

Theodore S Dibble

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2405860/publications.pdf>

Version: 2024-02-01

58
papers

1,704
citations

257101

24
h-index

301761

39
g-index

70
all docs

70
docs citations

70
times ranked

1440
citing authors

#	ARTICLE	IF	CITATIONS
1	A new mechanism for atmospheric mercury redox chemistry: implications for the global mercury budget. <i>Atmospheric Chemistry and Physics</i> , 2017, 17, 6353-6371.	1.9	296
2	Thermodynamics of reactions of ClHg and BrHg radicals with atmospherically abundant free radicals. <i>Atmospheric Chemistry and Physics</i> , 2012, 12, 10271-10279.	1.9	107
3	Impact of tunneling on hydrogen-migration of the n-propylperoxy radical. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17969.	1.3	74
4	Improved Mechanistic Model of the Atmospheric Redox Chemistry of Mercury. <i>Environmental Science & Technology</i> , 2021, 55, 14445-14456.	4.6	65
5	Isomerization of OH-Isoprene Adducts and Hydroxyalkoxy Isoprene Radicals. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6643-6650.	1.1	62
6	First kinetic study of the atmospherically important reactions BrHg \dot{E}^{TM} + NO ₂ and BrHg \dot{E}^{TM} + HOO. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1826-1838.	1.3	51
7	Reactions of the Alkoxy Radicals Formed Following OH-Addition to \hat{I}^{\pm} -Pinene and \hat{I}^2 -Pinene. C \hat{C} Bond Scission Reactions. <i>Journal of the American Chemical Society</i> , 2001, 123, 4228-4234.	6.6	50
8	Isomerization and Decomposition Reactions of Primary Alkoxy Radicals Derived from Oxygenated Solvents. <i>Journal of Physical Chemistry A</i> , 2003, 107, 63-72.	1.1	50
9	Intramolecular Hydrogen Bonding and Double H-Atom Transfer in Peroxy and Alkoxy Radicals from Isoprene. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2199-2207.	1.1	50
10	Effects of Olefin Group and Its Position on the Kinetics for Intramolecular H-Shift and HO ₂ Elimination of Alkenyl Peroxy Radicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 655-663.	1.1	46
11	A Quantum Chemical Study of the C \hat{C} Bond Fission Pathways of Alkoxy Radicals Formed following OH Addition to Isoprene. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8559-8565.	1.1	43
12	Optical diagnostics of a low power, low gas flow rates atmospheric-pressure argon plasma created by a microwave plasma torch. <i>Plasma Sources Science and Technology</i> , 2009, 18, 025030.	1.3	43
13	Mechanism and dynamics of the CH ₂ OH+O ₂ reaction. <i>Chemical Physics Letters</i> , 2002, 355, 193-200.	1.2	42
14	Exploration of the Potential Energy Surfaces, Prediction of Atmospheric Concentrations, and Prediction of Vibrational Spectra for the HO ₂ ·(H ₂ O) _n (n= 1 $\hat{2}$) Hydrogen Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 3686-3691.	1.1	39
15	Computational Studies of Intramolecular Hydrogen Atom Transfers in the \hat{I}^2 -Hydroxyethylperoxy and \hat{I}^2 -Hydroxyethoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5032-5042.	1.1	37
16	Failures and limitations of quantum chemistry for two key problems in the atmospheric chemistry of peroxy radicals. <i>Atmospheric Environment</i> , 2008, 42, 5837-5848.	1.9	35
17	Prompt Chemistry of Alkenoxy Radical Products of the Double H-Atom Transfer of Alkoxy Radicals from Isoprene. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2208-2215.	1.1	34
18	Modeling the OH-Initiated Oxidation of Mercury in the Global Atmosphere without Violating Physical Laws. <i>Journal of Physical Chemistry A</i> , 2020, 124, 444-453.	1.1	33

#	ARTICLE	IF	CITATIONS
19	Laser-Induced Fluorescence Excitation Spectra of tert-Butoxy and 2-Butoxy Radicals. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8207-8212.	1.1	32
20	Computational Study on the Photolysis of BrHgONO and the Reactions of BrHgO [•] with CH ₄ , C ₂ H ₆ , NO, and NO ₂ : Implications for Formation of Hg(II) Compounds in the Atmosphere. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1637-1647.	1.1	30
21	Direct kinetic studies of the reactions of 2-butoxy radicals with NO and O ₂ . <i>Chemical Physics Letters</i> , 2000, 330, 541-546.	1.2	29
22	Observation of the time evolution of phase changes in clusters. <i>Journal of the American Chemical Society</i> , 1990, 112, 890-891.	6.6	28
23	Observation and quantification of OH radicals in the far downstream part of an atmospheric microwave plasma jet using cavity ringdown spectroscopy. <i>Applied Physics Letters</i> , 2009, 95, 051501.	1.5	28
24	Quality Structures, Vibrational Frequencies, and Thermochemistry of the Products of Reaction of BrHg [•] with NO ₂ , HO ₂ , ClO, BrO, and IO. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10502-10510.	1.1	27
25	Direct Kinetic Studies of Reactions of 3-Pentoxo Radicals with NO and O ₂ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 8985-8990.	1.1	23
26	Quantum Chemistry, Reaction Kinetics, and Tunneling Effects in the Reaction of Methoxy Radicals with O ₂ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 14230-14242.	1.1	21
27	Structures, Vibrational Frequencies, and Bond Energies of the BrHgOX and BrHgXO Species Formed in Atmospheric Mercury Depletion Events. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7976-7985.	1.1	20
28	Observation of Fluorescence Excitation Spectra of tert-Pentoxo and 3-Pentoxo Radicals. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10368-10373.	1.1	19
29	Rate Constants and Kinetic Isotope Effects for Methoxy Radical Reacting with NO ₂ and O ₂ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 3552-3563.	1.1	19
30	Atmospheric chemistry of isopropyl formate and tert-butyl formate. <i>International Journal of Chemical Kinetics</i> , 2010, 42, 479-498.	1.0	18
31	Quantum Chemical Study of Autoignition of Methyl Butanoate. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7282-7292.	1.1	18
32	Cis-Trans Isomerization of Chemically Activated 1-Methylallyl Radical and Fate of the Resulting 2-Buten-1-peroxy Radical. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7603-7614.	1.1	17
33	Thermodynamics limits the reactivity of BrHg radical with volatile organic compounds. <i>Chemical Physics Letters</i> , 2016, 653, 283-284.		
34	LIF Spectra of Cyclohexoxy Radical and Direct Kinetic Studies of Its Reaction with O ₂ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 447-454.	1.1	16
35	Absorption Cross-Sections of the C-H Overtone of Volatile Organic Compounds: 2-Methyl-1,3-Butadiene (Isoprene), 1,3-Butadiene, and 2,3-Dimethyl-1,3-Butadiene. <i>Applied Spectroscopy</i> , 2007, 61, 230-236.	1.2	16
36	BrHgO [•] + CO: Analogue of OH + CO and Reduction Path for Hg(II) in the Atmosphere. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 1777-1784.	1.2	16

#	ARTICLE	IF	CITATIONS
37	Characterization of HOCH ₂ CH ₂ O and its dissociation pathway. Chemical Physics Letters, 1999, 301, 297-302.	1.2	13
38	Cyclization of 1,4-hydroxycarbonyls is not a homogenous gas phase process. Chemical Physics Letters, 2007, 447, 5-9.	1.2	13
39	Towards a Consistent Chemical Kinetic Model of Electron Beam Irradiation of Humid Air. Plasma Chemistry and Plasma Processing, 2009, 29, 347-362.	1.1	13
40	BrHgO [•] + C ₂ H ₄ and BrHgO [•] + 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.	1.1	13
41	Laser-Induced Fluorescence Spectra of 4-Methylcyclohexoxy Radical and Perdeuterated Cyclohexoxy Radical and Direct Kinetic Studies of Their Reactions with O ₂ . Journal of Physical Chemistry A, 2005, 109, 9232-9240.	1.1	12
42	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.	1.2	10
43	First experimental kinetic study of the atmospherically important reaction of BrHg [•] +NO ₂ . Chemical Physics Letters, 2020, 759, 137928.	1.2	10
44	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.	1.1	9
45	Tunneling effect in 1,5 H-migration of a prototypical OOQOOH. Chemical Physics Letters, 2016, 646, 153-157.	1.2	9
46	Temperature-Dependent Branching Ratios of Deuterated Methoxy Radicals (CH ₂ DO [•]) Reacting With O ₂ . Journal of Physical Chemistry A, 2012, 116, 6295-6302.	1.1	7
47	Critical Review of Atmospheric Chemistry of Alkoxy Radicals. , 2017, , 185-269.		6
48	Structure, Vibrational Frequencies, and Stability of a Reactive Intermediate: FOONO. Journal of the American Chemical Society, 1997, 119, 2894-2895.	6.6	5
49	Peroxy and alkoxy radicals from 2-methyl-3-buten-2-ol. Physical Chemistry Chemical Physics, 2006, 8, 456-463.	1.3	5
50	Pressure Dependence and Kinetic Isotope Effects in the Absolute Rate Constant for Methoxy Radical Reacting with NO ₂ . International Journal of Chemical Kinetics, 2014, 46, 501-511.	1.0	5
51	Computations on the $\tilde{\nu}_{1/2}$ transition of isoprene-OH-O ₂ peroxy radicals. Journal of Computational Chemistry, 2005, 26, 836-845.	1.5	3
52	Understanding OH Yields in Electron Beam Irradiation of Humid N ₂ . Plasma Chemistry and Plasma Processing, 2011, 31, 41-50.	1.1	3
53	Combined Experimental and Computational Kinetics Studies for the Atmospherically Important BrHg Radical Reacting with NO and O ₂ . Journal of Physical Chemistry A, 2022, 126, 3914-3925.	1.1	3
54	Comment on "Isomerization of the methoxy radical revisited: the impact of water dimers" by B. Bandyopadhyay et al., Phys. Chem. Chem. Phys., 2016, 18, 27728 and "Isomerization of methoxy radical in the troposphere: competition between acidic, neutral and basic catalysts" by P. Kumar, B. Bandyopadhyay et al., Phys. Chem. Chem. Phys., 2017, 19, 278. Physical Chemistry Chemical Physics, 2018, 20, 11481-11482.	1.3	2

#	ARTICLE	IF	CITATIONS
55	EXPERIMENTAL AND THEORETICAL PROGRESS IN UNDERSTANDING THE ROLE OF CX_3 RADICALS IN ATMOSPHERIC CHEMICAL PROCESSES. Advanced Series in Physical Chemistry, 1995, , 686-743.	1.5	2
56	Reaction mechanism and kinetics of the important but neglected reaction of Hg with NO ₂ at low temperature. Chemical Engineering Journal, 2022, 432, 134373.	6.6	2
57	Theoretical Study of the Monohydration of Mercury Compounds of Atmospheric Interest. Journal of Physical Chemistry A, 2021, 125, 5819-5828.	1.1	1
58	Modeling electron beam irradiation of methane. International Journal of Chemical Kinetics, 0, , .	1.0	1