

## 8 References

1. Finlayson-Pitts, B. J. and J. N. Pitts, *Chemistry of the Upper and Lower Atmosphere*. 2000, San Diego, California: Academic Press.
2. Seinfeld, J. H. and S. N. Pandis, *Atmospheric Chemistry and Physics- From Air Pollution to Climate Change*. 1998, New York: John Wiley and Sons.
3. Tonnesen, G. S., "Effects of uncertainty in the reaction of the hydroxyl radical with nitrogen dioxide on model-simulated ozone control strategies". *Atmospheric Environment*, 1999. **33**(10): p. 1587-1598.
4. Martien, P. T. and R. A. Harley, "Adjoint sensitivity analysis for a three-dimensional photochemical model: Application to Southern California". *Environmental Science & Technology*, 2006. **40**(13): p. 4200-4210.
5. Martien, P. T. and R. A. Harley, "Adjoint sensitivity analysis for a three-dimensional photochemical model: Implementation and method comparison". *Environmental Science & Technology*, 2006. **40**(8): p. 2663-2670.
6. Robertshaw, J. S. and I. W. M. Smith, "Kinetics of the hydroxyl + nitrogen dioxide + argon and hydroxyl + nitrogen dioxide + tetrafluoromethane reactions at high total pressures". *Journal of Physical Chemistry*, 1982. **86**(5): p. 785-790.
7. Bean, B. D., A. K. Mollner, S. A. Nizkorodov, G. Nair, M. Okumura, S. P. Sander, K. A. Peterson, and J. S. Francisco, "Cavity ringdown spectroscopy of cis-cis HOONO and the HOONO/HONO2 branching ratio in the reaction OH+NO2+M". *Journal of Physical Chemistry A*, 2003. **107**(36): p. 6974-6985.
8. Berden, G., R. Peeters, and G. Meijer, "Cavity ring-down spectroscopy: Experimental schemes and applications". *International Reviews of Physical Chemistry*, 2000. **19**(4): p. 565-607.

9. Jongma, R. T., M. G. H. Boogaarts, I. Holleman, and G. Meijer, "Trace gas detection with cavity ring down spectroscopy". *Reviews of Scientific Instruments*, 1995. **66**(4): p. 2821-2828.
10. Paldus, B. A. and A. A. Kachanov, "An historical overview of cavity-enhanced methods". *Canadian Journal of Physics*, 2005. **83**(10): p. 975-999.
11. Scherer, J. J., J. B. Paul, A. Okeefe, and R. J. Saykally, "Cavity ringdown laser absorption spectroscopy: History, development, and application to pulsed molecular beams". *Chemical Reviews*, 1997. **97**(1): p. 25-51.
12. Wheeler, M. D., S. M. Newman, A. J. Orr-Ewing, and M. N. R. Ashfold, "Cavity ring-down spectroscopy". *Journal of the Chemical Society - Faraday Transactions*, 1998. **94**(3): p. 337-351.
13. Meijer, G., M. G. H. Boogaarts, R. T. Jongma, D. H. Parker, and A. M. Wodtke, "Coherent cavity ring down spectroscopy". *Chemical Physics Letters*, 1994. **217**(1-2): p. 112-116.
14. Hodges, J. T., J. P. Looney, and R. D. van Zee, "Response of a ring-down cavity to an arbitrary excitation". *Journal of Chemical Physics*, 1996. **105**(23): p. 10287-10288.
15. Hodges, J. T., J. P. Looney, and R. D. van Zee, "Laser bandwidth effects in quantitative cavity ring-down spectroscopy". *Applied Optics*, 1996. **35**(21): p. 4112-4116.
16. O'Keefe, A. and D. A. G. Deacon, "Cavity ring-down optical spectrometer for absorption measurements using pulsed laser sources". *Review of Scientific Instruments*, 1988. **59**(12): p. 2544-2551.
17. Romanini, D. and K. K. Lehmann, "Ring-down cavity absorption spectroscopy of the very weak hydrogen cyanide overtone bands with six, seven, and eight stretching quanta". *Journal of Chemical Physics*, 1993. **99**(9): p. 6287-301.
18. Zalicki, P. and R. N. Zare, "Cavity ring-down spectroscopy for quantitative absorption measurements". *Journal of Chemical Physics*, 1995. **102**(7): p. 2708-2717.

19. Fuelberth, T. M., M.S. Thesis. "The building of an infrared source for use in free radical kinetics important in stratospheric ozone depletion: Cavity ringdown detection", California Institute of Technology, 1997.
20. Garland, E. R., Ph.D. Thesis. "Laboratory studies of atmospheric reactions using infrared cavity ringdown spectroscopy", California Institute of Technology, 2002.
21. Reid, S. A. and Y. Tang, "Generation of tunable, narrow-band mid-infrared radiation through a 532-nm-pumped KTP optical parametric amplifier". *Applied Optics*, 1996. **35**(9): p. 1473-1477.
22. Chackerian, C., S. W. Sharpe, and T. A. Blake, "Anhydrous nitric acid integrated absorption cross sections: 820-5300  $\text{cm}^{-1}$ ". *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2003. **82**(1-4): p. 429-441.
23. Lange, K. R., N. P. Wells, K. S. Plegge, and J. A. Phillips, "Integrated Intensities of O-H Stretching Bands: Fundamentals and Overtones in Vapor-Phase Alcohols and Acids". *Journal of Physical Chemistry A*, 2001. **105**: p. 3481-3486.
24. Phillips, J. A., J. J. Orlando, G. S. Tyndall, and V. Vaida, "Integrated Intensities of OH vibrational overtones in alcohols". *Chemical Physics Letters*, 1998. **296**: p. 377-383.
25. Biaueme, F., "Nitric Acid Vapour Absorption Cross-Section Spectrum and its Photodissociation in the Stratosphere". *Journal of Photochemistry*, 1973. **2**: p. 139-149.
26. Burkholder, J. A., R. K. Talukdar, A. R. Ravishankara, and S. Solomon, "Temperature Dependence of the  $\text{HNO}_3$  UV Absorption Cross Sections". *Journal of Geophysical Research*, 1993. **98**(D12): p. 22937-22948.
27. Johnston, H. and R. Graham, "Gas-phase ultraviolet absorption spectrum of nitric acid vapor". *Journal of Physical Chemistry*, 1973. **77**(1): p. 62-63.
28. Molina, L. T. and M. J. Molina, "UV Absorption Cross-Sections of  $\text{HO}_2\text{NO}_2$  Vapor". *Journal of Photochemistry*, 1981. **15**(2): p. 97-108.

29. Okabe, H., "Photodissociation of nitric acid and water in the vacuum ultraviolet; vibrational and rotational distributions of OH". *Journal of Chemical Physics*, 1980. **72**(12): p. 6642-6650.
30. Rattigan, O., E. Lutman, R. L. Jones, R. A. Cox, K. Clemitshaw, and J. Williams, "Temperature-dependent absorption cross sections of gaseous nitric acid and methyl nitrate". *Journal of Photochemistry and Photobiology A-Chemistry*, 1992. **66**(3): p. 313-326.
31. Suto, M. and L. C. Lee, "Photoabsorption and photodissociation of HONO<sub>2</sub> in the 105-220nm region". *Journal of Chemical Physics*, 1984. **81**(3): p. 1294-1297.
32. Connell, P. S. and C. J. Howard, "Kinetics study of the reaction HO + HNO<sub>3</sub>". *International Journal of Chemical Kinetics*, 1985. **17**: p. 17-31.
33. Wine, P. H., A. R. Ravishankara, N. M. Kreutter, R. C. Shah, J. M. Nicovich, and R. L. Thompson, "Rate of reaction of OH with HNO<sub>3</sub>". *Journal of Geophysical Research*, 1981. **86**(C2): p. 1105-1112.
34. Yalin, A. P. and R. N. Zare, "Effects of laser lineshape on the quantitative analysis of cavity ring-down signals". *Laser Physics*, 2002. **12**: p. 1065-1072.
35. Pine, A. S. and A. Goldman. *private communication*.
36. Sander, S. P., B. J. Finlayson-Pitts, D. M. Golden, R. E. Huie, C. E. Kolb, M. J. Kurylo, M. J. Molina, *et al.*, *Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 15*. 2006, Jet Propulsion Laboratory: Pasadena, CA.
37. Colmont, J., B. Bakri, F. Rohart, and G. Wlodarczak, "Experimental determination of pressure-broadening parameters of millimeter-wave transitions of HNO<sub>3</sub> perturbed by N<sub>2</sub> and O<sub>2</sub>, and of their temperature dependences". *Journal of Molecular Spectroscopy*, 2003. **220**: p. 52-57.
38. Schiffman, A. and D. Nesbitt, "Pressure broadening and collisional narrowing in OH( $v=1 \leftarrow 0$ ) rovibrational transitions with Ar, He, O<sub>2</sub>, and N<sub>2</sub>". *Journal of Chemical Physics*, 1994. **100**(4): p. 2677-2689.

39. Feierabend, K. J., D. K. Havey, and V. Vaida, "Gas phase spectroscopy of HNO<sub>3</sub> in the region 2000-8500 cm<sup>-1</sup>". *Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy*, 2004. **60**(12): p. 2775-2781.
40. Chen, W. J., W. J. Lo, B. M. Cheng, and Y. P. Lee, "Photolysis of nitric acid in solid nitrogen". *Journal of Chemical Physics*, 1992. **97**(10): p. 7167-73.
41. Cheng, B. M., J. W. Lee, and Y. P. Lee, "Photolysis of nitric acid in solid argon: the infrared absorption of peroxyxynitrous acid (HOONO)". *Journal of Physical Chemistry*, 1991. **95**(7): p. 2814-17.
42. Lo, W.-J. and Y.-P. Lee, "Ultraviolet absorption of cis-cis and trans-perp peroxyxynitrous acid (HOONO) in solid argon". *Chemical Physics Letters*, 1994. **229**(4-5): p. 357-361.
43. Lo, W.-J. and Y.-P. Lee, "Infrared absorption of cis-cis peroxyxynitrous acid (HOONO) in solid argon". *Journal of Chemical Physics*, 1994. **101**: p. 5494-5499.
44. Konen, I. M., I. B. Pollack, E. X. J. Li, M. I. Lester, M. E. Varner, and J. F. Stanton, "Infrared overtone spectroscopy and unimolecular decay dynamics of peroxyxynitrous acid". *Journal of Chemical Physics*, 2005. **122**(9). 094320.
45. Matthews, J. and A. Sinha, "State-resolved unimolecular dissociation of cis-cis HOONO: Product state distributions and action spectrum in the 2ν(OH) band region". *Journal of Chemical Physics*, 2005. **122**(10). 104313.
46. McCoy, A. B., J. L. Fry, J. S. Francisco, A. K. Mollner, and M. Okumura, "Role of OH-stretch/torsion coupling and quantum yield effects in the first OH overtone spectrum of cis-cis HOONO". *Journal of Chemical Physics*, 2005. **122**(10). 104311.
47. Hippler, H., N. Krasteva, S. Nasterlack, and F. Striebel, "Reaction of OH+NO<sub>2</sub>: High pressure experiments and falloff analysis". *Journal of Physical Chemistry A*, 2006. **110**(21): p. 6781-6788.
48. Dixon, D. A., D. Feller, C. G. Zhan, and J. S. Francisco, "Decomposition pathways of peroxyxynitrous acid: Gas-phase and solution energetics". *Journal of Physical Chemistry A*, 2002. **106**(13): p. 3191-3196.

49. Golden, D. M., J. R. Barker, and L. L. Lohr, "Master equation models for the pressure- and temperature-dependant reactions  $\text{HO}+\text{NO}_2 \rightarrow \text{HONO}_2$  and  $\text{HO}+\text{NO}_2 \rightarrow \text{HOONO}$ ". *Journal of Physical Chemistry A*, 2003. **107**(50): p. 11057-11071.
50. Li, Y. M. and J. S. Francisco, "High level ab initio molecular orbital theory study of the structure, vibrational spectrum, stability, and low-lying excited states of HOONO". *Journal of Chemical Physics*, 2000. **113**(18): p. 7976-7981.
51. McGrath, M. P. and F. S. Rowland, "Internal rotation in peroxyxynitrous acid (ONOOH)". *Journal of Chemical Physics*, 2005. **122**(13). 134312.
52. McGrath, M. P. and F. S. Rowland, "Determination of the barriers to internal rotation in ONOOX (X = H, Cl) and characterization of the minimum energy conformers". *Journal of Physical Chemistry*, 1994. **98**(4): p. 1061-1067.
53. Drouin, B. J., J. L. Fry, and C. E. Miller, "Rotational spectrum of cis-cis HOONO". *Journal of Chemical Physics*, 2004. **120**(12): p. 5505-5508.
54. Li, E. X. J., I. M. Konen, M. I. Lester, and A. B. McCoy, "Spectroscopic characterization of peroxyxynitrous acid in cis-perp configurations". *Journal of Physical Chemistry A*, 2006. **110**(17): p. 5607-5612.
55. Fry, J. L., S. A. Nizkorodov, M. Okumura, C. M. Roehl, J. S. Francisco, and P. O. Wennberg, "Cis-cis and trans-perp HOONO: Action spectroscopy and isomerization kinetics". *Journal of Chemical Physics*, 2004. **121**(3): p. 1432-1448.
56. Liu, Y. D. and R. G. Zhong, "Theoretical studies on HOONO, HONOO, and HNO<sub>3</sub> isomers and their isomerization reactions". *Journal of Molecular Structure-Theochem*, 2006. **765**(1-3): p. 143-149.
57. Zhu, R. S. and M. C. Lin, "Ab initio study of the HO<sub>2</sub>+NO reaction: Prediction of the total rate constant and product branching ratios for the forward and reverse processes". *Journal of Chemical Physics*, 2003. **119**(20): p. 10667-10677.
58. Zhang, J. Y. and N. M. Donahue, "Constraining the mechanism and kinetics of OH+NO<sub>2</sub> and HO<sub>2</sub>+NO using the multiple-well master equation". *Journal of Physical Chemistry A*, 2006. **110**(21): p. 6898-6911.

59. D'Ottone, L., D. Bauer, P. Campuzano-Jost, M. Fardy, and A. J. Hynes, "Kinetic and mechanistic studies of the recombination of OH with NO<sub>2</sub>: Vibrational deactivation, isotopic scrambling and product isomer branching ratios". *Faraday Discussions*, 2005. **130**: p. 111-123.
60. Hippler, H., S. Nasterlack, and F. Striebel, "Reaction of OH+NO<sub>2</sub>+M: Kinetic evidence of isomer formation". *Physical Chemistry Chemical Physics*, 2002. **4**(13): p. 2959-2964.
61. Donahue, N. M., R. Mohrschladt, T. J. Dransfield, J. G. Anderson, and M. K. Dubey, "Constraining the mechanism of OH+NO<sub>2</sub> using isotopically labeled reactants: Experimental evidence for HOONO formation". *Journal of Physical Chemistry A*, 2001. **105**(9): p. 1515-1520.
62. Nizkorodov, S. A. and P. O. Wennberg, "First spectroscopic observation of gas-phase HOONO". *Journal of Physical Chemistry A*, 2002. **106**(6): p. 855-859.
63. Williams, C. F., S. K. Pogrebnya, and D. C. Clary, "Quantum study on the branching ratio of the reaction NO<sub>2</sub> + OH". *Journal of Chemical Physics*, 2007. **126**. 154321.
64. Chakraborty, D., J. Park, and M. C. Lin, "Theoretical study of the OH+NO<sub>2</sub> reaction: formation of nitric acid and the hydroperoxyl radical". *Chemical Physics*, 1998. **231**(1): p. 39-49.
65. Golden, D. M. and G. P. Smith, "Reaction of OH+NO<sub>2</sub>+M: A new view". *Journal of Physical Chemistry A*, 2000. **104**(17): p. 3991-3997.
66. Matheu, D. M. and W. H. Green, "A priori falloff analysis for OH+NO<sub>2</sub>". *International Journal of Chemical Kinetics*, 2000. **32**(4): p. 245-262.
67. Troe, J., "Analysis of the Temperature and Pressure Dependence of the Reaction HO+NO<sub>2</sub>+M,<sub>2</sub><-> HONO<sub>2</sub>+M". *International Journal of Chemical Kinetics*, 2001. **33**(12): p. 878-889.
68. Schofield, D. P. and H. G. Kjaergaard, "Effect of OH internal torsion on the OH-stretching spectrum of cis,cis-HOONO". *Journal of Physical Chemistry A*, 2005. **109**(9): p. 1810-1814.

69. Frisch, M. J., G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, *et al.*, *Gaussian 03, Revision C.02*. 2004, Wallingford CT: Gaussian, Inc.
70. Smith, I. W. and M. D. Williams, "Vibrational-relaxation of OH (V=1) and OD(V=1) by HNO<sub>3</sub>, DNO<sub>3</sub>, H<sub>2</sub>O, NO and NO<sub>2</sub>". *Journal of the Chemical Society-Faraday Transactions II*, 1985. **81**: p. 1849-1860.
71. Park, C. R. and J. R. Wiesenfeld, "Full characterization of OH product energetics in the reaction of O(1D) with hydrocarbons". *Journal of Chemical Physics*, 1991. **95**(11): p. 8166-8177.
72. Aker, P. M. and J. J. Sloan, "The initial product vibrational energy distribution in the reaction between O(1D) and H<sub>2</sub>". *Journal of Chemical Physics*, 1986. **85**(3): p. 1412-1417.
73. Feierabend, K. J., D. K. Havey, M. E. Varner, J. F. Stanton, and V. Vaida, "A comparison of experimental and calculated spectra of HNO<sub>3</sub> in the near-infrared using Fourier transform infrared spectroscopy and vibrational perturbation theory". *Journal of Chemical Physics*, 2006. **124**(12). 124323.
74. Zhang, X., M. R. Nimlos, G. B. Ellison, M. E. Varner, and J. F. Stanton, "Infrared absorption spectra of matrix-isolated cis, cis-HOONO and its ab initio CCSD(T) anharmonic vibrational bands". *Journal of Chemical Physics*, 2006. **124**(8). 084305.
75. Matthews, J., A. Sinha, and J. S. Francisco, "Relative vibrational overtone intensity of cis-cis and trans-perp peroxyxynitrous acid". *Journal of Chemical Physics*, 2004. **120**(22): p. 10543-10553.
76. Russell, A. and R. Dennis, "NARSTO critical review of photochemical models and modeling". *Atmospheric Environment*, 2000. **34**(12-14): p. 2283-2324.
77. Orlando, J. J., G. S. Tyndall, and T. J. Wallington, "The atmospheric chemistry of alkoxy radicals". *Chemical Reviews*, 2003. **103**(12): p. 4657-4689.
78. Atkinson, R. and J. Arey, "Atmospheric degradation of volatile organic compounds". *Chemical Reviews*, 2003. **103**(12): p. 4605-4638.

79. Somnitz, H. and R. Zellner, "Theoretical studies of unimolecular reactions of C-2-C-5 alkoxy radicals. Part I. Ab initio molecular orbital calculations". *Physical Chemistry Chemical Physics*, 2000. **2**(9): p. 1899-1905.
80. Somnitz, H. and R. Zellner, "Theoretical studies of unimolecular reactions of C-2-C-5 alkoxy radicals. Part II. RRKM dynamical calculations". *Physical Chemistry Chemical Physics*, 2000. **2**(9): p. 1907-1918.
81. Jungkamp, T. P. W., J. N. Smith, and J. H. Seinfeld, "Atmospheric oxidation mechanism of n-butane: The fate of alkoxy radicals". *Journal of Physical Chemistry A*, 1997. **101**(24): p. 4392-4401.
82. Atkinson, R., "Atmospheric reactions of alkoxy and beta-hydroxyalkoxy radicals". *International Journal of Chemical Kinetics*, 1997. **29**(2): p. 99-111.
83. Atkinson, R., E. S. C. Kwok, J. Arey, and S. M. Aschmann, "Reactions of alkoxy radicals in the atmosphere". *Faraday Discussions*, 1995(100): p. 23-37.
84. Atkinson, R. and S. M. Aschmann, "Alkoxy radical isomerization products from the gas-phase OH radical-initiated reactions of 2,4-dimethyl-2-pentanol and 3,5-dimethyl-3-hexanol". *Environmental Science & Technology*, 1995. **29**(2): p. 528-536.
85. Kwok, E. S. C., J. Arey, and R. Atkinson, "Alkoxy radical isomerization in the OH radical-initiated reactions of C-4-C-8 n-alkanes". *Journal of Physical Chemistry*, 1996. **100**(1): p. 214-219.
86. Niki, H., P. D. Maker, C. M. Savage, and L. P. Breitenbach, "An Ft Ir Study of the Isomerization and O-2 Reaction of Normal-Butoxy Radicals". *Journal of Physical Chemistry*, 1981. **85**(18): p. 2698-2700.
87. Atkinson, R., "Gas-phase tropospheric chemistry of volatile organic compounds .1. Alkanes and alkenes". *Journal of Physical and Chemical Reference Data*, 1997. **26**(2): p. 215-290.
88. Atkinson, R., D. L. Baulch, R. A. Cox, J. N. Crowley, R. F. Hampson, R. G. Hynes, M. E. Jenkin, M. J. Rossi, and J. Troe, "Evaluated kinetic and

- photochemical data for atmospheric chemistry: Volume II-Gas phase reactions of organic species". *Atmospheric Chemistry and Physics*, 2006. **6**: p. 3625-4055.
89. Devolder, P., "Atmospheric fate of small alkoxy radicals: recent experimental and theoretical advances". *Journal of Photochemistry and Photobiology A-Chemistry*, 2003. **157**(2-3): p. 137-147.
90. Carter, W. P. L., K. R. Darnall, R. A. Graham, A. M. Winer, and J. N. Pitts, "Reactions of C2 and C-4 Alpha-hydroxy Radicals with Oxygen". *Journal of Physical Chemistry*, 1979. **83**(18): p. 2305-2311.
91. Cox, R. A., K. F. Patrick, and S. A. Chant, "Mechanism of atmospheric photo-oxidation of organic compounds-Reactions of alkoxy radicals in oxidation of normal-butane and simple ketones". *Environmental Science & Technology*, 1981. **15**(5): p. 587-592.
92. Heiss, A. and K. Sahetchian, "Isomerization reactions of the n-C4H9O and n-OOC4H8OH radicals in oxygen". *International Journal of Chemical Kinetics*, 1996. **28**(7): p. 531-544.
93. Dobe, S., T. Berces, and F. Marta, "Gas-phase decomposition and isomerization reactions of 2-pentoxy radicals". *International Journal of Chemical Kinetics*, 1986. **18**(3): p. 329-344.
94. Cassanelli, P., R. A. Cox, J. J. Orlando, and G. S. Tyndall, "An FT-IR study of the isomerization of 1-butoxy radicals under atmospheric conditions". *Journal of Photochemistry and Photobiology A-Chemistry*, 2006. **177**(2-3): p. 109-115.
95. Cassanelli, P., D. Johnson, and R. A. Cox, "A temperature-dependent relative-rate study of the OH initiated oxidation of n-butane: The kinetics of the reactions of the 1-and 2-butoxy radicals". *Physical Chemistry Chemical Physics*, 2005. **7**(21): p. 3702-3710.
96. Hein, H., A. Hoffmann, and R. Zellner, "Direct investigations of reactions of 1-butoxy and 1-pentoxy radicals using laser pulse initiated oxidation: reaction with

- O-2 and isomerisation at 293 K and 50 mbar". *Physical Chemistry Chemical Physics*, 1999. **1**(16): p. 3743-3752.
97. Geiger, H., I. Barnes, K. H. Becker, B. Bohn, T. Brauers, B. Donner, H. P. Dorn, *et al.*, "Chemical mechanism development: Laboratory studies and model applications". *Journal of Atmospheric Chemistry*, 2002. **42**(1): p. 323-357.
98. Atkinson, D. B., "Solving chemical problems of environmental importance using cavity ring-down spectroscopy". *Analyst*, 2003. **128**(2): p. 117-125.
99. Vallance, C., "Innovations in cavity ringdown spectroscopy". *New Journal of Chemistry*, 2005. **29**(7): p. 867-874.
100. *Organic syntheses. Collective volume*. 1941, Wiley: New York.
101. Glover, B. G. and T. A. Miller, "Near-IR cavity ringdown spectroscopy and kinetics of the isomers and conformers of the butyl peroxy radical". *Journal of Physical Chemistry A*, 2005. **109**(49): p. 11191-11197.
102. Stein, S. E., J. M. Rukkers, and R. L. Brown, *NIST Standard Reference Database 69*, P. J. Linstrom and W. G. Mallard, Editors. 2005, National Institute of Standards and Technology: Gaithersburg, MD (<http://webbook.nist.gov>).
103. Sharpe, S. W., T. J. Johnson, R. L. Sams, P. M. Chu, G. C. Rhoderick, and P. A. Johnson, "Gas-phase databases for quantitative infrared spectroscopy". *Applied Spectroscopy*, 2004. **58**(12): p. 1452-1461.
104. Somnitz, H. and R. Zellner, "Kinetics and dynamics of multi-channel unimolecular reactions of alkoxy radicals over an extended range of temperature and pressure. A combined quantum chemical/RRKM dynamical study". *Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics*, 2006. **220**(8): p. 1029-1048.
105. Parkinson, W. H., J. Rufus, and K. Yoshino, "Absolute absorption cross section measurements of CO<sub>2</sub> in the wavelength region 163-2000 nm and the temperature dependence". *Chemical Physics*, 2003. **290**: p. 251-256.