

## Papers by Theodore S. Dibble

Last updated May 16, 2016

- 64) A Quantum Chemistry Guide to PTRMS Studies of as-yet Undetected Products of the Bromine-Atom Initiated Oxidation of Gaseous Elemental Mercury. T. S. Dibble, M. J. Zelie, and Y. Jiao, *J. Phys. Chem. A*, submitted.
- 63) Pressure Dependence and Kinetic Isotope Effects in the Absolute Rate Constant for Methoxy Radical Reacting with NO<sub>2</sub>. J. Chai and T. S. Dibble, *Int. J. Chem. Kinet.*, **2014**, in press.
- 62) Rate Constants and Kinetic Isotope Effects for Methoxy Radical Reacting with NO<sub>2</sub> and O<sub>2</sub>. J. Chai, H. Hu, T. S. Dibble, G. S. Tyndall, and J. J. Orlando. *J. Phys. Chem. A*, **2014**, in press (<http://pubs.acs.org/doi/abs/10.1021/jp501205d>).
- 61) Quantum Chemistry, Reaction Kinetics, and Tunneling Effects in the Reaction of Methoxy Radicals with O<sub>2</sub>. H. Hu and T. S. Dibble. *J. Phys. Chem. A*, **2013**, 117, 14230–42.
- 60) Thermodynamics of reactions of ClHg and BrHg radicals with atmospherically abundant free radicals. T. S. Dibble, M. J. Zelie, and H. Mao. *Atmos. Chem. Phys.*, **2012**. <http://dx.doi.org/0.5194/acp-12-10271-2012>.
- 59) Cis-trans isomerization of chemically activated 1-methylallyl radical and fate of the resulting 2-buten-1-peroxy radical. T. S. Dibble, Y. Sha, W. F. Thornton, and F. Zhang. *J. Phys. Chem. A*, **2012**, 116, 7603–7614.
- 57) Impact of Tunneling on hydrogen-migration of n-propylperoxy radical. F. Zhang and T. S. Dibble, *Phys. Chem. Chem. Phys.*, **2011**, 13, 17969-77.
- 56) Understanding OH Yields in Electron Beam Irradiation of Humid N<sub>2</sub>. K. L. Schmitt and T. S. Dibble. *Plasma Chem. Plasma Proc.*, **31**, 41-50 (2011).
- 55) Effects of Olefin Group and Its Position on the Kinetics for Intramolecular H-Shift and HO<sub>2</sub> Elimination of Alkenyl Peroxy Radicals. F. Zhang and T. S. Dibble, *J. Phys. Chem. A*, **115**, 655-63 (2011).
- 54) Potential Energy Profiles for the N + HOCO Reaction and Products of the Chemically Activated Reactions N + HOCO and H + HOCO. T. S. Dibble and Y. Zeng, *Chem. Phys. Lett.*, **2010**, 495, 170-4.
- 53) Atmospheric Chemistry of Isopropyl Formate and tert-Butyl Formate. A. S. Pimentel, G. S. Tyndall, J. J. Orlando, M. D. Hurley, and T. J. Wallington, M. P. Sulbaek Andersen, P. Marshall, and T. S. Dibble, *Int. J. Chem. Kinet.*, **2010**, 42, 479-498.
- 52) Towards a Consistent Chemical Kinetic Model of Electron Beam Irradiation of Humid Air. K. L. Schmitt, D. M. Murray, and T. S. Dibble. *Plasma Chem. Plasma Proc.*, 29, 347-362 (2009).
- 51) Observation of OH Radicals in the Far Downstream Part of an Atmospheric Microwave Plasma Jet Using Cavity Ringdown Spectroscopy. C. Wang, N. Shrivastava, and T. S. Dibble, *Appl. Phys. Lett.*, 95, 051501 (2009).
- 50) A study of OH radicals in an atmospheric AC discharge plasma using near infrared diode laser cavity ringdown spectroscopy combined with optical emission spectroscopy, *Eur. J. Phys. D*, 54, 77-86 (2009).

- 49) Optical diagnostics of a low power - low gas flow rates atmospheric-pressure argon microwave induced plasma, C. Wang, N. Srivastava, S. Scherrer, P.-R. Jang, T. S. Dibble, and Y. Duan, *Plasma Sources Sci. and Technol.*, **18**, 025030 (2009).
- 48) Failures and Limitations of Quantum Chemistry for Two Key Problems in the Atmospheric Chemistry of Peroxy Radicals. T. S. Dibble, *Atmos. Environ.*, **42**, 5837-48 (2008).
- 47) Cyclization of 1,4-hydroxycarbonyls is not a homogenous gas-phase process. T. S. Dibble, *Chem. Phys. Lett.*, **447**, 5-9 (2007).
- 46) Computational studies of intramolecular hydrogen atom transfers in the  $\beta$ -hydroxyethoxy and  $\beta$ -hydroxyethylperoxy radicals. K. T. Kuwata, T. S. Dibble, E. Sliz, and E. B. Petersen. *J. Phys. Chem. A*, **111**, 5032-42 (2007).
- 45) Absorption cross-sections of CH-overtone of volatile organic compounds: 2 methyl-1,3-butadiene (isoprene), 1,3-butadiene, and 2,3-dimethyl-1,3-butadiene, P. Cias, C. Wang, and T. S. Dibble, *Appl. Spect.*, **61**, 230-6 (2007).
- 44) Exploration of the Potential Energy Surface and Prediction of the Atmospheric Abundance and Vibrational Spectra of the  $\text{HO}_2 \cdots (\text{H}_2\text{O})_n$  ( $n=1-2$ ) Hydrogen-Bonded Complexes, K. S. Alongi, T. S. Dibble, G. C. Shields, and K. N. Kirschner, *J. Phys. Chem. A*, **110**, 3686-3691 (2006).
- 43) Peroxy and alkoxy radicals from 2-methyl-3-buten-2-ol. T. S. Dibble and T. Pham, *Phys Chem. Chem. Phys.*, **8**, 456-463 (2006).
- 42) LIF spectra of 4-methylcyclohexoxy radical and perdeuterated cyclohexoxy radicals and direct kinetic studies of their reaction with  $\text{O}_2$ . L. Zhang, K. M. Callahan, D. Derbyshire, and T. S. Dibble, *J. Phys. Chem. A*, **109**, 9232-9240 (2005).
- 41) Computations on the  $\tilde{A} - \tilde{X}$  Transition of Isoprene-OH- $\text{O}_2$  Peroxy Radicals. T. S. Dibble. *J. Comput. Chem.* **26**, 836-845 (2005).
- 40) Prompt chemistry of alkenoxy radical products of the double H-atom transfer of alkoxy radicals from isoprene. T. S. Dibble, *J. Phys. Chem. A*, **108**, 2208-2215 (2004).
- 39) Intramolecular hydrogen bonding and double H-atom transfer in peroxy and alkoxy radicals from isoprene. T. S. Dibble, *J. Phys. Chem. A*, **108**, 2199-2207 (2004).
- 38) LIF spectra of cyclohexoxy radical and direct kinetic studies of its reaction with  $\text{O}_2$ . L. Zhang, K. A. Kitney, M. A. Ferenac, W. Deng and T. S. Dibble, *J. Phys. Chem. A* **108**, 447-454 (2004).
- 37) Isomerization and decomposition reactions of primary alkoxy radicals derived from oxygenated solvents, M. A. Ferenac, A. J. Davis, A. S. Holloway, and T. S. Dibble, *J. Phys. Chem. A*, **107**, 63-72 (2003).
- 36) Do aerosols act as catalysts in the OH radical initiated atmospheric oxidation of volatile organic compounds? M. Sørensen, M. D. Hurley, T. J. Wallington, T. S. Dibble, and O. J. Nielsen, *Atmos. Environ.*, **36**, 5947-5952 (2002).
- 35) Isomerization of OH-isoprene adducts and hydroxyalkoxy isoprene radicals, T. S. Dibble, *J. Phys. Chem. A*, **106** 6643-6650 (2002).
- 34) Mechanism and dynamics of the  $\text{CH}_2\text{OH} + \text{O}_2$  reaction. T. S. Dibble, *Chem. Phys. Lett.*, **355** 193-200 (2002).

- 33) Direct Kinetic Studies of Reactions of 3-Pentoxy Radicals with NO and O<sub>2</sub>. W. Deng, A. J. Davis, L. Zhang, D. R. Katz, and T. S. Dibble, *J. Phys. Chem. A*, **105** 8985-90 (2001).
- 32) Reactions of the Alkoxy Radicals Formed Following OH-addition to  $\alpha$ -pinene and  $\beta$ -pinene. C-C Bond Scission Reactions. T. S. Dibble, *J. Am. Chem. Soc.*, **123** 4228-4234 (2001).
- 31) Direct kinetic studies of the reactions of 2-butoxy radicals with NO and O<sub>2</sub>. W. Deng, C. Wang, D. R. Katz, G. R. Gawinski, A. J. Davis, and T. S. Dibble, *Chem. Phys. Lett.*, **330** 541-6 (2000).
- 30) Observation of Fluorescence Excitation Spectra of tert-Pentoxy and 3-Pentoxy Radicals, C. Wang, W. Deng, L. G. Shemesh, M. D. Lilien, D. R. Katz, and T. S. Dibble, *J. Phys. Chem. A*, **104** 10368-73 (2000).
- 29) A Quantum Chemical Study of the C-C Bond Fission Pathways of Alkoxy Radicals Formed Following OH Addition to Isoprene. T. S. Dibble, *J. Phys. Chem. A*, **103** 8559-65 (1999).
- 28) Laser-Induced Fluorescence Excitation Spectra of tert-Butoxy and 2-Butoxy Radicals. C. Wang, L. G. Shemesh, W. Deng, M. D. Lilien, and T. S. Dibble, *J. Phys. Chem. A*, **103** 8207-12 (1999).
- 27) Structure and Vibrational Frequencies of the Alkoxy Radicals CH<sub>2</sub>FO and CHF<sub>2</sub>O. T. S. Dibble, *J. Molec. Structure*, Invited paper for Special Issue to Honor Professor Lawrence S. Bartell, **485-6** 67-71 (1999).
- 26) Characterization of HOCH<sub>2</sub>CH<sub>2</sub>O• and its Dissociation Pathway. T. S. Dibble, *Chem. Phys. Letts.*, **301** 297-302 (1999).
- 25) Generation of Energetic He Atoms by a Pulsed Positive Corona Discharge. S-Y. Lo, J.D. Lobo, S. Blumberg, T. S. Dibble, C-C. Tsao, and M. Okumura, *J. Appl. Phys.*, **81** 5896-904 (1997).
- 24) Structure, Vibrational Frequencies, and Stability of a Reactive Intermediate: FOONO. T. S. Dibble and J. S. Francisco, *J. Am. Chem. Soc.*, **119** 2894-5 (1997).
- 23) Evaluating the Accuracy of Density-Functional Methods for ClOO. V. R. Morris, S. C. Bhatia, T. S. Dibble, and J. S. Francisco. *J. Chem. Phys.* **104**, 5345-6 (1996).
- 22) Kinetics of the Reaction of CF<sub>3</sub>O with NO. T. S. Dibble, M.M. Maricq, J. J. Szente, and J. S. Francisco. *J. Phys. Chem.* **99** 17394-402 (1995).
- 21) CF<sub>3</sub>CO Dissociation Kinetics. M.M. Maricq, J. J. Szente, G. A. Khitrov, T. S. Dibble, and J. S. Francisco, *J. Phys. Chem.* **99** 11875-82 (1995).
- 20) Dissociation of Acetyl Bromide. An Experimental and Theoretical Study. Y. Su, T. S. Dibble, Z. Li, and J. S. Francisco. *Chem. Phys.* **196** 59-67 (1995).
- 19) Ab Initio Study of the Structure, Binding Energy, and Vibrational Frequencies of the HOCl-H<sub>2</sub>O complex, T. S. Dibble and J. S. Francisco, *J. Phys. Chem.* **99**, 1919-22 (1995).
- 18) Experimental and Theoretical Progress in Understanding the Role of CX<sub>3</sub> Radicals in Atmospheric Chemical Kinetics. Z. Li, T. S. Dibble, and J. S. Francisco, In *Progress and Problems in Atmospheric Chemistry*, J. R. Barker, Ed.; World Scientific, Singapore, 1995, 646-743.

- 17) Reply to Comment on the Atmospheric Chemistry of FNO. T. S. Dibble and J. S. Francisco, *J. Phys. Chem.* **98** 10374 (1994).
- 16) Atmospheric Chemical Kinetics of FC(O)O. M.M. Maricq, J. J. Szente, T. S. Dibble, and J. S. Francisco, *J. Phys. Chem.* **98**, 12294-309 (1994).
- 15) An Ab Initio Study of the Heat of Formation of FC(O)O and FC(O)OH, T. S. Dibble and J. S. Francisco, *J. Phys. Chem.* **98**, 11694-6 (1994).
- 14) The Last Chapter in Chlorofluorocarbon Photo-oxidation Processes: Formation and Dissociation of FC(O)ONO. T. S. Dibble and J. S. Francisco, *J. Phys. Chem.* **98**, 5010-8 (1994).
- 13) A CASSCF and Density Functional Theory Study of FNO, T. S. Dibble, J. S. Francisco, R. J. Deeth, M. R. Hand, and I. H. Williams. *J. Chem. Phys.* **100**, 459-63 (1994).
- 12) Ab Initio Study of the Reaction  $\text{CF}_3\text{CHO} + \text{X} \rightarrow \text{CF}_3\text{CO} + \text{HX}$  ( $\text{X}=\text{F}, \text{Cl}$ ), T. S. Dibble and J. S. Francisco, *Chem. Phys. Lett.* **215** 409-15 (1993).
- 11) FNO<sub>2</sub>: Improving Calculated Structures at the Second-Order Moller-Plesset Level of Theory, T. S. Dibble and J. S. Francisco. *Chem. Phys. Lett.* **215**, 423-6 (1993).
- 10) FNO: Another Challenging Molecule for Electron Correlation Methods. T. S. Dibble and J. S. Francisco. *J. Chem. Phys.* **99**, 397-402 (1993).
- 9) Observation of a Crystalline Phase Predicted for Transition Metal Hexafluorides. L. S. Bartell, J. W. Hovick, T. S. Dibble, and P.J. Lennon, *J. Phys. Chem.* **97**, 230-2 (1993).
- 8) Electron Diffraction Studies of the Kinetics of Phase Changes in Molecular Clusters. 3. Solid State Transitions in SeF<sub>6</sub> and (CH<sub>3</sub>)<sub>3</sub>CCl. T. S. Dibble and L. S. Bartell, *J. Phys. Chem.* **96**, 8603-10 (1992).
- 7) Structure and Transformation. Clusters as Models for Condensed Phases. L. S. Bartell, T. S. Dibble, J. W. Hovick, and S. Xu. NATO ASI Ser. C (1992), **374** (Physics and Chemistry of Finite Systems: Clusters Cryst., Vol. 1), 71-6.
- 6) Kinetics of Phase Changes in Large Molecular Clusters. L. S. Bartell and T. S. Dibble, *Z. fur Physik D* **20**, 255 (1991).
- 5) Electron Diffraction Studies of the Kinetics of Phase Changes in Molecular Clusters. 2. Freezing of CH<sub>3</sub>CCl<sub>3</sub> in Supersonic Flow. T. S. Dibble and L. S. Bartell, *J. Phys. Chem.* **96**, 2317-22 (1991).
- 4) Electron Diffraction Studies of the Kinetics of Phase Changes in Molecular Clusters. Freezing of CCl<sub>4</sub> in Supersonic Flow. L. S. Bartell and T. S. Dibble, *J. Phys. Chem.* **95**, 1159-67 (1991).
- 3) Factors Governing the Phase of Clusters Nucleated in Supersonic Flow. L. S. Bartell, L. Harsanyi, T. S. Dibble, and P. J. Lennon, *J. Phys. Chem.* **94**, 6009-12 (1990).
- 2) Test of an Empirical Criterion for Predicting Cluster Phase. L. S. Bartell, E. J. Valente, and T. S. Dibble, *J. Phys. Chem.* **94**, 1452-3 (1990).
- 1) Observation of the Time Evolution of Phase Changes in Clusters. L. S. Bartell and T. S. Dibble, *J. Amer. Chem. Soc.* **112**, 890-1 (1990).