Theodore S Dibble

List of Publications by Year
in descending order

58 papers	1,704 citations	257450 24 h-index	302126 39 g-index
70 all docs	70 docs citations	70 times ranked	1440 citing authors

#	Article	IF	Citations
1	Reaction mechanism and kinetics of the important but neglected reaction of Hg with NO2 at low temperature. Chemical Engineering Journal, 2022, 432, 134373.	12.7	2
2	Combined Experimental and Computational Kinetics Studies for the Atmospherically Important BrHg Radical Reacting with NO and O₂. Journal of Physical Chemistry A, 2022, 126, 3914-3925.	2.5	3
3	Theoretical Study of the Monohydration of Mercury Compounds of Atmospheric Interest. Journal of Physical Chemistry A, 2021, 125, 5819-5828.	2.5	1
4	Improved Mechanistic Model of the Atmospheric Redox Chemistry of Mercury. Environmental Science & Technology, 2021, 55, 14445-14456.	10.0	65
5	Modeling the OH-Initiated Oxidation of Mercury in the Global Atmosphere without Violating Physical Laws. Journal of Physical Chemistry A, 2020, 124, 444-453.	2.5	33
6	First experimental kinetic study of the atmospherically important reaction of BrHgÂ+ÂNO2. Chemical Physics Letters, 2020, 759, 137928.	2.6	10
7	BrHgO^{â€¢} + CO: Analogue of OH + CO and Reduction Path for Hg(II) in the Atmosphere. ACS Earth and Space Chemistry, 2020, 4, 1777-1784.	2.7	16
8	BrHgO^{â€¢} + C₂H₄ and BrHgO^{â€¢} + HCHO in Atmospheric Oxidation of Mercury: Determining Rate Constants of Reactions with Prereactive Complexes and Bifurcation. Journal of Physical Chemistry A, 2019, 123, 6045-6055.	2.5	13
9	Computational Study on the Photolysis of BrHgONO and the Reactions of BrHgO^{â€¢} with CH₄, C₂H₆, NO, and NO₂: Implications for Formation of Hg(II) Compounds in the Atmosphere. Journal of Physical Chemistry A, 2019, 123, 1637-1647.	2.5	30
10	Comment on â€œIsomerization of the methoxy radical revisited: the impact of water dimersâ€•by B. Bandyopadhyay <i>et al.</i>, <i>Phys. Chem. Chem. Phys.</i>, 2016, 18, 27728 and â€œIsomerization of methoxy radical in the troposphere: competition between acidic, neutral and basic catalystsâ€•by P. Kumar, B. Bandyopadhyay <i>et al.</i>, <i>Phys. Chem. Chem. Phys.</i>, 2017, 19, 278. Physical Chemistry Chemical Physics, 2018, 20, 11481-11482.	2.8	2
11	Critical Review of Atmospheric Chemistry of Alkoxy Radicals. , 2017, , 185-269.		6
12	First kinetic study of the atmospherically important reactions BrHgË™ + NO2 and BrHgË™ + HOO. Physical Chemistry Chemical Physics, 2017, 19, 1826-1838.	2.8	51
13	Structures, Vibrational Frequencies, and Bond Energies of the BrHgOX and BrHgXO Species Formed in Atmospheric Mercury Depletion Events. Journal of Physical Chemistry A, 2017, 121, 7976-7985.	2.5	20
14	A new mechanism for atmospheric mercury redox chemistry: implications for the global mercury budget. Atmospheric Chemistry and Physics, 2017, 17, 6353-6371.	4.9	296
15	Thermodynamics limits the reactivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>BrHg</mml:mtext></mml:mrow><mml:mrow><mml:mtext /></mml:mrow></mml:msup></mml:mrow></mml:math> radical with volatile organic compounds. Chemical Physics Letters, 2016, 659, 289-294.	2.6	17
16	Tunneling effect in 1,5 H-migration of a prototypical OOQOOH. Chemical Physics Letters, 2016, 646, 153-157.	2.6	9
17	Quantum Chemical Study of Autoignition of Methyl Butanoate. Journal of Physical Chemistry A, 2015, 119, 7282-7292.	2.5	18
18	Quality Structures, Vibrational Frequencies, and Thermochemistry of the Products of Reaction of BrHg^{â€¢} with NO₂, HO₂, ClO, BrO, and IO. Journal of Physical Chemistry A, 2015, 119, 10502-10510.	2.5	27

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19	Quantum Chemistry Guide to PTRMS Studies of As-Yet Undetected Products of the Bromine-Atom Initiated Oxidation of Gaseous Elemental Mercury. Journal of Physical Chemistry A, 2014, 118, 7847-7854.	2.5	9
20	Rate Constants and Kinetic Isotope Effects for Methoxy Radical Reacting with NO₂ and O₂. Journal of Physical Chemistry A, 2014, 118, 3552-3563.	2.5	19
21	Pressure Dependence and Kinetic Isotope Effects in the Absolute Rate Constant for Methoxy Radical Reacting with NO₂. International Journal of Chemical Kinetics, 2014, 46, 501-511.	1.6	5
22	Quantum Chemistry, Reaction Kinetics, and Tunneling Effects in the Reaction of Methoxy Radicals with O2. Journal of Physical Chemistry A, 2013, 117, 14230-14242.	2.5	21
23	Thermodynamics of reactions of ClHg and BrHg radicals with atmospherically abundant free radicals. Atmospheric Chemistry and Physics, 2012, 12, 10271-10279.	4.9	107
24	Cisâ€“Trans Isomerization of Chemically Activated 1-Methylallyl Radical and Fate of the Resulting 2-Buten-1-peroxy Radical. Journal of Physical Chemistry A, 2012, 116, 7603-7614.	2.5	17
25	Temperature-Dependent Branching Ratios of Deuterated Methoxy Radicals (CH2DOâ€¢) Reacting With O2. Journal of Physical Chemistry A, 2012, 116, 6295-6302.	2.5	7
26	Effects of Olefin Group and Its Position on the Kinetics for Intramolecular H-Shift and HO₂ Elimination of Alkenyl Peroxy Radicals. Journal of Physical Chemistry A, 2011, 115, 655-663.	2.5	46
27	Impact of tunneling on hydrogen-migration of the n-propylperoxy radical. Physical Chemistry Chemical Physics, 2011, 13, 17969.	2.8	74
28	Understanding OH Yields in Electron Beam Irradiation of Humid N2. Plasma Chemistry and Plasma Processing, 2011, 31, 41-50.	2.4	3
29	Potential energy profiles for the N+HOCO reaction and products of the chemically activated reactions N+HOCO and H+HOCO. Chemical Physics Letters, 2010, 495, 170-174.	2.6	10
30	Atmospheric chemistry of isopropyl formate and <i>tert</i>â€butyl formate. International Journal of Chemical Kinetics, 2010, 42, 479-498.	1.6	18
31	Towards a Consistent Chemical Kinetic Model of Electron Beam Irradiation of Humid Air. Plasma Chemistry and Plasma Processing, 2009, 29, 347-362.	2.4	13
32	Observation and quantification of OH radicals in the far downstream part of an atmospheric microwave plasma jet using cavity ringdown spectroscopy. Applied Physics Letters, 2009, 95, 051501.	3.3	28
33	Optical diagnostics of a low powerâ€"low gas flow rates atmospheric-pressure argon plasma created by a microwave plasma torch. Plasma Sources Science and Technology, 2009, 18, 025030.	3.1	43
34	Failures and limitations of quantum chemistry for two key problems in the atmospheric chemistry of peroxy radicals. Atmospheric Environment, 2008, 42, 5837-5848.	4.1	35
35	Absorption Cross-Sections of the Câ€"H Overtone of Volatile Organic Compounds: 2 Methyl-1,3-Butadiene (Isoprene), 1,3-Butadiene, and 2,3-Dimethyl-1,3-Butadiene. Applied Spectroscopy, 2007, 61, 230-236.	2.2	16
36	Computational Studies of Intramolecular Hydrogen Atom Transfers in the Î²-Hydroxyethylperoxy and Î²-Hydroxyethoxy Radicals. Journal of Physical Chemistry A, 2007, 111, 5032-5042.	2.5	37

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37	Cyclization of 1,4-hydroxycarbonyls is not a homogenous gas phase process. Chemical Physics Letters, 2007, 447, 5-9.	2.6	13
38	Peroxy and alkoxy radicals from 2-methyl-3-buten-2-ol. Physical Chemistry Chemical Physics, 2006, 8, 456-463.	2.8	5
39	Exploration of the Potential Energy Surfaces, Prediction of Atmospheric Concentrations, and Prediction of Vibrational Spectra for the HO2Â·Â·Â·(H2O)n(n= 1â^'2) Hydrogen Bonded Complexes. Journal of Physical Chemistry A, 2006, 110, 3686-3691.	2.5	39
40	Computations on the ï¿½-?? transition of isoprene-OH-O2 peroxy radicals. Journal of Computational Chemistry, 2005, 26, 836-845.	3.3	3
41	Laser-Induced Fluorescence Spectra of 4-Methylcyclohexoxy Radical and Perdeuterated Cyclohexoxy Radical and Direct Kinetic Studies of Their Reactions with O2. Journal of Physical Chemistry A, 2005, 109, 9232-9240.	2.5	12
42	LIF Spectra of Cyclohexoxy Radical and Direct Kinetic Studies of Its Reaction with O2. Journal of Physical Chemistry A, 2004, 108, 447-454.	2.5	16
43	Intramolecular Hydrogen Bonding and Double H-Atom Transfer in Peroxy and Alkoxy Radicals from Isoprene. Journal of Physical Chemistry A, 2004, 108, 2199-2207.	2.5	50
44	Prompt Chemistry of Alkenoxy Radical Products of the Double H-Atom Transfer of Alkoxy Radicals from Isoprene. Journal of Physical Chemistry A, 2004, 108, 2208-2215.	2.5	34
45	Isomerization and Decomposition Reactions of Primary Alkoxy Radicals Derived from Oxygenated Solvents. Journal of Physical Chemistry A, 2003, 107, 63-72.	2.5	50
46	Isomerization of OH-Isoprene Adducts and Hydroxyalkoxy Isoprene Radicals. Journal of Physical Chemistry A, 2002, 106, 6643-6650.	2.5	62
47	Mechanism and dynamics of the CH2OH+O2 reaction. Chemical Physics Letters, 2002, 355, 193-200.	2.6	42
48	Reactions of the Alkoxy Radicals Formed Following OH-Addition to Î±-Pinene and Î²-Pinene. Câ^'C Bond Scission Reactions. Journal of the American Chemical Society, 2001, 123, 4228-4234.	13.7	50
49	Direct Kinetic Studies of Reactions of 3-Pentoxy Radicals with NO and O2. Journal of Physical Chemistry A, 2001, 105, 8985-8990.	2.5	23
50	Direct kinetic studies of the reactions of 2-butoxy radicals with NO and O2. Chemical Physics Letters, 2000, 330, 541-546.	2.6	29
51	Observation of Fluorescence Excitation Spectra oftert-Pentoxy and 3-Pentoxy Radicalsâ€. Journal of Physical Chemistry A, 2000, 104, 10368-10373.	2.5	19
52	Characterization of HOCH2CH2O and its dissociation pathway. Chemical Physics Letters, 1999, 301, 297-302.	2.6	13
53	A Quantum Chemical Study of the Câ^'C Bond Fission Pathways of Alkoxy Radicals Formed following OH Addition to Isoprene. Journal of Physical Chemistry A, 1999, 103, 8559-8565.	2.5	43
54	Laser-Induced Fluorescence Excitation Spectra oftert-Butoxy and 2-Butoxy Radicals. Journal of Physical Chemistry A, 1999, 103, 8207-8212.	2.5	32

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55	Structure, Vibrational Frequencies, and Stability of a Reactive Intermediate:Â FOONO. Journal of the American Chemical Society, 1997, 119, 2894-2895.	13.7	5
56	EXPERIMENTAL AND THEORETICAL PROGRESS IN UNDERSTANDING THE ROLE OF CX₃ RADICALS IN ATMOSPHERIC CHEMICAL PROCESSES. Advanced Series in Physical Chemistry, 1995, , 686-743.	1.5	2
57	Observation of the time evolution of phase changes in clusters. Journal of the American Chemical Society, 1990, 112, 890-891.	13.7	28
58	Modeling electron beam irradiation of methane. International Journal of Chemical Kinetics, 0, , .	1.6	1