexadienone. Journal of Physical Chemistry A, 2003, 107, 3696-3703.	2.5	70
24	Kinetic Study on Pyrolysis and Oxidation of CH ₃ Cl in Ar/H ₂ /O ₂ Mixtures. Combustion Science and Technology, 1992, 85, 23-63.	2.3	66
25	Bond dissociation energy of the phenol OH bond from ab initio calculations. Chemical Physics Letters, 2006, 424, 42-45.	2.6	66
26	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
27	Molecular density of states from estimated vapor phase heat capacities. International Journal of Chemical Kinetics, 1997, 29, 161-170.	1.6	62
28	Analysis of Tertiary Butyl Radical + O ₂ , Isobutene + HO ₂ , Isobutene + OH, and Isobutene + OH Adducts + O ₂ : A Detailed Tertiary Butyl Oxidation Mechanism. Journal of Physical Chemistry A, 1999, 103, 9731-9769.	2.5	62
29	Kinetic Analysis for HO ₂ Addition to Ethylene, Propene, and Isobutene, and Thermochemical Parameters of Alkyl Hydroperoxides and Hydroperoxide Alkyl Radicals. Journal of Physical Chemistry A, 2000, 104, 4997-5012.	2.5	62
30	Elementary Reaction Mechanism for Benzene Oxidation in Supercritical Water. Journal of Physical Chemistry A, 2000, 104, 10576-10586.	2.5	61
31	Structures, thermochemical properties (enthalpy, entropy and heat capacity), rotation barriers, and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxides Electronic supplementary information (ESI) available. Structures, geometry parameters, thermochemical properties, rotation barriers and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b1/b111303h/ Presented at the Bunsen Discussion on Formation and Degradation of Hydrocarbons I. Physical Chemistry Chemical Physics, 2002, 4, 3691-3703.	2.8	60
32	Thermochemical Properties, Rotation Barriers, Bond Energies, and Group Additivity for Vinyl, Phenyl, Ethynyl, and Allyl Peroxides. Journal of Physical Chemistry A, 2004, 108, 8353-8366.	2.5	60
33	Kinetic modeling of the benzyl+HO ₂ reaction. Proceedings of the Combustion Institute, 2009, 32, 287-294.	3.9	59
34	Thermochemical Property, Pathway and Kinetic Analysis on the Reactions of Allylic Isobutenyl Radical with O ₂ : an Elementary Reaction Mechanism for Isobutene Oxidation. Journal of Physical Chemistry A, 2000, 104, 9715-9732.	2.5	58
35	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
36	Thermochemical Properties, $\Delta H^\circ(298)$, $\Delta S^\circ(298)$, and $C_p(T)$, for n-Butyl and n-Pentyl Hydroperoxides and the Alkyl and Peroxy Radicals, Transition States, and Kinetics for Intramolecular Hydrogen Shift Reactions of the Peroxy Radicals. Journal of Physical Chemistry A, 2007, 111, 6361-6377.	2.5	58

#	ARTICLE	IF	CITATIONS
37	Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions. Journal of Physical Chemistry A, 2010, 114, 2275-2283.	2.5	57
38	Decomposition of Methylbenzyl Radicals in the Pyrolysis and Oxidation of Xylenes. Journal of Physical Chemistry A, 2009, 113, 10264-10278.	2.5	55
39	Thermochemistry, Reaction Paths, and Kinetics on the Hydroperoxy-Ethyl Radical Reaction with O ₂ : New Chain Branching Reactions in Hydrocarbon Oxidation. Journal of Physical Chemistry A, 2002, 106, 1113-1121.	2.5	54
40	Thermochemical and Kinetic Analysis of the Formyl Methyl Radical + O ₂ Reaction System. Journal of Physical Chemistry A, 2003, 107, 3778-3791.	2.5	53
41	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. ChemPhysChem, 2006, 7, 1119-1126.	2.1	53
42	CATALYTIC HYDRODECHLORINATION OF 1,2-DICHLOROETHANE AND TRICHLOROETHYLENE OVER Rh/SiO ₂ CATALYSTS. Chemical Engineering Communications, 1992, 115, 1-11.	2.6	52
43	Ab Initio Calculations and Internal Rotor: Contribution for Thermodynamic Properties S [°] ₂₉₈ and Cp(T)'s (300 < T/K < 1500): Group Additivity for Fluoroethanes. Journal of Physical Chemistry A, 1998, 102, 7286-7293.	2.5	52
44	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	2.5	52
45	Thermochemical and Kinetic Analysis on the Reactions of Neopentyl and Hydroperoxy-Neopentyl Radicals with Oxygen: Part I. OH and Initial Stable HC Product Formation. Journal of Physical Chemistry A, 2004, 108, 1694-1711.	2.5	50
46	Benzoyl Radical Decomposition Kinetics: Formation of Benzaldehyde + H, Phenyl + CH ₂ O, and Benzene + HCO. Journal of Physical Chemistry A, 2009, 113, 6979-6986.	2.5	50
47	Kinetic and Thermodynamic Analysis on OH Addition to Ethylene: Adduct Formation, Isomerization, and Isomer Dissociations. Journal of Physical Chemistry A, 1999, 103, 7646-7655.	2.5	49
48	Thermochemical and Kinetic Analysis of the Acetyl Radical (CH ₃ C=O) + O ₂ Reaction System. Journal of Physical Chemistry A, 2002, 106, 7155-7170.	2.5	49
49	Thermochemical Properties, Pathway, and Kinetic Analysis on the Reactions of Benzene with OH: An Elementary Reaction Mechanism. Journal of Physical Chemistry A, 2004, 108, 4632-4652.	2.5	49
50	Formation of a Criegee intermediate in the low-temperature oxidation of dimethyl sulfoxide. Physical Chemistry Chemical Physics, 2008, 10, 1769.	2.8	49
51	Chain Branching and Termination in the Low-Temperature Combustion of <i>n</i> -Alkanes: 2-Pentyl Radical + O ₂ , Isomerization and Association of the Second O ₂ . Journal of Physical Chemistry A, 2010, 114, 7693-7708.	2.5	49
52	Chloroform Pyrolysis: Experiment and Detailed Reaction Model. Combustion Science and Technology, 1992, 85, 345-373.	2.3	47
53	Correlations between lead and coronene concentrations at urban, suburban, and industrial sites in New Jersey. Environmental Science & Technology, 1981, 15, 566-570.	10.0	46
54	Thermochemical and Kinetic Analysis on the Reactions of O ₂ with Products from OH Addition to Isobutene, 2-Hydroxy-1,1-dimethylethyl, and 2-Hydroxy-2-methylpropyl Radicals: HO ₂ Formation from Oxidation of Neopentane, Part II. Journal of Physical Chemistry A, 2007, 111, 4974-4986.	2.5	46

#	ARTICLE	IF	CITATIONS
55	Thermochemistry and Bond Dissociation Energies of Ketones. Journal of Physical Chemistry A, 2012, 116, 5707-5722.	2.5	45
56	Time-integrated pointers for enabling the analysis of detailed reaction mechanisms. AIChE Journal, 2004, 50, 2956-2970.	3.6	44
57	Thermochemistry of Methyl and Ethyl Nitro, RNO ₂ , and Nitrite, RONO, Organic Compounds. Journal of Physical Chemistry A, 2008, 112, 3172-3185.	2.5	44
58	Thermochemistry of C ₇ H ₁₆ to C ₁₀ H ₂₂ Alkane Isomers: Primary, Secondary, and Tertiary C-H Bond Dissociation Energies and Effects of Branching. Journal of Physical Chemistry A, 2014, 118, 9364-9379.	2.5	44
59	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Radicals Derived from H Atom Loss in Mono-, Di-, and Trichloromethanol and Parent Chloromethanols. Journal of Physical Chemistry A, 2001, 105, 4504-4516.	2.5	43
60	Role of the $\dot{\text{I}}\text{-hydroxyethylperoxy}$ radical in the reactions of acetaldehyde and vinyl alcohol with HO ₂ . Chemical Physics Letters, 2009, 483, 25-29.	2.6	43
61	Thermodynamic Parameters and Group Additivity Ring Corrections for Three- to Six-Membered Oxygen Heterocyclic Hydrocarbons. Journal of Physical Chemistry A, 1997, 101, 2471-2477.	2.5	42
62	Thermochemical Properties of <i>exo</i> -Tricyclo[5.2.1.0 ^{2,6}]decane (JP-10 Jet Fuel) and Derived Tricyclodecyl Radicals. Journal of Physical Chemistry A, 2010, 114, 9545-9553.	2.5	42
63	Mercury Oxidation via Chlorine, Bromine, and Iodine under Atmospheric Conditions: Thermochemistry and Kinetics. Journal of Physical Chemistry A, 2014, 118, 2959-2975.	2.5	41
64	Development of a detailed high-pressure reaction model for methane/methanol mixtures under pyrolytic and oxidative conditions and comparison with experimental data. Fuel Processing Technology, 2003, 83, 111-145.	7.2	40
65	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Methyl Ethyl, Methyl Isopropyl, and Methyl <i>tert</i> -Butyl Ethers and the Corresponding Radicals. Journal of Physical Chemistry A, 2003, 107, 4531-4546.	2.5	40
66	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
67	Reaction of H + ketene to formyl methyl and acetyl radicals and reverse dissociations. International Journal of Chemical Kinetics, 2003, 35, 20-44.	1.6	37
68	Thermochemical Properties, Rotation Barriers, and Group Additivity for Unsaturated Oxygenated Hydrocarbons and Radicals Resulting from Reaction of Vinyl and Phenyl Radical Systems with O ₂ . Journal of Physical Chemistry A, 2005, 109, 2233-2253.	2.5	37
69	On the reactivity of methylbenzenes. Combustion and Flame, 2010, 157, 2175-2183.	5.2	37
70	Structures, Intramolecular Rotation Barriers, and Thermodynamic Properties (Enthalpies, Entropies) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Journal of Physical Chemistry A, 2000, 104, 8270-8282.	2.5	36
71	Theoretical Study of the Oxidation Catalyst N-Hydroxyphthalimide (NHPI): $\hat{\alpha}\%$ 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
72	Thermochemical and kinetic analysis on the addition reactions of H, O, OH, and HO ₂ with 1,3 cyclopentadiene. International Journal of Chemical Kinetics, 1997, 29, 893-913.	1.6	35

#	ARTICLE	IF	CITATIONS
73	Formation of Chlorinated Aromatics by Reactions of Cl•, Cl ₂ , and HCl with Benzene in the Cool-Down Zone of a Combustor. <i>Environmental Science & Technology</i> , 2003, 37, 1684-1689.	10.0	35
74	Thermochemistry for enthalpies and reaction paths of nitrous acid isomers. <i>International Journal of Chemical Kinetics</i> , 2007, 39, 378-398.	1.6	35
75	Measurement of Selected Volatile Organic Compounds at Three Locations in New Jersey during the Summer Season. <i>Journal of the Air Pollution Control Association</i> , 1983, 33, 1177-1183.	0.5	34
76	Conversion of chloroform to hydrochloric acid by reaction with hydrogen and water vapor. <i>Environmental Science & Technology</i> , 1986, 20, 568-574.	10.0	34
77	Presence of Chlorine Radicals and Formation of Molecular Chlorine in the Post-Flame Region of Chlorocarbon Combustion. <i>Environmental Science & Technology</i> , 2000, 34, 4565-4570.	10.0	34
78	Molecular Products and Fundamentally Based Reaction Pathways in the Gas-Phase Pyrolysis of the Lignin Model Compound <i>p</i> -Coumaryl Alcohol. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3352-3371.	2.5	34
79	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O ₂ reaction system. <i>International Journal of Chemical Kinetics</i> , 2000, 32, 435-452.	1.6	33
80	Kinetics of the Multichannel Reaction of Methanethiyl Radical (CH ₃ S•) with SO ₂ . <i>Journal of Physical Chemistry A</i> , 2006, 110, 6923-6937.	2.5	33
81	Thermodynamic properties of the species resulting from the phenyl radical with O ₂ reaction system. <i>International Journal of Chemical Kinetics</i> , 2008, 40, 583-604.	1.6	33
82	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
83	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6235-6249.	2.5	33
84	Thermodynamic Properties (H ^o (298), S(298), and Cp(T) (300 ≤ T ≤ 1500)) of Fluorinated Propanes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 5602-5610.	2.5	32
85	Standard Chemical Thermodynamic Properties of Multichloro Alkanes and Alkenes: A Modified Group Additivity Scheme. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4551-4558.	2.5	31
86	The multi-channel reaction of CH ₃ S + SO ₂ : Thermochemistry and kinetic barriers. <i>Computational and Theoretical Chemistry</i> , 2005, 728, 147-157.	1.5	30
87	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
88	Thermochemical Properties Enthalpy, Entropy, and Heat Capacity of C ₁ –C ₄ Fluorinated Hydrocarbons: Fluorocarbon Group Additivity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 8202-8215.	2.5	30
89	Hydroxyl Radical Initiated Oxidation of <i>s</i> -Triazine: Hydrogen Abstraction Is Faster than Hydroxyl Addition. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8596-8606.	2.5	28
90	Kinetic Study of Di- <i>t</i> -Butyl Peroxide: Thermal Decomposition and Product Reaction Pathways. <i>International Journal of Chemical Kinetics</i> , 2015, 47, 133-161.	1.6	27

#	ARTICLE	IF	CITATIONS
91	Soil and Water Decontamination by Extraction with Surfactants. Separation Science and Technology, 1993, 28, 793-804.	2.5	26
92	Thermochemistry and Kinetics for 2-Butanone-3-yl Radical ($\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3$) Reactions with O_2 . Zeitschrift Fur Physikalische Chemie, 2011, 225, 993-1018.	2.8	26
93	Thermochemistry and Kinetics for 2-Butanone-1-yl Radical ($\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3$) Reactions with O_2 . Journal of Physical Chemistry A, 2014, 118, 21-37.	2.5	26
94	Pathways to Chlorinated Dibenzodioxins and Dibenzofurans from Partial Oxidation of Chlorinated Aromatics by OH Radical: Thermodynamic and Kinetic Insights. Combustion Science and Technology, 1994, 101, 153-169.	2.3	25
95	Structures, Rotational Barriers, Thermochemical Properties, and Additivity Groups for 2-Propanol, 2-Chloro-2-propanol and the Corresponding Alkoxy and Hydroxyalkyl Radicals. Journal of Physical Chemistry A, 2002, 106, 3947-3956.	2.5	25
96	Thermochemistry, Reaction Paths, and Kinetics on the <i>tert</i> -Isooctane Radical Reaction with O_2 . Journal of Physical Chemistry A, 2014, 118, 4631-4646.	2.5	25
97	Volatile organic compounds at hazardous waste sites and a sanitary landfill in New Jersey. Environmental Progress, 1986, 5, 18-27.	0.7	24
98	Vibrational relaxation of highly excited diatomics. I. Method, analysis, and application to $\text{HCl}(v=7)+\text{CO}_2$ and N_2O . Journal of Chemical Physics, 1982, 76, 2972-2983.	3.0	23
99	Structures, Rotation Barrier, and Thermodynamic Properties $\hat{H}^\circ(298)$, $S^\circ(298)$, and $C_p(T)$ of Chloromethyl Hypochlorites CH_3OCl , CH_2ClOCl , CHCl_2OCl , and CCl_3OCl . Journal of Physical Chemistry A, 2000, 104, 9581-9590.	2.5	23
100	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties: \hat{H}° Ethanol, \hat{H}° -Monoethanols, Dichloroethanols, and Corresponding Radicals Derived from H Atom Loss. Journal of Physical Chemistry A, 2001, 105, 9543-9552.	2.5	23
101	Reactions of water vapor or molecular hydrogen with trichloroethylene in a microwave plasma reactor. Plasma Chemistry and Plasma Processing, 1988, 8, 293-314.	2.4	22
102	Thermochemical Properties ($\hat{H}^\circ(298\text{ K})$, $S^\circ(298\text{ K})$, $C_p(T)$) and Bond Dissociation Energies for C_1 - C_4 Normal Hydroperoxides and Peroxy Radicals. Journal of Chemical & Engineering Data, 2016, 61, 1836-1849.	1.9	22
103	Reactions of Chlorinated Benzenes in H_2 and in H_2/O_2 Mixtures: Thermodynamic Implications on Pathways to Dioxin. Combustion Science and Technology, 1990, 74, 117-135.	2.3	21
104	Chlorocarbon-Induced Incomplete Combustion In A Jet-Stirred Reactor. Combustion Science and Technology, 1992, 85, 87-100.	2.3	21
105	An experimental and numerical study of the high-temperature oxidation of 1,1,1- $\text{C}_2\text{H}_3\text{Cl}_3$. Combustion and Flame, 1994, 98, 155-169.	5.2	21
106	Reaction of OH Radical with $\text{C}_2\text{H}_3\text{Cl}$: Rate Constant and Reaction Pathway Analysis. Journal of Physical Chemistry A, 1999, 103, 7800-7810.	2.5	20
107	Structures, Rotational Barriers, and Thermodynamic Properties of C_2 Vinyl and Chlorovinyl Alcohols and Additivity Groups. Journal of Physical Chemistry A, 2000, 104, 9197-9206.	2.5	20
108	Thermochemical Properties for Isooctane and Carbon Radicals: Computational Study. Journal of Physical Chemistry A, 2013, 117, 421-429.	2.5	20

#	ARTICLE	IF	CITATIONS
109	Thermochemical Properties and Bond Dissociation Enthalpies of 3- to 5-Member Ring Cyclic Ether Hydroperoxides, Alcohols, and Peroxy Radicals: Cyclic Ether Radical + 3O ₂ Reaction Thermochemistry. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3147-3167.	2.5	20
110	Enthalpy of formation and bond energies on unsaturated oxygenated hydrocarbons using G3MP2B3 calculation methods. <i>International Journal of Chemical Kinetics</i> , 2005, 37, 633-648.	1.6	19
111	Thermochemistry and kinetics of acetonylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7139.	2.8	19
112	Thermochemistry and Reaction Paths in the Oxidation Reaction of Benzoyl Radical: C ₆ H ₅ C [•] . <i>Journal of Physical Chemistry A</i> , 2011, 115, 11897-11914.	2.5	19
113	Thermochemical Properties of Methyl-Substituted Cyclic Alkyl Ethers and Radicals for Oxiranes, Oxetanes, and Oxolanes: C-H Bond Dissociation Enthalpy Trends with Ring Size and Ether Site. <i>Journal of Physical Chemistry A</i> , 2013, 117, 378-392.	2.5	19
114	Gas Phase Mercury Oxidation by Halogens (Cl, Br, I) in Combustion Effluents: Influence of Operating Conditions. <i>Energy & Fuels</i> , 2016, 30, 603-615.	5.1	19
115	Thermochemistry of Hydroxyl and Hydroperoxide Substituted Furan, Methylfuran, and Methoxyfuran. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4523-4544.	2.5	19
116	Monitoring volatile organic compounds at hazardous and sanitary landfills in New Jersey. <i>Journal of Environmental Science and Health Part A, Environmental Science and Engineering</i> , 1985, 20, 491-501.	0.1	18
117	Reaction of chlorocarbons to hydrochloric acid and hydrocarbons in a hydrogen-rich microwave induced plasma reactor. <i>Environmental Science & Technology</i> , 1989, 23, 666-671.	10.0	18
118	Thermodynamic Properties, $\Delta_f H^\circ(298.15 \text{ K})$, $\Delta_f S^\circ(298.15 \text{ K})$, and $\Delta_f G^\circ(T)$, of 2-Fluoro-2-Methylpropane, Fluorinated Ethanes, and Group Additivity for Fluoroalkanes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 7373-7379.	2.5	18
119	Comparison of selected volatile organic compounds during the summer and winter at urban sites in New Jersey. <i>Science of the Total Environment</i> , 1984, 38, 259-274.	8.0	17
120	Chemical makeup and physical characterization of a synthetic fuel and methods of heat content evaluation for studies on MSW incineration. <i>Fuel</i> , 2002, 81, 211-217.	6.4	17
121	Thermochemical Properties, $\Delta_f H^\circ(298.15 \text{ K})$, $\Delta_f S^\circ(298.15 \text{ K})$, and $\Delta_f G^\circ(T)$, of 1,4-Dioxin, 2,3-Benzodioxin, Furan, 2,3-Benzofuran, and Twelve Monochloro and Dichloro Dibenzo-p-dioxins and Dibenzofurans. <i>Journal of Physical and Chemical Reference Data</i> , 2003, 32, 1713-1735.	4.2	17
122	Thermochemical Similarities Among Three Reaction Systems: Vinyl + O ₂ Phenyl + O ₂ Dibenzofuranyl + O ₂ . <i>Combustion Science and Technology</i> , 2008, 180, 959-974.	2.3	17
123	Structures, Rotational Barriers, and Thermochemical Properties of Chlorinated Aldehydes and the Corresponding Acetyl (CCO) and Formyl Methyl Radicals (COCO) and Additivity Groups. <i>Journal of Physical Chemistry A</i> , 2002, 106, 345-355.	2.5	16
124	Structure and Thermochemical Properties of 2-Methoxyfuran, 3-Methoxyfuran, and Their Carbon-Centered Radicals Using Computational Chemistry. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7984-7995.	2.5	16
125	Dihydrogen Catalysis: A Degradation Mechanism for N ₂ -Fixation Intermediates. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11618-11642.	2.5	16
126	Simulation of a Three-Stage Chlorocarbon Incinerator through the Use of a Detailed Reaction Mechanism: Chlorine to Hydrogen Mole Ratios below 0.15. <i>Environmental Science & Technology</i> , 1995, 29, 3059-3063.	10.0	15

#	ARTICLE	IF	CITATIONS
127	Bond Energies and Thermochemical Properties of Ring-Opened Diradicals and Carbenes of <i>exo</i> -Tricyclo[5.2.1.0 ^{2,6}]decane. Journal of Physical Chemistry A, 2015, 119, 9857-9878.	2.5	15
128	Analysis and Optimization of Chlorocarbon Incineration through Use of a Detailed Reaction Mechanism. Industrial & Engineering Chemistry Research, 1995, 34, 4185-4192.	3.7	14
129	Polymer Pyrolysis and Oxidation Studies in a Continuous Feed and Flow Reactor: Cellulose and Polystyrene. Environmental Science & Technology, 1999, 33, 2584-2592.	10.0	14
130	Kinetics and mechanism for the thermal chlorination of chloroform in the gas phase: Inclusion of HCl elimination from CHCl ₃ . International Journal of Chemical Kinetics, 2003, 35, 647-660.	1.6	14
131	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	2.5	14
132	Reaction of the <i>i</i> -C ₄ H ₅ (CH ₂ CCHCH ₂) Radical with O ₂ . Journal of Physical Chemistry A, 2011, 115, 1018-1026.	2.5	14
133	OH-Initiated Reactions of <i>p</i> -Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part I. Potential Energy Surface Analysis. Journal of Physical Chemistry A, 2019, 123, 2570-2585.	2.5	14
134	Airborne asbestos levels in several school buildings before and after bulk asbestos removal. International Journal of Environmental Studies, 1982, 20, 27-30.	1.6	13
135	Enthalpies of formation of cyclic alkyl peroxides: dioxirane, 1,2-dioxetane, 1,2-dioxolane, and 1,2-dioxane. Chemical Physics Letters, 1997, 268, 175-179.	2.6	13
136	Pyrolysis and Oxidation of Cellulose in a Continuous-Feed and -Flow Reactor: Effects of NaCl. Industrial & Engineering Chemistry Research, 2002, 41, 3526-3539.	3.7	13
137	Thermodynamic properties (S ₂₉₈ , Cp(T), internal rotations and group additivity parameters) in vinyl and phenyl hydroperoxides Electronic supplementary information (ESI) available: Internal rotation barriers, Fourier expansion coefficients for internal rotation potentials for vinyl and phenyl hydroperoxides. See http://www.rsc.org/suppdata/cp/b2/b207030h/ . Physical Chemistry Chemical Physics, 2003, 5, 300-307.	2.8	13
138	Thermochemistry of oxabicycloheptenes: enthalpy of formation, entropy and heat capacity. Journal of Physical Organic Chemistry, 2006, 19, 93-103.	1.9	13
139	Thermochemical Properties and Bond Dissociation Energies of C ₃ -C ₅ Cycloalkyl Hydroperoxides and Peroxy Radicals: Cycloalkyl Radical + 3O ₂ Reaction Thermochemistry. Journal of Physical Chemistry A, 2012, 116, 7550-7563.	2.5	13
140	Propagation of uncertainty in chemically activated systems. AIChE Journal, 2006, 52, 3246-3256.	3.6	12
141	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
142	Thermochemistry and Kinetic Analysis of the Unimolecular Oxiranyl Radical Dissociation Reaction: A Theoretical Study. ChemPhysChem, 2016, 17, 1983-1992.	2.1	12
143	Cyclopentadienone Oxidation Reaction Kinetics and Thermochemistry for the Alcohols, Hydroperoxides, and Vinylic, Alkoxy, and Alkylperoxy Radicals. Journal of Physical Chemistry A, 2016, 120, 433-451.	2.5	12
144	Thermochemical Properties: Enthalpy, Entropy, and Heat Capacity of C ₂ -C ₃ Fluorinated Aldehydes. Radicals and Fluorocarbon Group Additivity. Journal of Physical Chemistry A, 2019, 123, 650-665.	2.5	12

#	ARTICLE	IF	CITATIONS
145	Thermal Reactions of Methylene Chloride in Methane/Argon Mixtures. Combustion Science and Technology, 1994, 101, 135-152.	2.3	11
146	Thermodynamic properties of chloroacetylene, dichloroacetylene, ethynyl radical, and chloroethynyl radical. Chemical Physics Letters, 2002, 362, 445-452.	2.6	11
147	Structures, Rotational Barriers, and Thermochemical Properties of $\hat{1}^2$ -Chlorinated Ethyl Hydroperoxides. Journal of Physical Chemistry A, 2003, 107, 1018-1024.	2.5	11
148	Thermodynamic and kinetic analysis on the reaction of dimethyl sulfide radical with oxygen. International Journal of Quantum Chemistry, 2012, 112, 1945-1958.	2.0	11
149	Thermochemistry, bond energies and internal rotor barriers of methyl sulfinic acid, methyl sulfinic acid ester and their radicals. Journal of Physical Organic Chemistry, 2011, 24, 366-377.	1.9	10
150	Di-tertiary-butyl Peroxide Decomposition and Combustion with Air: Reaction Mechanism, Ignition, Flame Structures, and Laminar Flame Velocities. Energy & Fuels, 2017, 31, 2260-2273.	5.1	10
151	Kinetic parameters for coupled bulk and wall reactions in a tubular flow reactor. AIChE Journal, 1987, 33, 1207-1211.	3.6	9
152	Computational study on structures, thermochemical properties, and bond energies of disulfide oxygen ($\hat{S}^{\bullet}-\hat{S}^{\bullet}(O)$)-bridged CH_3SSOH and $CH_3SS(=O)H$ and radicals. Journal of Physical Organic Chemistry, 2012, 25, 475-485.	1.9	9
153	Removal of Cr(VI) from Chromium Contaminated Sites by Washing with Hot Water. Hazardous Waste and Hazardous Materials, 1994, 11, 511-517.	0.4	8
154	ab initio molecular orbital and density functional analysis of acetylene + O ₂ reactions with CHEMKIN evaluation. International Journal of Chemical Kinetics, 2000, 32, 623-641.	1.6	8
155	Structure, Torsional Potentials, and Thermochemical Properties $\hat{1}^2$ H $\hat{A}^{\bullet}f_{298}$, $S\hat{A}^{\bullet}298$, and $Cp(T)$ of Chloro-Dimethyl Ethers: \hat{A} CH ₂ ClOCH ₃ , CHCl ₂ OCH ₃ , and CCl ₃ OCH ₃ . Density Functional and ab Initio Calculations. Journal of Physical Chemistry A, 2001, 105, 5420-5430.	2.5	8
156	Cl ₂ molecular elimination reaction from 1,2-dichloroethane. Chemical Physics Letters, 2002, 357, 65-72.	2.6	8
157	Thermochemistry, Reaction Paths, and Kinetics on the Secondary Isooctane Radical Reaction with 3 O ₂ . International Journal of Chemical Kinetics, 2014, 46, 71-103.	1.6	8
158	S ₂ + Air Combustion: Reaction Kinetics, Flame Structure, and Laminar Flame Behavior. Energy & Fuels, 2018, 32, 10184-10193.	5.1	8
159	Reaction between atomic fluorine and CF ₃ Br: Evidence for a pseudotrihalogen radical intermediate. Journal of Chemical Physics, 1973, 59, 3669-3675.	3.0	7
160	Analysis of selected volatile organic compounds associated with residential kerosene heater use. International Journal of Environmental Studies, 1995, 49, 125-131.	1.6	7
161	Study of Volatile Organic Compounds Destruction by Dielectric Barrier Corona Discharge. Journal of Advanced Oxidation Technologies, 1997, 2, .	0.5	7
162	Comparison of AM1 and PM3 in MOPAC6 with Literature for the Thermodynamic Parameters of C1 and C2 Chlorocarbons. Industrial & Engineering Chemistry Research, 1998, 37, 3497-3507.	3.7	7

#	ARTICLE	IF	CITATIONS
163	Theoretical Investigation on Stability of the CÂ-H2OCl Radical. Journal of Physical Chemistry A, 2001, 105, 3941-3946.	2.5	7
164	Structure, Intramolecular Rotation Barrier, and Thermochemical Properties of Hydroxycyclohexadienyl Radical. Journal of Physical Chemistry A, 2003, 107, 6451-6456.	2.5	7
165	Thermochemical properties for <i>n</i> -propyl, <i>iso</i> -propyl, and <i>tert</i> -butyl nitroalkanes, alkyl nitrites, and their carbon-centered radicals. International Journal of Chemical Kinetics, 2010, 42, 181-199.	1.6	7
166	Structures, Internal Rotor Potentials, and Thermochemical Properties for a Series of Nitrocarbonyls, Nitroolefins, Corresponding Nitrites, and Their Carbon Centered Radicals. Journal of Physical Chemistry A, 2011, 115, 13921-13930.	2.5	7
167	Calculated Entropies for n-Heptane, 2-Methylhexane, 2,3-Dimethylpentane, and Radicals from the Loss of H Atoms. Advances in Physical Chemistry, 2013, 2013, 1-7.	2.0	7
168	Thermochemical Properties and Bond Dissociation Energies for Fluorinated Methanol, CH ₃ CF ₂ OH, and Fluorinated Methyl Hydroperoxides, CH ₃ CF ₂ OOH: Group Additivity. Journal of Physical Chemistry A, 2016, 120, 6998-7010.	2.5	7
169	Thermodynamics of OHgX, XHgOH, XHgOCl, XHgOBr, and HOHgY Gaseous Oxidized Mercury Molecules from Isodesmic, Isogyric, and Atomization Work Reactions (X = Halogen, Y = OH, OCl, OBr). Journal of Physical Chemistry A, 2019, 123, 4452-4464.	2.5	7
170	Thermochemistry and kinetics of the 2-butanone + O ₂ reaction system. International Journal of Chemical Kinetics, 2019, 51, 541-562.	1.6	7
171	ab initio calculations and thermochemical analysis on C1 atom abstractions of chlorine from chlorocarbons and the reverse alkyl abstractions: Cl ₂ + R ₁ · → R ₁ Cl + Cl·. International Journal of Chemical Kinetics, 2000, 32, 548-565.	1.6	6
172	Terahertz study of trichloroanisole by time-domain spectroscopy. Chemical Physics, 2008, 353, 185-188.	1.9	6
173	Comparison of RC(O)OOH, RC(O)OH and R(CO)OOH bond dissociation energies with RC(O)OOH, RCOOH and RCOOH, R as phenyl, vinyl and alkyl groups. Chemical Physics Letters, 2015, 629, 102-112.	2.6	6
174	Mass Transfer of Hazardous Organic Compounds in Soil Matrices Experiment and Model. Combustion Science and Technology, 1992, 85, 151-163.	2.3	5
175	Standard chemical thermodynamic properties of monochloroalkanes. Industrial & Engineering Chemistry Research, 1993, 32, 3184-3188.	3.7	5
176	REACT for Windows: Chemical Kinetics Emulation and Application (Manka, Michael). Journal of Chemical Education, 2000, 77, 165.	2.3	5
177	Structural and thermochemical studies on CH ₃ SCH ₂ CHO, CH ₃ CH ₂ SCHO, CH ₃ SC(=O)CH ₃ and radicals corresponding to loss of H atom. Journal of Physical Organic Chemistry, 2017, 30, e3688.	1.9	5
178	OH-Initiated Reactions of <i>p</i> -Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part II. Kinetic Analysis. Journal of Physical Chemistry A, 2020, 124, 4875-4904.	2.5	5
179	Thermodynamic Properties: Enthalpy, Entropy, Heat Capacity, and Bond Energies of Fluorinated Carboxylic Acids. Journal of Physical Chemistry A, 2022, 126, 3-15.	2.5	5
180	A fluorescence lecture demonstration. Journal of Chemical Education, 1982, 59, 787.	2.3	4

#	ARTICLE	IF	CITATIONS
181	Pyrolysis and Oxidation of 1,1,1-Trichloroethane in Methane/Oxygen/Argon. Hazardous Waste and Hazardous Materials, 1993, 10, 381-395.	0.4	4
182	Subatmospheric Extinction of Opposed-Jet Diffusion Flames of Jet Fuel and Its Surrogates. AIAA Journal, 2010, 48, 158-165.	2.6	4
183	Chemical activation reactions of cyclic alkanes and ethers and tricyclodecane ring-opened diradicals with O ₂ : Thermochemistry, reaction paths, kinetics, and modeling. International Journal of Chemical Kinetics, 2012, 44, 232-256.	1.6	4
184	Thermochemical Properties of Hydroxycyclohexadienyl Peroxy Isomers from Reaction of O ₂ with the Benzene-OH adduct. Zeitschrift Fur Physikalische Chemie, 2015, 229, 999-1036.	2.8	4
185	Structures and thermochemistry of methyl ethyl sulfide and its hydroperoxides: HOOCH ₂ SCH ₂ CH ₃ , CH ₃ SCH(OOH)CH ₃ , CH ₃ SCH ₂ CH ₂ OOH, and radicals. Journal of Physical Organic Chemistry, 2018, 31, e3751.	1.9	4
186	Thermochemistry of Intermediates and Products in the Oxidation Reaction of 1,1,2-Trifluoroethene via OH Radical. Journal of Physical Chemistry A, 2019, 123, 8017-8027.	2.5	4
187	Variable power microwave discharge and cavity. Review of Scientific Instruments, 1981, 52, 612-614.	1.3	3
188	Mass Transfer Studies Related to Thermal Adsorption-Desorption of Benzene and Chlorobenzene on Soil Matrices. Hazardous Waste and Hazardous Materials, 1994, 11, 227-236.	0.4	3
189	Thermochemistry of Oxabicyclo-Heptanes, Oxabicyclo-Heptene: Enthalpy of Formation, Entropy, Heat Capacity, and Group Additivity. Journal of Physical and Chemical Reference Data, 2007, 36, 663-681.	4.2	3
190	Extinction of Opposed Jet Diffusion Flames of Scramjet Fuel Components at Subatmospheric Pressures. , 2008, , .		3
191	Reaction Paths and Chemical Activation Reactions of 2-Methyl-5-Furanyl Radical with ³ O ₂ . Journal of Physical Chemistry A, 2017, 121, 7309-7323.	2.5	3
192	Structural and thermochemical properties of methyl ethyl sulfide alcohols: HOCH ₂ SCH ₂ CH ₃ , CH ₃ SCH(OH)CH ₃ , CH ₃ SCH ₂ CH ₂ OH, and radicals corresponding to loss of H atom. Journal of Physical Organic Chemistry, 2018, 31, e3836.	1.9	3
193	OH-Initiated Reactions of <i>p</i> -Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part III. Kinetics of H-Abstraction by H, OH, and CH ₃ Radicals. Journal of Physical Chemistry A, 2020, 124, 4905-4915.	2.5	3
194	Thermochemistry, Bond Energies and Internal Rotor Potentials of Acetic Acid Hydrazide, Acetamide, N-Methyl Acetamide (NMA) and Radicals. Thermo, 2021, 1, 15-31.	1.3	3
195	Kinetic Analysis of Unimolecular Reactions Following the Addition of the Hydroxyl Radical to 1,1,2-Trifluoroethene. Journal of Physical Chemistry A, 2021, 125, 5375-5384.	2.5	3
196	High Pressure Capillary Flow Meter for GC. Journal of Chromatographic Science, 1983, 21, 226-228.	1.4	2
197	Removal of chromium from a highly contaminated soil/slag matrix by washing at low pH. International Journal of Environmental Studies, 1993, 44, 285-297.	1.6	2
198	Thermochemistry of Fluorinated Dimethyl and Ethyl Methyl Ethers and Corresponding Radical Species. Journal of Chemical & Engineering Data, 2020, 65, 1594-1616.	1.9	2

#	ARTICLE	IF	CITATIONS
199	Total hydrocarbon pollutants from a non-vented radiant kerosene heater. International Journal of Environmental Studies, 1988, 32, 75-83.	1.6	1
200	Gas-Phase Mercury Conversion in H_2 , O_2 , Chloro C_1 -Hydrocarbon, and NO_x Combustion Effluent from Use of an Elementary Kinetic Mechanism. Combustion Science and Technology, 2010, 182, 529-543.	2.3	1
201	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O_2 reaction system. , 2000, 32, 435.		1
202	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O_2 reaction system. International Journal of Chemical Kinetics, 2000, 32, 435-452.	1.6	1
203	Gaussian M-062x/6-31+g (d,p) Calculation of Standard Enthalpy, Entropy and Heat Capacity of Some Fluorinated Alcohol TM s and Its Radicals at Different Temperatures. American Journal of Physical Chemistry, 2020, 9, 101.	0.1	1
204	Alcohol-fueled missile. Journal of Chemical Education, 1983, 60, 1069.	2.3	0
205	A study of the concentrations of selected organic vapors in the ambient atmosphere of suburban and rural New Jersey locations. International Journal of Environmental Studies, 1985, 26, 125-135.	1.6	0
206	Toward a Pressure-Dependent Detailed Chemical Kinetic Model for JP-10 Combustion. , 2012, , .		0
207	Reaction kinetics and thermochemistry of the chemically activated and stabilized primary ethyl radical of methyl ethyl sulfide, $CH_3SCH_2CH_2$, with O_2 to $CH_3SCH_2CH_2OO$. International Journal of Chemical Kinetics, 2019, 51, 618-633.	1.6	0
208	Reaction pathways, kinetics and thermochemistry of the chemically-activated and stabilized primary methyl radical of methyl ethyl sulfide, $CH_3CH_2SCH_2$, with $3O_2$ to $CH_2CH_3SCH_2OO$. Combustion and Flame, 2019, 204, 368-379.	5.2	0
209	Heat Capacity and Bond Dissociation Energy Calculations of Some Fluorinated Ethanol TM s and its Radicals: CH_3 , CH_2 , F , OH , CH_3 , CH_2 , F , OH . Open Journal of Physical Chemistry, 2021, 11, 13-53.	0.6	0