Joseph Bozzelli

List of Publications by Year
in descending order

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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	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
2	Heat Capacity and Bond Dissociation Energy Calculations of Some Fluorinated Ethanolâ€™s and its Radicals: CH_{3-x}CH₂F_xOH, CH₃CH_{2-x}F_xOH. Open Journal of Physical Chemistry, 2021, 11, 13-53.	0.6	0
3	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
4	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
5	OH-Initiated Reactions of para-Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part II. Kinetic Analysis. Journal of Physical Chemistry A, 2020, 124, 4875-4904.	2.5	5
6	OH-Initiated Reactions of para-Coumaryl Alcohol Relevant to the Lignin Pyrolysis. Part III. Kinetics of H-Abstraction by H, OH, and CH₃ Radicals. Journal of Physical Chemistry A, 2020, 124, 4905-4915.	2.5	3
7	Thermochemistry of Fluorinated Dimethyl and Ethyl Methyl Ethers and Corresponding Radical Species. Journal of Chemical & Engineering Data, 2020, 65, 1594-1616.	1.9	2
8	Gaussian M-062x/6-31+g (d,p) Calculation of Standard Enthalpy, Entropy and Heat Capacity of Some Fluorinated Alcoholâ€™s and Its Radicals at Different Temperatures. American Journal of Physical Chemistry, 2020, 9, 101.	0.1	1
9	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
10	Reaction kinetics and thermochemistry of the chemically activated and stabilized primary ethyl radical of methyl ethyl sulfide, CH₃SCH₂CH₂â€¢, with O₂ to CH₃SCH₂CH₂OOâ€¢. International Journal of Chemical Kinetics, 2019, 51, 618-633.	1.6	0
11	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
12	Thermochemistry and kinetics of the 2â€butanoneâ€4â€yl CH₃C(=O)CH₂CH₂â€¢ + O₂ reaction system. International Journal of Chemical Kinetics, 2019, 51, 541-562.	1.6	7
13	OH-Initiated Reactions of p-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
14	Reaction pathways, kinetics and thermochemistry of the chemically-activated and stabilized primary methyl radical of methyl ethyl sulfide, CH3CH2SCH2â€¢, with 3O2 to CH2CH3SCH2OOâ€¢. Combustion and Flame, 2019, 204, 368-379.	5.2	0
15	Thermochemical Properties: Enthalpy, Entropy, and Heat Capacity of C2â€“C3 Fluorinated Aldehydes. Radicals and Fluorocarbon Group Additivity. Journal of Physical Chemistry A, 2019, 123, 650-665.	2.5	12
16	Structural and thermochemical properties of methyl ethyl sulfide alcohols: HOCH₂SCH₂CH₃, CH₃SCH(OH)CH₃, CH₃SCH₂CH₂OH, and radicals corresponding to loss of H atom. Journal of Physical Organic Chemistry, 2018, 31, e3836.	1.9	3
17	Structures and thermochemistry of methyl ethyl sulfide and its hydroperoxides: HOOCH₂SCH₂CH₃, CH₃SCH(OOH)CH₃, CH₃SCH₂CH₂OOH, and radicals. Journal of Physical Organic Chemistry, 2018, 31, e3751.	1.9	4
18	S₂ + Air Combustion: Reaction Kinetics, Flame Structure, and Laminar Flame Behavior. Energy & Fuels, 2018, 32, 10184-10193.	5.1	8

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19	Structural and thermochemical studies on CH₃SCH₂CHO, CH₃CH₂SCHO, CH₃SC(â•Ö)CH_{3,} and radicals corresponding to loss of H atom. Journal of Physical Organic Chemistry, 2017, 30, e3688.	1.9	5
20	Molecular Products and Fundamentally Based Reaction Pathways in the Gas-Phase Pyrolysis of the Lignin Model Compound p-Coumaryl Alcohol. Journal of Physical Chemistry A, 2017, 121, 3352-3371.	2.5	34
21	Thermochemistry of Hydroxyl and Hydroperoxide Substituted Furan, Methylfuran, and Methoxyfuran. Journal of Physical Chemistry A, 2017, 121, 4523-4544.	2.5	19
22	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
23	Reaction Paths and Chemical Activation Reactions of 2-Methyl-5-Furanyl Radical with ³O₂. Journal of Physical Chemistry A, 2017, 121, 7309-7323.	2.5	3
24	Thermochemistry and Kinetic Analysis of the Unimolecular Oxiranyl Radical Dissociation Reaction: A Theoretical Study. ChemPhysChem, 2016, 17, 1983-1992.	2.1	12
25	Thermochemical Properties (Î”fHÂ°(298 K), SÂ°(298 K), Cp(T)) and Bond Dissociation Energies for C1â€“C4 Normal Hydroperoxides and Peroxy Radicals. Journal of Chemical & Engineering Data, 2016, 61, 1836-1849.	1.9	22
26	Thermochemical Properties and Bond Dissociation Energies for Fluorinated Methanol, CH_{3â€“x}F_xOH, and Fluorinated Methyl Hydroperoxides, CH_{3â€“x}F_xOOH: Group Additivity. Journal of Physical Chemistry A, 2016, 120, 6998-7010.	2.5	7
27	Gas Phase Mercury Oxidation by Halogens (Cl, Br, I) in Combustion Effluents: Influence of Operating Conditions. Energy & Fuels, 2016, 30, 603-615.	5.1	19
28	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
29	Thermochemical Properties of Hydroxycyclohexadienyl Peroxy Isomers from Reaction of O2 with the Benzene-OH adduct. Zeitschrift Fur Physikalische Chemie, 2015, 229, 999-1036.	2.8	4
30	Kinetic Study of Diâ€Tertâ€Butyl Peroxide: Thermal Decomposition and Product Reaction Pathways. International Journal of Chemical Kinetics, 2015, 47, 133-161.	1.6	27
31	Thermochemical Properties Enthalpy, Entropy, and Heat Capacity of C1â€“C4 Fluorinated Hydrocarbons: Fluorocarbon Group Additivity. Journal of Physical Chemistry A, 2015, 119, 8202-8215.	2.5	30
32	Comparison of RC(O) OOH, RC(O)O OH and R(C O)OO H bond dissociation energies with RC OOH, RCO OH and RCOO H, R as phenyl, vinyl and alkyl groups. Chemical Physics Letters, 2015, 629, 102-112.	2.6	6
33	Bond Energies and Thermochemical Properties of Ring-Opened Diradicals and Carbenes of exo-Tricyclo[5.2.1.0^{2,6}]decane. Journal of Physical Chemistry A, 2015, 119, 9857-9878.	2.5	15
34	Thermochemistry and Kinetics for 2-Butanone-1-yl Radical (CH₂Â·C(â•Ö)CH₂CH₃) Reactions with O₂. Journal of Physical Chemistry A, 2014, 118, 21-37.	2.5	26
35	Thermochemistry, Reaction Paths, and Kinetics on the Secondary Isooctane Radical Reaction with 3 O2. International Journal of Chemical Kinetics, 2014, 46, 71-103.	1.6	8
36	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

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37	Thermochemistry of C₇H₁₆ to C₁₀H₂₂ Alkane Isomers: Primary, Secondary, and Tertiary Câ€“H Bond Dissociation Energies and Effects of Branching. Journal of Physical Chemistry A, 2014, 118, 9364-9379.	2.5	44
38	Thermochemical Properties and Bond Dissociation Enthalpies of 3- to 5-Member Ring Cyclic Ether Hydroperoxides, Alcohols, and Peroxy Radicals: Cyclic Ether Radical + 3O2 Reaction Thermochemistry. Journal of Physical Chemistry A, 2014, 118, 3147-3167.	2.5	20
39	Thermochemistry, Reaction Paths, and Kinetics on the tert-Isooctane Radical Reaction with O₂. Journal of Physical Chemistry A, 2014, 118, 4631-4646.	2.5	25
40	Thermochemical Properties for Isooctane and Carbon Radicals: Computational Study. Journal of Physical Chemistry A, 2013, 117, 421-429.	2.5	20
41	Thermochemical Properties of Methyl-Substituted Cyclic Alkyl Ethers and Radicals for Oxiranes, Oxetanes, and Oxolanes: Câ€“H Bond Dissociation Enthalpy Trends with Ring Size and Ether Site. Journal of Physical Chemistry A, 2013, 117, 378-392.	2.5	19
42	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
43	Toward a Pressure-Dependent Detailed Chemical Kinetic Model for JP-10 Combustion. , 2012, , .		0
44	Dihydrogen Catalysis: A Degradation Mechanism for N₂-Fixation Intermediates. Journal of Physical Chemistry A, 2012, 116, 11618-11642.	2.5	16
45	Thermochemistry and Bond Dissociation Energies of Ketones. Journal of Physical Chemistry A, 2012, 116, 5707-5722.	2.5	45
46	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
47	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
48	Computational study on structures, thermochemical properties, and bond energies of disulfide oxygen (Sâ€“Sâ€“O)â€bridged CH₃SSOH and CH₃SS(=O)H and radicals. Journal of Physical Organic Chemistry, 2012, 25, 475-485.	1.9	9
49	Thermochemical Properties and Bond Dissociation Energies of C3â€“C5 Cycloalkyl Hydroperoxides and Peroxy Radicals: Cycloalkyl Radical + 3O2 Reaction Thermochemistry. Journal of Physical Chemistry A, 2012, 116, 7550-7563.	2.5	13
50	Chemical activation reactions of cyclic alkanes and ethers and tricyclodecane ringâ€opened diradicals with O₂: Thermochemistry, reaction paths, kinetics, and modeling. International Journal of Chemical Kinetics, 2012, 44, 232-256.	1.6	4
51	Reaction of the i-C₄H₅ (CH₂CCHCH₂) Radical with O₂. Journal of Physical Chemistry A, 2011, 115, 1018-1026.	2.5	14
52	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
53	Thermochemistry and Reaction Paths in the Oxidation Reaction of Benzoyl Radical: C₆H₅C^{â€¢}(â•O). Journal of Physical Chemistry A, 2011, 115, 11897-11914.	2.5	19
54	Thermochemistry and Kinetics for 2-Butanone-3yl Radical (CH₃C(=O)CH^{â€¢}CH₃) Reactions with O₂. Zeitschrift Fur Physikalische Chemie, 2011, 225, 993-1018.	2.8	26

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55	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
56	Gas-Phase Mercury Conversion in H₂, O₂, Chloro C₁-Hydrocarbon, and NO_xCombustion Effluent from Use of an Elementary Kinetic Mechanism. Combustion Science and Technology, 2010, 182, 529-543.	2.3	1
57	Structure and Thermochemical Properties of 2-Methoxyfuran, 3-Methoxyfuran, and Their Carbon-Centered Radicals Using Computational Chemistry. Journal of Physical Chemistry A, 2010, 114, 7984-7995.	2.5	16
58	Thermochemical properties for nâ€propyl, isoâ€propyl, and tertâ€butyl nitroalkanes, alkyl nitrites, and their carbonâ€centered radicals. International Journal of Chemical Kinetics, 2010, 42, 181-199.	1.6	7
59	On the reactivity of methylbenzenes. Combustion and Flame, 2010, 157, 2175-2183.	5.2	37
60	Subatmospheric Extinction of Opposed-Jet Diffusion Flames of Jet Fuel and Its Surrogates. AIAA Journal, 2010, 48, 158-165.	2.6	4
61	Thermochemical Properties of exo-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
62	Formation and Decomposition of Chemically Activated and Stabilized Hydrazine. Journal of Physical Chemistry A, 2010, 114, 6235-6249.	2.5	33
63	Kinetics of the Cyclopentadienyl + Acetylene, Fulvenallene + H, and 1-Ethynylcyclopentadiene + H Reactions. Journal of Physical Chemistry A, 2010, 114, 2275-2283.	2.5	57
64	Chain Branching and Termination in the Low-Temperature Combustion ofn-Alkanes: 2-Pentyl Radical + O₂, Isomerization and Association of the Second O₂. Journal of Physical Chemistry A, 2010, 114, 7693-7708.	2.5	49
65	Quantum Chemical Study of the Acrolein (CH₂CHCHO) + OH + O₂ Reactions. Journal of Physical Chemistry A, 2010, 114, 8302-8311.	2.5	63
66	Kinetic modeling of the benzyl+HO2 reaction. Proceedings of the Combustion Institute, 2009, 32, 287-294.	3.9	59
67	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
68	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
69	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
70	Decomposition of Methylbenzyl Radicals in the Pyrolysis and Oxidation of Xylenes. Journal of Physical Chemistry A, 2009, 113, 10264-10278.	2.5	55
71	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
72	Thermal Decomposition of the Benzyl Radical to Fulvenallene (C₇H₆) + H. Journal of Physical Chemistry A, 2009, 113, 6111-6120.	2.5	100

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73	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
74	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
75	Ethanol Oxidation: Kinetics of the Î±-Hydroxyethyl Radical + O₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 8923-8933.	2.5	118
76	Thermodynamic properties of the species resulting from the phenyl radical with O₂ reaction system. International Journal of Chemical Kinetics, 2008, 40, 583-604.	1.6	33
77	Terahertz study of trichloroanisole by time-domain spectroscopy. Chemical Physics, 2008, 353, 185-188.	1.9	6
78	Formation of a Criegee intermediate in the low-temperature oxidation of dimethyl sulfoxide. Physical Chemistry Chemical Physics, 2008, 10, 1769.	2.8	49
79	Thermochemistry of Methyl and Ethyl Nitro, RNO₂, and Nitrite, RONO, Organic Compounds. Journal of Physical Chemistry A, 2008, 112, 3172-3185.	2.5	44
80	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
81	Extinction of Opposed Jet Diffusion Flames of Scramjet Fuel Components at Subatmospheric Pressures. , 2008, , .		3
82	Variational Analysis of the Phenyl + O₂ and Phenoxy + O Reactions. Journal of Physical Chemistry A, 2008, 112, 3566-3575.	2.5	82
83	Thermochemistry and kinetics of acetonylperoxy radical isomerisation and decomposition: a quantum chemistry and CVT/SCT approach. Physical Chemistry Chemical Physics, 2008, 10, 7139.	2.8	19
84	Thermochemical Similarities Among Three Reaction Systems: VinylÂ+ÂO2â€“ PhenylÂ+ÂO2â€“ DibenzofuranylÂ+ÂO2. Combustion Science and Technology, 2008, 180, 959-974.	2.3	17
85	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
86	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
87	Thermochemical and Kinetic Analysis on the Reactions of O2 with Products from OH Addition to Isobutene, 2-Hydroxy-1,1-dimethylethyl, and 2-Hydroxy-2-methylpropyl Radicals:â€‰ HO2 Formation from Oxidation of Neopentane, Part II. Journal of Physical Chemistry A, 2007, 111, 4974-4986.	2.5	46
88	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
89	Thermochemical Properties, Î”fHÂ°(298), SÂ°(298), and CpÂ°(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
90	Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels:Â Ethyl Propanoate and Methyl Butanoateâ€. Journal of Physical Chemistry A, 2007, 111, 3727-3739.	2.5	145

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91	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
92	Thermochemistry for enthalpies and reaction paths of nitrous acid isomers. International Journal of Chemical Kinetics, 2007, 39, 378-398.	1.6	35
93	Thermochemistry, Bond Energies, and Internal Rotor Potentials of Dimethyl Tetraoxide. Journal of Physical Chemistry A, 2007, 111, 12026-12036.	2.5	14
94	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
95	Thermochemistry of Acetonyl and Related Radicals. Journal of Physical Chemistry A, 2006, 110, 13618-13623.	2.5	52
96	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
97	Kinetics of the Multichannel Reaction of Methanethiyl Radical (CH3Sâ€¢) with3O2â€. Journal of Physical Chemistry A, 2006, 110, 6923-6937.	2.5	33
98	Thermochemistry of oxabicycloheptenes: enthalpy of formation, entropy and heat capacity. Journal of Physical Organic Chemistry, 2006, 19, 93-103.	1.9	13
99	Bond dissociation energy of the phenol OH bond from ab initio calculations. Chemical Physics Letters, 2006, 424, 42-45.	2.6	66
100	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
101	Thermodynamic and Ab Initio Analysis of the Controversial Enthalpy of Formation of Formaldehyde. ChemPhysChem, 2006, 7, 1119-1126.	2.1	53
102	Propagation of uncertainty in chemically activated systems. AICHE Journal, 2006, 52, 3246-3256.	3.6	12
103	The multi-channel reaction of CH3S+3O2: Thermochemistry and kinetic barriers. Computational and Theoretical Chemistry, 2005, 728, 147-157.	1.5	30
104	Enthalpy of formation and bond energies on unsaturated oxygenated hydrocarbons using G3MP2B3 calculation methods. International Journal of Chemical Kinetics, 2005, 37, 633-648.	1.6	19
105	Thermochemical Properties, Rotation Barriers, and Group Additivity for Unsaturated Oxygenated Hydrocarbons and Radicals Resulting from Reaction of Vinyl and Phenyl Radical Systems with O2. Journal of Physical Chemistry A, 2005, 109, 2233-2253.	2.5	37
106	Time-integrated pointers for enabling the analysis of detailed reaction mechanisms. AICHE Journal, 2004, 50, 2956-2970.	3.6	44
107	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
108	Thermochemical and Kinetic Analysis on the Reactions of Neopentyl and Hydroperoxy-Neopentyl Radicals with Oxygen:â€‰ Part I. OH and Initial Stable HC Product Formation. Journal of Physical Chemistry A, 2004, 108, 1694-1711.	2.5	50

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109	Thermochemical Properties, Pathway, and Kinetic Analysis on the Reactions of Benzene with OH:â€‰ An Elementary Reaction Mechanism. Journal of Physical Chemistry A, 2004, 108, 4632-4652.	2.5	49
110	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
111	Kinetics and mechanism for the thermal chlorination of chloroform in the gas phase: Inclusion of HCl elimination from CHCl3. International Journal of Chemical Kinetics, 2003, 35, 647-660.	1.6	14
112	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
113	Thermochemical and Kinetic Analysis of the Formyl Methyl Radical + O2 Reaction System. Journal of Physical Chemistry A, 2003, 107, 3778-3791.	2.5	53
114	Structure, Intramolecular Rotation Barrier, and Thermochemical Properties of Hydroxycyclohexadienyl Radical. Journal of Physical Chemistry A, 2003, 107, 6451-6456.	2.5	7
115	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties of Methyl Ethyl, Methyl Isopropyl, and Methyl tert-Butyl Ethers and the Corresponding Radicals. Journal of Physical Chemistry A, 2003, 107, 4531-4546.	2.5	40
116	Structures, Rotational Barriers, and Thermochemical Properties of Î²-Chlorinated Ethyl Hydroperoxides. Journal of Physical Chemistry A, 2003, 107, 1018-1024.	2.5	11
117	Formation of Chlorinated Aromatics by Reactions of Clâ€¢, Cl2, and HCl with Benzene in the Cool-Down Zone of a Combustor. Environmental Science & Technology, 2003, 37, 1684-1689.	10.0	35
118	Kinetics and Thermochemistry for the Gas-Phase Ketoâ^'Enol Tautomerism of Phenol â†" 2,4-Cyclohexadienone. Journal of Physical Chemistry A, 2003, 107, 3696-3703.	2.5	70
119	Thermodynamic properties (S298, Cp(T), internal rotations and group additivity parameters) in vinyl and phenyl hydroperoxidesElectronic 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, 299-307.	2.8	13
120	Thermochemical Properties, Î"fHÂ°(298.15â€‰K), SÂ°(298.15â€‰K), and CpÂ°(T), of 1,4-Dioxin, 2,3-Benzodioxin, Furan, 2,3-Benzofuran, and Twelve Monochloro and Dichloro Dibenzo-p-dioxins and Dibenzofurans. Journal of Physical and Chemical Reference Data, 2003, 32, 1713-1735.	4.2	17
121	Pyrolysis and Oxidation of Cellulose in a Continuous-Feed and -Flow Reactor:Â Effects of NaCl. Industrial & Engineering Chemistry Research, 2002, 41, 3526-3539.	3.7	13
122	Structures, Rotational Barriers, and Thermochemical Properties of Chlorinated Aldehydes and the Corresponding Acetyl (CCâ€¢O) and Formyl Methyl Radicals (Câ€¢CO) and Additivity Groups. Journal of Physical Chemistry A, 2002, 106, 345-355.	2.5	16
123	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
124	Thermochemistry, Reaction Paths, and Kinetics on the Hydroperoxy-Ethyl Radical Reaction with O2:â€‰ New Chain Branching Reactions in Hydrocarbon Oxidation. Journal of Physical Chemistry A, 2002, 106, 1113-1121.	2.5	54
125	Thermochemical and Kinetic Analysis of the Acetyl Radical (CH3Câ€¢O) + O2Reaction System. Journal of Physical Chemistry A, 2002, 106, 7155-7170.	2.5	49
126	Detailed Kinetics and Thermochemistry of C2H5+ O2:Â Reaction Kinetics of the Chemically-Activated and Stabilized CH3CH2OOâ€¢Adduct. Journal of Physical Chemistry A, 2002, 106, 7276-7293.	2.5	140

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127	structures, thermochemical properties (enthalpy, entropy and heat capacity), rotation barriers, and peroxide bond energies of vinyl, allyl, ethynyl and phenyl hydroperoxidesElectronic 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
128	Chemical makeup and physical characterization of a synthetic fuel and methods of heat content evaluation for studies on MSW incineration. Fuel, 2002, 81, 211-217.	6.4	17
129	Cl2 molecular elimination reaction from 1,2-dichloroethane. Chemical Physics Letters, 2002, 357, 65-72.	2.6	8
130	Thermodynamic properties of chloroacetylene, dichloroacetylene, ethynyl radical, and chloroethynyl radical. Chemical Physics Letters, 2002, 362, 445-452.	2.6	11
131	Structures, Intramolecular Rotation Barriers, and Thermochemical Properties:Â Ethanol, Î±-Monoethanols, Dichloroethanols, and Corresponding Radicals Derived from H Atom Loss. Journal of Physical Chemistry A, 2001, 105, 9543-9552.	2.5	23
132	Detailed Kinetic Study of the Growth of Small Polycyclic Aromatic Hydrocarbons. 1. 1-Naphthyl + Ethyneâ€. Journal of Physical Chemistry A, 2001, 105, 1561-1573.	2.5	97
133	Structure, Torsional Potentials, and Thermodynamic Properties Î”HÂ°f298, SÂ°298, andCp(T) of Chloro-Dimethyl Ethers:Â CH2ClOCH3, CHCl2OCH3, and CCl3OCH3. Density Functional and ab Initio Calculations. Journal of Physical Chemistry A, 2001, 105, 5420-5430.	2.5	8
134	Theoretical Investigation on Stability of the CÂ·H2OCl Radical. Journal of Physical Chemistry A, 2001, 105, 3941-3946.	2.5	7
135	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
136	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O2 reaction system. International Journal of Chemical Kinetics, 2000, 32, 435-452.	1.6	33
137	ab initio molecular orbital and density functional analysis of acetylene + O2 reactions with CHEMKIN evaluation. International Journal of Chemical Kinetics, 2000, 32, 623-641.	1.6	8
138	ab initio calculations and thermochemical analysis on C1 atom abstractions of chlorine from chlorocarbons and the reverse alkyl abstractions: Cl2 + Rï¿½ ? Clï¿½ + RCl. International Journal of Chemical Kinetics, 2000, 32, 548-565.	1.6	6
139	REACT for Windows: Chemical Kinetics Emulation and Application (Manka, Michael). Journal of Chemical Education, 2000, 77, 165.	2.3	5
140	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
141	Elementary Reaction Mechanism for Benzene Oxidation in Supercritical Waterâ€. Journal of Physical Chemistry A, 2000, 104, 10576-10586.	2.5	61
142	Kinetic Analysis for HO2Addition 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
143	Structures, Rotational Barriers, and Thermodynamic Properties of C2Vinyl and Chlorovinyl Alcohols and Additivity Groups. Journal of Physical Chemistry A, 2000, 104, 9197-9206.	2.5	20
144	Structures, Rotation Barrier, and Thermodynamic Properties Î”HfÂ°298, SÂ°298, and Cp(T) of Chloromethyl Hypochlorites CH3OCl, CH2ClOCl, CHCl2OCl, and CCl3OCl. Journal of Physical Chemistry A, 2000, 104, 9581-9590.	2.5	23

#	Article	IF	Citations
145	Thermochemical Property, Pathway and Kinetic Analysis on the Reactions of Allylic Isobutenyl Radical with O2:â€‰ an Elementary Reaction Mechanism for Isobutene Oxidation. Journal of Physical Chemistry A, 2000, 104, 9715-9732.	2.5	58
146	Presence of Chlorine Radicals and Formation of Molecular Chlorine in the Post-Flame Region of Chlorocarbon Combustion. Environmental Science & Technology, 2000, 34, 4565-4570.	10.0	34
147	Comparisons of CBS-q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethyl-ether + O2 reaction system. , 2000, 32, 435.		1
148	Comparisons of CBSâ€q and G2 calculations on thermodynamic properties, transition states, and kinetics of dimethylâ€ether + O2 reaction system. International Journal of Chemical Kinetics, 2000, 32, 435-452.	1.6	1
149	Kinetic and Thermodynamic Analysis on OH Addition to Ethylene:Â Adduct Formation, Isomerization, and Isomer Dissociations. Journal of Physical Chemistry A, 1999, 103, 7646-7655.	2.5	49
150	Thermodynamic Properties (Î”Hf(298),S(298), andCp(T) (300 â‰¤Tâ‰¤ 1500)) of Fluorinated Propanes. Journal of Physical Chemistry A, 1999, 103, 5602-5610.	2.5	32
151	Thermodynamic Properties Î”HfÂ°298, SÂ°298, and Cp(T) for 2-Fluoro-2-Methylpropane, Î”HfÂ°298 of Fluorinated Ethanes, and Group Additivity for Fluoroalkanes. Journal of Physical Chemistry A, 1999, 103, 7373-7379.	2.5	18
152	Analysis of Tertiary Butyl Radical + O2, Isobutene + HO2, Isobutene + OH, and Isobuteneâ˙OH Adducts + O2:Â A Detailed Tertiary Butyl Oxidation Mechanism. Journal of Physical Chemistry A, 1999, 103, 9731-9769.	2.5	62
153	Reaction of OH Radical with C2H3Cl:Â Rate Constant and Reaction Pathway Analysis. Journal of Physical Chemistry A, 1999, 103, 7800-7810.	2.5	20
154	Polymer Pyrolysis and Oxidation Studies in a Continuous Feed and Flow Reactor:Â Cellulose and Polystyrene. Environmental Science & Technology, 1999, 33, 2584-2592.	10.0	14
155	Thermochemical and Kinetic Analysis of the H, OH, HO2, O, and O2Association Reactions with Cyclopentadienyl Radical. Journal of Physical Chemistry A, 1998, 102, 3537-3555.	2.5	91
156	Standard Chemical Thermodynamic Properties of Multichloro Alkanes and Alkenes:Â A Modified Group Additivity Scheme. Journal of Physical Chemistry A, 1998, 102, 4551-4558.	2.5	31
157	Ab Initio Calculations and Internal Rotor:â€‰ Contribution for Thermodynamic Properties SÂ°298 and Cp(T)'s (300 < T/K < 1500):â€‰ Group Additivity for Fluoroethanes. Journal of Physical Chemistry A, 1998, 102, 7286-7293.	2.5	52
158	Comparison of AM1 and PM3 in MOPAC6 with Literature for the Thermodynamic Parameters of C1and C2Chlorocarbons. Industrial & Engineering Chemistry Research, 1998, 37, 3497-3507.	3.7	7
159	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
160	Enthalpies of Formation and Group Additivity of Alkyl Peroxides and Trioxides. Journal of Physical Chemistry A, 1997, 101, 9505-9510.	2.5	105
161	Study of Volatile Organic Compounds Destruction by Dielectric Barrier Corona Discharge. Journal of Advanced Oxidation Technologies, 1997, 2, .	0.5	7
162	Thermochemical and kinetic analysis on the addition reactions of H, O, OH, and HO2 with 1,3 cyclopentadiene. International Journal of Chemical Kinetics, 1997, 29, 893-913.	1.6	35

#	Article	IF	Citations
163	Molecular density of states from estimated vapor phase heat capacities. International Journal of Chemical Kinetics, 1997, 29, 161-170.	1.6	62
164	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
165	Impact of SO2 and NO on CO oxidation under post-flame conditions. International Journal of Chemical Kinetics, 1996, 28, 773-790.	1.6	140
166	Ab InitioStudy of Î±-Chlorinated Ethyl Hydroperoxides CH3CH2OOH, CH3CHClOOH, and CH3CCl2OOH:Â Conformational Analysis, Internal Rotation Barriers, Vibrational Frequencies, and Thermodynamic Properties. The Journal of Physical Chemistry, 1996, 100, 8240-8249.	2.9	104
167	O + NNH: A possible new route for NOX formation in flames. International Journal of Chemical Kinetics, 1995, 27, 1097-1109.	1.6	222
168	Analysis of selected volatile organic compounds associated with residential kerosene heater use. International Journal of Environmental Studies, 1995, 49, 125-131.	1.6	7
169	Analysis and Optimization of Chlorocarbon Incineration through Use of a Detailed Reaction Mechanism. Industrial & Engineering Chemistry Research, 1995, 34, 4185-4192.	3.7	14
170	Simulation of a Three-Stage Chlorocarbon Incinerator through the Use of a Detailed Reaction Mechanism: Chlorine to Hydrogen Mole Ratios below 0.15. Environmental Science & Technology, 1995, 29, 3059-3063.	10.0	15
171	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
172	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
173	Thermal Reactions of Methylene Chloride in Methane/Argon Mixtures. Combustion Science and Technology, 1994, 101, 135-152.	2.3	11
174	An experimental and numerical study of the high-temperature oxidation of 1,1,1-C2H3Cl3. Combustion and Flame, 1994, 98, 155-169.	5.2	21
175	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
176	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
177	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
178	Soil and Water Decontaminaton by Extraction with Surfactants. Separation Science and Technology, 1993, 28, 793-804.	2.5	26
179	Standard chemical thermodynamic properties of monochloroalkanes. Industrial & Engineering Chemistry Research, 1993, 32, 3184-3188.	3.7	5
180	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

#	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	CATALYTIC HYDRODECHLORINATION OF 1,2-DICHLOROETHANE AND TRICHLOROETHYLENE OVER Rh/Si0 2 CATALYSTS. Chemical Engineering Communications, 1992, 115, 1-11.	2.6	52
183	Mass Transfer of Hazardous Organic Compounds in Soil Matrices Experiment and Model. Combustion Science and Technology, 1992, 85, 151-163.	2.3	5
184	Chloroform Pyrolysis: Experiment and Detailed Reaction Model. Combustion Science and Technology, 1992, 85, 345-373.	2.3	47
185	Kinetic Study on Pyrolysis and Oxidation of CH3Cl in Ar/H2/O2Mixtures. Combustion Science and Technology, 1992, 85, 23-63.	2.3	66
186	Chlorocarbon-Induced Incomplete Combustion In A Jet-Stirred Reactor. Combustion Science and Technology, 1992, 85, 87-100.	2.3	21
187	Thermal reactions of CH2Cl2 in H2/O2 mixtures: Implications for chlorine inhibition of CO conversion to CO2. Combustion and Flame, 1992, 88, 265-295.	5.2	82
188	CHEMACT: A Computer Code to Estimate Rate Constants for Chemically-Activated Reactions. Combustion Science and Technology, 1991, 80, 63-85.	2.3	84
189	THERM: Thermodynamic property estimation for gas phase radicals and molecules. International Journal of Chemical Kinetics, 1991, 23, 767-778.	1.6	460
190	Reactions of Chlorinated Benzenes in H2 and in H2/O2Mixtures: Thermodynamic Implications on Pathways to Dioxin. Combustion Science and Technology, 1990, 74, 117-135.	2.3	21
191	Chemical activation analysis of the reaction of ethyl radical with oxygen. The Journal of Physical Chemistry, 1990, 94, 3313-3317.	2.9	107
192	Reaction of chlorocarbons to hydrochloric acid and hydrocarbons in a hydrogen-rich microwave induced plasma reactor. Environmental Science & Technology, 1989, 23, 666-671.	10.0	18
193	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
194	Total hydrocarbon pollutants from a nonâ€vented radiant kerosene heater. International Journal of Environmental Studies, 1988, 32, 75-83.	1.6	1
195	Kinetic parameters for coupled bulk and wall reactions in a tubular flow reactor. AICHE Journal, 1987, 33, 1207-1211.	3.6	9
196	Conversion of chloroform to hydrochloric acid by reaction with hydrogen and water vapor. Environmental Science & Technology, 1986, 20, 568-574.	10.0	34
197	Volatile organic compounds at hazardous waste sites and a sanitary landfill in New Jersey. Environmental Progress, 1986, 5, 18-27.	0.7	24
198	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

#	Article	IF	Citations
199	Monitoring volatile organic compounds at hazardous and sanitary landfills in New Jersey. Journal of Environmental Science and Health Part A, Environmental Science and Engineering, 1985, 20, 491-501.	0.1	18
200	Comparison of selected volatile organic compounds during the summer and winter at urban sites in New Jersey. Science of the Total Environment, 1984, 38, 259-274.	8.0	17
201	Alcohol-fueled missile. Journal of Chemical Education, 1983, 60, 1069.	2.3	0
202	High Pressure Capillary Flow Meter for GC. Journal of Chromatographic Science, 1983, 21, 226-228.	1.4	2
203	Measurement of Selected Volatile Organic Compounds at Three Locations in New Jersey during the Summer Season. Journal of the Air Pollution Control Association, 1983, 33, 1177-1183.	0.5	34
204	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
205	Vibrational relaxation of highly excited diatomics. I. Method, analysis, and application to HCl(vâ‰7)+CO2 and N2O. Journal of Chemical Physics, 1982, 76, 2972-2983.	3.0	23
206	A fluorescence lecture demonstration. Journal of Chemical Education, 1982, 59, 787.	2.3	4
207	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
208	Variable power microwave discharge and cavity. Review of Scientific Instruments, 1981, 52, 612-614.	1.3	3
209	Reaction between atomic fluorine and CF3Br: Evidence for a pseudotrihalogen radical intermediate. Journal of Chemical Physics, 1973, 59, 3669-3675.	3.0	7