



## REFERENCES and SOURCES for HITRAN

(Last updated: 14 July 2011)

The reference 0 (zero) is used for all data surviving from the 1986 HITRAN Database. For further details, refer to: L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).

### *Subsequent articles describing HITRAN:*

- L.S. Rothman, R.R. Gamache, R.H. Tipping, C.P. Rinsland, M.A.H. Smith, D.Chris Benner, V.Malathy Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S. Massie, L.R. Brown, and R.A. Toth, "The HITRAN Molecular Database: Editions of 1991 and 1992," *JQSRT* **48**, 469-507 (1992)
- L.S. Rothman, C.P. Rinsland, A. Goldman, S.T. Massie, D.P. Edwards, J.-M. Flaud, A. Perrin, C. Camy-Peyret, V. Dana, J.-Y. Mandin, J. Schroeder, A. McCann, R.R. Gamache, R.B. Wattson, K. Yoshino, K.V. Chance, K.W. Jucks, L.R. Brown, V. Nemtchinov, and P. Varanasi, "The HITRAN Molecular Spectroscopic Database and HAWKS (HITRAN Atmospheric Workstation): 1996 Edition," *JQSRT* **60**, 665-710 (1998)
- L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003)
- L.S. Rothman, D. Jacquemart, A. Barbe, C. Chris Benner, M. Birk, L.R. Brown, M.R. Carleer, C. Chackerian Jr., K. Chance, L.H. Coudert, V. Dana, V.M. Devi, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S.T. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, "The HITRAN 2004 molecular spectroscopic database," *JQSRT* **96**, 139-204 (2005)
- L.S. Rothman, I.E. Gordon, A. Barbe, D.Chris Benner, P.F. Bernath, M. Birk, et al, "The HITRAN 2008 molecular spectroscopic database," *JQSRT* **110**, 533-572 (2009).

---

**H<sub>2</sub>O [1] 161, 181, 171, 162, 182, 172**

### Positions

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
- 1.** C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, J.P. Chevillard, J. Brault, D.A. Ramsay, M. Vervloet, and J. Chauville, "The High-Resolution Spectrum of Water Vapor between 16500 and 25250 cm<sup>-1</sup>," *J.Mol.Spectrosc.* **113**, 208-228 (1985); J.-Y. Mandin, J.-P. Chevillard, C. Camy-Peyret, J.-M. Flaud, and J.W. Brault, "The High-Resolution Spectrum of Water Vapor between 13 200 and 16 500 cm<sup>-1</sup>," *J.Mol.Spectrosc.* **116**, 167-190 (1986).
- 2.** J.-Y. Mandin, J.P. Chevillard, J.-M. Flaud, and C. Camy-Peyret, "H<sub>2</sub><sup>16</sup>O: Line positions and intensities between 8000 and 9500 cm<sup>-1</sup>: the second hexad of interacting vibrational states:

- {(050),(130),(031),(210),(111),(012)},” *Can.J.Phys.* **66**, 997 (1988).
3. R.A. Toth, “Measurements of H<sub>2</sub><sup>16</sup>O Line Positions and Strengths: 11 610 to 12 861 cm<sup>-1</sup>,” *J.Mol.Spectrosc.* **166**, 176-183 (1994).
  4. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, “H<sub>2</sub><sup>16</sup>O: line positions and intensities between 9500 and 11 500 cm<sup>-1</sup>. The (041), (220), (121), (201), (102), and (003) interacting states,” *Can.J.Phys.* **67**, 1065-1084 (1989).
  5. R.A. Toth, “ $\nu_2$  band of H<sub>2</sub><sup>16</sup>O: line strengths and transition frequencies,” *JOSA B* **8**, 2236-2255 (1991); R.A. Toth, “ $2\nu_2 - \nu_2$  and  $2\nu_2$  bands of H<sub>2</sub><sup>16</sup>O, H<sub>2</sub><sup>17</sup>O, and H<sub>2</sub><sup>18</sup>O: line positions and strengths,” *JOSA B* **10**, 1526-1544 (1993).
  6. Preliminary results from R.A. Toth, “Extensive measurements of H<sub>2</sub><sup>16</sup>O line frequencies and strengths: 5750-7965 cm<sup>-1</sup>,” *Appl.Opt.* **33**, 4851-4867 (1994).
  7. J.-M. Flaud, C. Camy-Peyret, and R.A. Toth, “Water Vapor Parameters from Microwave to Medium Infrared,” Pergamon Press, Paris (1981).
  8. J.-M. Flaud, C. Camy-Peyret, J.-P. Maillard, and G. Guelachvili, “The H<sub>2</sub>O Spectrum between, 4200 and 5000 cm<sup>-1</sup>,” *J.Mol.Spectrosc.* **65**, 219-228 (1977).
  9. J.-M. Flaud, C. Camy-Peyret, and J.-P. Maillard, “Higher ro-vibrational levels of H<sub>2</sub>O deduced from high resolution oxygen-hydrogen flame spectra between 2800-6200 cm<sup>-1</sup>,” *Mol.Phys.* **32**, 499-521 (1976).
  10. C. Camy-Peyret and J.-M. Flaud, *J.Phys.Lett.* **41**, 23 (1980).
  11. J.-M. Flaud, C. Camy-Peyret, K.Narahari Rao, Da-Wun Chen, Yan-Shek Ho, and J.-P. Maillard, “Spectrum of Water Vapor between 8050 and 9370 cm<sup>-1</sup>,” *J.Mol.Spectrosc.* **75**, 339-362 (1979).
  12. C. Camy-Peyret, J.-M. Flaud, and N. Papineau, “La Bande  $\nu_2$  des espèces isotopiques H<sub>2</sub><sup>17</sup>O et H<sub>2</sub><sup>18</sup>O,” *C.R.Acad.Sc.Paris*, **t 290, Serie B**, 537-540 (1980).
  13. R.A. Toth, J.-M. Flaud, and C. Camy-Peyret, “Spectrum of H<sub>2</sub><sup>18</sup>O and H<sub>2</sub><sup>17</sup>O in the 5030 to 5640 cm<sup>-1</sup> region,” *J.Mol.Spectrosc.* **67**, 185-205 (1977).
  14. R.A. Toth, V.D. Gupta, and J.W. Brault, “Line positions and strengths of HDO in the 2400-3300 cm<sup>-1</sup> region,” *Appl.Opt.* **21**, 3337-3347 (1982).
  15. Estimate based on combination differences.
  16. M.P. Esplin, R.B. Wattson, and M.L. Hoke, “H<sub>2</sub>O Line Position Measurements at 1000K,” Paper ME04, Ohio State University International Symposium on Molecular Spectroscopy, June (1994).
  17. Taken from Smithsonian Astrophysical Observatory balloon data, K. Chance and K. Jucks, Harvard-Smithsonian Center for Astrophysics, private communication (1994).
  18. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, “The Smithsonian Astrophysical Observatory Database SAO92,” *JQSRT* **52**, 447-457 (1994).
  19. R.B. Wattson, “Extended Water Databases Calculated by Direct Numerical Diagonalization,” paper P2, Third HITRAN Spectroscopic Database Conference, Hanscom AFB, MA (1993).
  20. R.A. Toth, “HD<sup>16</sup>O, HD<sup>18</sup>O, and HD<sup>17</sup>O Transition Frequencies and Strengths in the  $\nu_2$  Bands,” *J.Mol.Spectrosc.* **162**, 20-40 (1993).
  21. R.A. Toth, “ $\nu_1 - \nu_2$ ,  $\nu_3 - \nu_2$ ,  $\nu_1$ , and  $\nu_3$  bands of H<sub>2</sub><sup>16</sup>O: line positions and strengths,” *JOSA B* **10**, 2006-2029 (1993).
  22. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, “H<sub>2</sub><sup>16</sup>O: line positions and intensities between 9500 and 11 500 cm<sup>-1</sup>. The (041), (220), (121), (201), (102), and (003) interacting states,” *Can.J.Phys.* **67**, 1065-1084 (1989). Line identified using D.W. Schwenke, “New H<sub>2</sub>O Rovibrational Line Assignments,” *J.Mol.Spectrosc.* **190**, 397-402 (1998).

23. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, " $\text{H}_2^{16}\text{O}$ : line positions and intensities between 9500 and 11 500  $\text{cm}^{-1}$ . The (041), (220), (121), (201), (102), and (003) interacting states," *Can.J.Phys.* **67**, 1065-1084 (1989). Line identified using D.W. Schwenke, "New  $\text{H}_2\text{O}$  Rovibrational Line Assignments," *J.Mol.Spectrosc.* **190**, 397-402 (1998); L.P. Giver, C. Chackerian, Jr, and P. Varanasi, "Long-Path near-Infrared Line Intensities for  $\text{H}_2\text{O}$ ," Proceedings of the 5<sup>th</sup> ASA Conference, page 141, Reims, France (1999).
24. L.R. Brown, R.A. Toth, and M. Dulick, "Empirical Line Parameters of  $\text{H}_2^{16}\text{O}$  near 0.94  $\mu\text{m}$ : Positions, Intensities and Air-Broadening Coefficients," *J.Mol.Spectrosc.* **212**, 57-82 (2002).
25. R.A. Toth, "Water vapor measurements between 590 and 2582  $\text{cm}^{-1}$ : Line positions and strengths," *J.Mol.Spectrosc.* **190**, 379-396 (1998); R.A. Toth, "HDO and  $\text{D}_2\text{O}$  low pressure, long path spectra in the 600-3100  $\text{cm}^{-1}$  region I. HDO line positions and strengths," *J.Mol.Spectrosc.* **195**, 73-97 (1999); R.A. Toth, "Analysis of line positions and strengths of  $\text{H}_2^{16}\text{O}$  ground and hot bands connecting to interacting upper states: (020), (100), and (001)," *J.Mol.Spectrosc.* **194**, 28-42 (1999).
26. H. Partridge and D.W. Schwenke, "The determination of an accurate isotope dependent potential energy surface for water from extensive ab initio calculations and experimental data," *J.Chem.Phys.* **106**, 4618-4639 (1997).
27. C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, A. Bykov, O. Naumenko, L. Sinita, and B. Voronin, "Fourier-transform absorption spectrum of the  $\text{H}_2^{17}\text{O}$  molecule in the 9711-11 335  $\text{cm}^{-1}$  spectral region: the first decade of resonating states," *JQSRT* **61**, 795-812 (1999).
28. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, " $\text{H}_2^{18}\text{O}$ : line positions and intensities between 9500 and 11 500  $\text{cm}^{-1}$ . The (041), (220), (121), (201), (102), and (003) interacting states," *Can.J.Phys.* **65**, 777-789 (1987).
29. P.F. Coheur, S. Fally, M. Carleer, C. Clerboux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, "New water vapor line parameters in the 26000-13000  $\text{cm}^{-1}$  region," *JQSRT* **74**, 493-510 (2002); M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, P.F. Coheur, R. Colin, S. Fally, and M. Bach, "Water vapor line parameters in the 13 000-9250  $\text{cm}^{-1}$  region," *JQSRT* **82**, 99-117 (2003).
30. R.A. Toth, "Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ," see <http://mark4sun.jpl.nasa.gov/h2o.html>.
31. Same as Ref. 30, but these lines are doubled with the weaker unassigned line hidden beneath the stronger component.
32. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
33. R. Lanquetin, L.H. Coudert, and C. Camy-Peyret, "High-lying rotational levels of water: an analysis of the energy of the five first vibrational states," *J.Mol.Spectrosc.* **206**, 83-103 (2001).
34. Calculation from K.V. Jucks, private communication (2000).
35. J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L.H. Coudert, J.-L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment," *Atmos.Oceanic Opt.* **16**, 172-181 (2003).
36. M. Tanaka, J.W. Brault, and J. Tennyson, "Absorption spectrum of  $\text{H}_2^{18}\text{O}$  in the 12,400 – 14,520  $\text{cm}^{-1}$  range," *J.Mol.Spectrosc.* **216**, 77-80 (2002).
37. J. Tennyson, University College London, private communication (2005).
38. M. Tanaka, O. Naumenko, J. Brault, and J. Tennyson, "Fourier transform absorption spectra of  $\text{H}_2^{18}\text{O}$  and  $\text{H}_2^{17}\text{O}$  in the  $3\nu+\delta$  and  $4\nu$  polyad region," *J.Mol.Spectrosc.* **234**, 1-9 (2005).
39. R. Tolchenov and J. Tennyson, "Water Line Parameters from Refitted Spectra constrained by empirical upper state levels: study of the 9500 - 14500  $\text{cm}^{-1}$  region," *JQSRT* **109**, 559-568

(2008).

- 40. R.N. Tolchenov, O. Naumenko, N.F. Zobov, S.V. Shirin, O.L. Polyansky, J. Tennyson, M. Carleer, P.-F. Coheur, S. Fally, A. Jenouvrier, and A.C. Vandaele, "Water vapour line assignments in the 9250-26 000  $\text{cm}^{-1}$  frequency range," *J.Mol.Spectrosc.* **233**, 68-76 (2005).
- 41. B.A. Voronin, O.V. Naumenko, M. Carleer, P.-F. Coheur, S. Fally, A. Jenouvrier, R.N. Tolchenov, A.C. Vandaele, and J. Tennyson, "HDO absorption spectrum above 11 500  $\text{cm}^{-1}$ : Assignment and dynamics," *J.Mol.Spectrosc.* **244**, 87-101 (2007).
- 42. R.J. Barber, J. Tennyson, G.J. Harris, R.N. Tolchenov, "A high-accuracy computed water line list," *Mon.Not.R.Astron.Soc.* **368**, 1087-1094 (2006).
- 43. Line positions generated from the database of experimentally-determined energy levels, I.E. Gordon (2008).

### Intensities

- 0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
- 1. C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, J.P. Chevillard, J. Brault, D.A. Ramsay, M. Vervloet, and J. Chauville, "The High-Resolution Spectrum of Water Vapor between 16500 and 25250  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **113**, 208-228 (1985); J.-Y. Mandin, J.-P. Chevillard, C. Camy-Peyret, J.-M. Flaud, and J.W. Brault, "The High-Resolution Spectrum of Water Vapor between 13 200 and 16 500  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **116**, 167-190 (1986).
- 2. J.-Y. Mandin, J.P. Chevillard, J.-M. Flaud, and C. Camy-Peyret, " $\text{H}_2^{16}\text{O}$ : Line positions and intensities between 8000 and 9500  $\text{cm}^{-1}$ : the second hexad of interacting vibrational states:  $\{(050),(130),(031),(210),(111),(012)\}$ ," *Can.J.Phys.* **66**, 997 (1988).
- 3. R.A. Toth, "Measurements of  $\text{H}_2^{16}\text{O}$  Line Positions and Strengths: 11 610 to 12 861  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **166**, 176-183 (1994).
- 4. J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, " $\text{H}_2^{16}\text{O}$ : line positions and intensities between 9500 and 11 500  $\text{cm}^{-1}$ . The (041), (220), (121), (201), (102), and (003) interacting states," *Can.J.Phys.* **67**, 1065-1084 (1989).
- 5. R.A. Toth, " $\nu_2$  band of  $\text{H}_2^{16}\text{O}$ : line strengths and transition frequencies," *JOSA B* **8**, 2236-2255 (1991); R.A. Toth, " $2\nu_2 - \nu_2$  and  $2\nu_2$  bands of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$ : line positions and strengths," *JOSA B* **10**, 1526-1544 (1993).
- 6. Preliminary results from R.A. Toth, "Extensive measurements of  $\text{H}_2^{16}\text{O}$  line frequencies and strengths: 5750-7965  $\text{cm}^{-1}$ ," *Appl.Opt.* **33**, 4851-4867 (1994).
- 7. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
- 8. R.B. Wattson, "Extended Water Databases Calculated by Direct Numerical Diagonalization," paper P2, Third HITRAN Spectroscopic Database Conference, Hanscom AFB, MA (1993).
- 9. C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, J.P. Chevillard, J. Brault, D.A. Ramsay, M. Vervloet, and J. Chauville, "The High-Resolution Spectrum of Water Vapor between 16500 and 25250  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **113**, 208-228 (1985); J.-Y. Mandin, J.-P. Chevillard, C. Camy-Peyret, J.-M. Flaud, and J.W. Brault, "The High-Resolution Spectrum of Water Vapor between 13 200 and 16 500  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **116**, 167-190 (1986). Intensity units corrected from HITRAN92 and HITRAN96 editions by L.P. Giver, C. Chackerian, Jr, and P. Varanasi, "Visible and Near-infrared  $\text{H}_2^{16}\text{O}$  Line Intensity Corrections for HITRAN-96," *JQSRT* **66**, 101-105 (2000).
- 10. J.-Y. Mandin, J.P. Chevillard, J.-M. Flaud, and C. Camy-Peyret, " $\text{H}_2^{16}\text{O}$ : Line positions and



intensities between 8000 and 9500  $\text{cm}^{-1}$ : the second hexad of interacting vibrational states:  $\{(050),(130),(031),(210),(111),(012)\}$ ,” *Can.J.Phys.* **66**, 997 (1988). Intensity units corrected from HITRAN92 and HITRAN96 editions by L.P. Giver, C. Chackerian, Jr, and P. Varanasi, “Visible and Near-infrared  $\text{H}_2^{16}\text{O}$  Line Intensity Corrections for HITRAN-96,” *JQSRT* **66**, 101-105 (2000).

**11.** R.A. Toth,  $3\nu_3 + \nu_2$  region (11661-12741  $\text{cm}^{-1}$ ), Jet Propulsion Laboratory, private communication (1990). Intensity units corrected from HITRAN92 and HITRAN96 editions by L.P. Giver, C. Chackerian, Jr, and P. Varanasi, “Visible and Near-infrared  $\text{H}_2^{16}\text{O}$  Line Intensity Corrections for HITRAN-96,” *JQSRT* **66**, 101-105 (2000).

**12.** J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, “ $\text{H}_2^{16}\text{O}$ : line positions and intensities between 9500 and 11 500  $\text{cm}^{-1}$ . The (041), (220), (121), (201), (102), and (003) interacting states,” *Can.J.Phys.* **67**, 1065-1084 (1989). Intensity units corrected from HITRAN92 and HITRAN96 editions by L.P. Giver, C. Chackerian, Jr, and P. Varanasi, “Visible and Near-infrared  $\text{H}_2^{16}\text{O}$  Line Intensity Corrections for HITRAN-96,” *JQSRT* **66**, 101-105 (2000).

**13.** R.A. Toth, “Water vapor measurements between 590 and 2582  $\text{cm}^{-1}$ : Line positions and strengths,” *J.Mol.Spectrosc.* **190**, 379-396 (1998); R.A. Toth, “HDO and  $\text{D}_2\text{O}$  low pressure, long path spectra in the 600-3100  $\text{cm}^{-1}$  region I. HDO line positions and strengths,” *J.Mol.Spectrosc.* **195**, 73-97 (1999); R.A. Toth, “Analysis of line positions and strengths of  $\text{H}_2^{16}\text{O}$  ground and hot bands connecting to interacting upper states: (020), (100), and (001),” *J.Mol.Spectrosc.* **194**, 28-42 (1999).

**14.** C. Camy-Peyret, J.-M. Flaud, J.-Y. Mandin, A. Bykov, O. Naumenko, L. Sinita, and B. Voronin, “Fourier-transform absorption spectrum of the  $\text{H}_2^{17}\text{O}$  molecule in the 9711-11 335  $\text{cm}^{-1}$  spectral region: the first decade of resonating states,” *JQSRT* **61**, 795-812 (1999).

**15.** L.R. Brown, R.A. Toth, and M. Dulick, “Empirical Line Parameters of  $\text{H}_2^{16}\text{O}$  near 0.94  $\mu\text{m}$ : Positions, Intensities and Air-Broadening Coefficients,” *J.Mol.Spectrosc.* **212**, 57-82 (2002).

**16.** Rescaled intensities of H. Partridge and D.W. Schwenke, “The determination of an accurate isotope dependent potential energy surface for water from extensive ab initio calculations and experimental data,” *J.Chem.Phys.* **106**, 4618-4639 (1997) as described in Ref.15 above. Observed intensities from J.P. Chevillard, J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, “ $\text{H}_2^{18}\text{O}$ : line positions and intensities between 9500 and 11 500  $\text{cm}^{-1}$ . The (041), (220), (121), (201), (102), and (003) interacting states,” *Can.J.Phys.* **65**, 777-789 (1987) were used to determine the scaling factors.

**17.** P.F. Coheur, S. Fally, M. Carleer, C. Clerboux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, “New water vapor line parameters in the 26000-13000  $\text{cm}^{-1}$  region,” *JQSRT* **74**, 493-510 (2002); M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, P.F. Coheur, R. Colin, S. Fally, and M. Bach, “Water vapor line parameters in the 13 000-9250  $\text{cm}^{-1}$  region,” *JQSRT* **82**, 99-117 (2003).

**18.** R.A. Toth, “Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ,” see <http://mark4sun.jpl.nasa.gov/h2o.html>.

**19.** Same as Ref. 18, but these lines are doubled with the weaker unassigned line hidden beneath the stronger component.

**20.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, “Submillimeter, Millimeter, and Microwave Spectral Line Catalog,” *JQSRT* **60**, 883-890 (1998).

**21.** L.H. Coudert, “Line frequency and line intensity analysis of water vapor,” *Mol.Phys.* **96**, 941-954 (1999).

**22.** J.C. Pearson, JPL, private communication (2000).

23. L.H. Coudert, Université Paris-Sud, private communication (2004).
24. M. Tanaka, J.W. Brault, and J. Tennyson, "Absorption spectrum of  $\text{H}_2^{18}\text{O}$  in the 12,400 – 14,520  $\text{cm}^{-1}$  range," *J.Mol.Spectrosc.* **216**, 77-80 (2002).
25. J. Tennyson, University College London, private communication (2005).
26. M. Tanaka, O. Naumenko, J. Brault, and J. Tennyson, "Fourier transform absorption spectra of  $\text{H}_2^{18}\text{O}$  and  $\text{H}_2^{17}\text{O}$  in the  $3\nu+\delta$  and  $4\nu$  polyad region," *J.Mol.Spectrosc.* **234**, 1-9 (2005).
27. R. Tolchenov and J. Tennyson, "Water Line Parameters from Refitted Spectra constrained by empirical upper state levels: study of the 9500 - 14500  $\text{cm}^{-1}$  region," *JQSRT* **109**, 559-568 (2008).
28. R.N. Tolchenov, O. Naumenko, N.F. Zobov, S.V. Shirin, O.L. Polyansky, J. Tennyson, M. Carleer, P.-F. Coheur, S. Fally, A. Jenouvrier, and A.C. Vandaele, "Water vapour line assignments in the 9250-26 000  $\text{cm}^{-1}$  frequency range," *J.Mol.Spectrosc.* **233**, 68-76 (2005).
29. B.A. Voronin, O.V. Naumenko, M. Carleer, P.-F. Coheur, S. Fally, A. Jenouvrier, R.N. Tolchenov, A.C. Vandaele, and J. Tennyson, "HDO absorption spectrum above 11 500  $\text{cm}^{-1}$ : Assignment and dynamics," *J.Mol.Spectrosc.* **244**, 87-101 (2007).
30. L.H. Coudert, G. Wagner, M. Birk, Y.I. Baranov, W.J. Lafferty, and J.-M. Flaud, "The  $\text{H}_2^{16}\text{O}$  molecule: Line position and line intensity analyses up to the second triad," *J.Mol.Spectrosc.* **251**, 339-357 (2008).
31. L. Lodi and J. Tennyson, "A line list of allowed and forbidden rotational transition intensities for water," *JQSRT* **109**, 1219-1233 (2008).
32. R.J. Barber, J. Tennyson, G.J. Harris, R.N. Tolchenov, "A high-accuracy computed water line list," *Mon.Not.R.Astron.Soc.* **368**, 1087-1094 (2006).

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. S.D. Gasster, C.H. Townes, D. Goorvitch, and F.P.J. Valero, "Foreign-gas collision broadening of the far-infrared spectrum of water vapor," *JOSA B* **5**, 593-601 (1988).
2. V.Ya. Ryadov and N.I. Furashov, *Opt.Spectrosc.(USSR)* **35**, 255-257(1973).
3. R. Emery, "Atmospheric Absorption Measurements in the Region of 1 mm Wavelength," *Infrared Phys.* **12**, 65-79 (1972).
4. R.B. Sanderson and N. Ginsburg, "Line Widths and Line Strengths in the Rotational Spectrum of Water Vapor," *JQSRT* **3**, 435-444 (1963).
5. G.E. Becker and S.H. Autler, "Water Vapor Absorption of Electromagnetic Radiation in the Centimeter Wave-Length Range," *Phys.Rev.* **70**, 300-307 (1946).
6. J.R. Rusk, "Line-Breadth Study of the 1.64-mm Absorption in Water Vapor," *J.Chem.Phys.* **42**, 493-500 (1965).
7. H.J. Liebe and T.A. Dillon, "Accurate Foreign-Gas-Broadening Parameters of the 22-GHz  $\text{H}_2\text{O}$  Line from Refraction Spectroscopy," *J.Chem.Phys.* **50**, 727-732 (1969).
8. L. Frenkel and D. Woods, "Microwave absorption by  $\text{H}_2\text{O}$  vapor and its mixtures with other gases between 100 and 300 Gc/s," *Proc IEEE* **54**, 498-505 (1966).
9. J.E. Pearson, D.T. Llewellyn-Jones, and R.J. Knight, "Water Vapour Absorption near a Wavelength of 0.79 mm," *Infrared Phys.* **9**, 53-58 (1969).
10. V.Ya. Ryadov and N.I. Furashov, *Opt.Spectrosc.(USSR)* **24**, 93-97 (1968).
11. C.P. Rinsland, A. Goldman, M.A.H. Smith, and V. Malathy Devi, "Measurements of Lorentz air-broadening coefficients and relative intensities in the  $\text{H}_2^{16}\text{O}$  pure rotational and  $\nu_2$  bands from

long horizontal path atmospheric spectra,” *Appl.Opt.* **30**, 1427-1438 (1991).

12. B.E. Grossmann and E.V. Browell, “Spectroscopy of Water Vapor in the 720-nm Wavelength Region: Line Strengths, Self-Induced Pressure Broadenings and Shifts, and Temperature Dependence of Linewidths and Shifts,” *J.Mol.Spectrosc.* **136**, 264-294 (1989); B.E. Grossmann and E.V. Browell, “Water-Vapor Line Broadening and Shifting by Air, Nitrogen, Oxygen, and Argon in the 720-nm Wavelength Region,” *J.Mol.Spectrosc.* **138**, 562-595 (1989).
13. J.J. Remedios, D.Phil.thesis, Oxford University (1990); J.J. Remedios and J. Ballard, “Experimental Determinations of the Air- and N<sub>2</sub>-broadened Line Widths of Strong Lines in the  $\nu_2$  Band of H<sub>2</sub><sup>16</sup>O: Line Widths and their Temperature Dependences between 243K and 298K,” to be published.
14. R.R. Gamache and R.W. Davies, “Theoretical calculations of N<sub>2</sub>-broadened halfwidths of H<sub>2</sub>O using quantum Fourier transform theory,” *Appl.Opt.* **22**, 4013-4019 (1983).
15. R.R. Gamache and L.S. Rothman, “Temperature Dependence of N<sub>2</sub>-Broadened Halfwidths of Water Vapor: The Pure Rotation and  $\nu_2$  Bands,” *J.Mol.Spectrosc.* **128**, 360-369 (1988).
16. R.R. Gamache, scaled average values, unpublished data (1993).
17. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, “The Smithsonian Astrophysical Observatory Database SAO92,” *JQSRT* **52**, 447-457 (1994).
18. R.A. Toth, “Air- and N<sub>2</sub>-Broadening parameters of water vapor: 604 to 2271 cm<sup>-1</sup>,” *J.Mol.Spectrosc.* **201**, 218-243 (2000); R.A. Toth, “Air- and N<sub>2</sub>-broadening parameters of HDO and D<sub>2</sub>O, 709 to 1936 cm<sup>-1</sup>,” *J.Mol.Spectrosc.* **198**, 358-370 (1999); R.A. Toth, L.R. Brown, and C. Plymate, “Self-broadened widths and frequency shifts of water vapor lines between 590 and 2400 cm<sup>-1</sup>,” *JQSRT* **59**, 529-562 (1998). Default values as a function of the running index  $m$  were used for the temperature-dependence coefficient of  $\gamma_{\text{air}}$ ,  $n_{\text{air}}$ .
19. Same as Ref. 18, using temperature-dependence of widths from J.J. Remedios (Ref. 13 above); used measured values for specific transitions, L.R. Brown, JPL, private communication (2000).
20. Determined from average of many bands, L.R. Brown, JPL, private communication (2000).
21. L.R. Brown, R.A. Toth, and M. Dulick, “Empirical Line Parameters of H<sub>2</sub><sup>16</sup>O near 0.94  $\mu\text{m}$ : Positions, Intensities and Air-Broadening Coefficients,” *J.Mol.Spectrosc.* **212**, 57-82 (2002).
22. Unassigned lines using default value 0.077 cm<sup>-1</sup>/atm, L.R. Brown, JPL, private communication (2000).
23. R.R. Gamache and J. Fischer, “Calculated Halfwidths and Lineshifts of Water-vapor transitions in the 0.7  $\mu\text{m}$  Region and a Comparison with Published Data,” *J.Mol.Spectrosc.* **207**, 254-262 (2001).
24. R.A. Toth, “Linelist of water vapor parameters from 500 to 8000 cm<sup>-1</sup>,” measured values, see <http://mark4sun.jpl.nasa.gov/h2o.html>.
25. Use of the semi-empirical coefficients of section 4.1 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
26. Default value of 0.07 cm<sup>-1</sup>/atm used for unassigned lines, D. Jacquemart, private communication (2004).
27. Use of air-widths of HD<sup>16</sup>O from Ref. 24 supposing no vibrational dependence.
28. Use of the semi-empirical coefficients of section 4.2.1 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
29. Use of the semi-empirical coefficients of section 4.2.2 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-

- induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
- 30.** Use of the semi-empirical coefficients of section 4.2.3 corresponding to Table 4 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
  - 31.** Use of the semi-empirical coefficients of section 4.2.3 corresponding to Table 9 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
  - 32.** Use of the semi-empirical coefficients of section 4.2.3 corresponding to Table 10 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, “Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines,” *JQSRT* **96**, 205-239 (2005).
  - 33.** L.P. Giver, B. Gentry, G. Schwemmer, and T.D. Wilkerson, “Water absorption lines, 931-961 nm: selected intensities, N<sub>2</sub>-collision-broadening coefficients, self-broadening coefficients, and pressure shifts in air,” *JQSRT* **27**, 423-436 (1982).
  - 34.** V. Malathy Devi, D.C. Benner, C.P. Rinsland, M.A.H. Smith, and B.D. Sidney, “Diode Laser Measurements of air and nitrogen broadening in the  $\nu_2$  bands of HDO, H<sub>2</sub><sup>16</sup>O, and H<sub>2</sub><sup>18</sup>O,” *J.Mol.Spectrosc.* **117**, 403-407 (1986).
  - 35.** F.M. Nicolaisen, ASA workshop, paper 5.8, Moscow June 6-8, (1990).
  - 36.** P. Cardinet, F. Sverin, A. Valentin, M.L. Claude, and A. Henri, “Wavenumber, intensity and width of water vapour lines in the region of 5.3  $\mu\text{m}$ ,” *CR.Acad.Sc.Paris* **284**, 37-39 (1977).
  - 37.** R.S. Eng, P.L. Kelley, A. Mooradian, A.R. Calawa, and T.C. Harman, “Tunable laser measurements of water vapor transitions in the vicinity of 5  $\mu\text{m}$ ,” *Chem.Phys.Lett.* **19**, 524-528 (1973).
  - 38.** Y.S. Chang and J.H. Shaw, “Intensities and widths of H<sub>2</sub>O lines between 1800 and 2100  $\text{cm}^{-1}$ ,” *JQSRT* **18**, 491-499 (1977).
  - 39.** J.R. Izatt, H. Sakai, H., and W.S. Benedict, “Positions, intensities, and widths of water-vapor lines between 475 and 692  $\text{cm}^{-1}$ ,” *JOSA* **59**, 19-26 (1969).
  - 40.** M.M. Johnson and A.H. LaGrone, “Determination of atmospheric water-vapor densities from measurements of the 6943.8-Å absorption line strength,” *Radio.Sci.* **8**, 407-410 (1973).
  - 41.** F.A. Blum, K.W. Nill, P.L. Kelley, A.R. Calawa, and T.C. Harman, “Tunable infrared laser spectroscopy of atmospheric water vapour,” *Science* **177**, 694-695 (1972).
  - 42.** A. Bauer, M. Godon, and B. Duterage, “Self- and air-broadened linewidth of the 183 GHz absorption in water vapour,” *JQSRT* **33**, 167-175 (1985).
  - 43.** R.S. Eng, P.L. Kelley, A.R. Calawa, T.C. Harman, and K.W. Nill, “Tunable diode laser measurements of water vapour absorption line parameters,” *Mol.Phys.* **28**, 653-664 (1974).
  - 44.** M.P. Arroyo and R.K. Hanson, 30th Aerospace Sciences Meetings & Exhibits paper AIAA 92-510, Reno NV, Jan. 6-9, (1992).
  - 45.** B.G. Aggev, Yu.N. Ponomarev, B.A. Tikhomirov, and I.S. Tyryshkin, 1990 ASA workshop paper 5.9, Moscow June 6-8, (1990).
  - 46.** T. Giesen, R. Schieder, G. Winnewisser, and K.M.T. Yamada, “Precise measurements of pressure broadening and shift for several H<sub>2</sub>O lines in the  $\nu_2$  band by argon, nitrogen, oxygen, and air,” *J.Mol.Spectrosc.* **153**, 406-418 (1992).
  - 47.** C.K.N. Patel, “Linewidth of tunable stimulated Raman scattering,” *Phys.Rev.Lett.* **28**, 649-652 (1972).
  - 48.** T.G. Adiks, A.A. Vinogradova, and I.P. Malkov, “Measurement of the absorption line



parameters of water vapor in the 5.8  $\mu\text{m}$  region using a tunable laser diode spectrometer,” *J.Appl.Spectrosc.* **45**, 778-781 (1986).

**49.** V.Ya. Ryadov, N.I. Furashov, “The width of the water vapor absorption line  $\lambda=0.92$  mm,” *Radiophys.Quant.Electron.* **9**, 621-623 (1966).

**50.** S. Adler-Golden, J. Lee, and N. Goldstein, “Diode laser measurements of temperature dependent line parameters for water vapor near 820 nm,” *JQSRT* **48**, 527-535 (1992).

**51.** V.Y. Ryadov and N.I. Furashov, *Radiophys. & Quantum Electron.* **18**, 256-266 (1975).

**52.** N. Goldstein, S. Adler-Golden, J. Lee, and F. Bien, “Measurement of molecular concentrations and line parameters using line-locked second harmonic spectroscopy with an AlGaAs diode laser,” *Appl.Opt.* **31**, 3409-3415 (1992).

**53.** A. Adel, *Phys.Rev.* **71**, 806-808 (1947).

**54.** K.M.T. Yamada, M. Harter, and T. Giesen, “Survey study of air-broadened water vapor lines in the  $\nu_2$  band by high-resolution FTIR spectroscopy,” *J.Mol.Spectrosc.* **157**, 84-94 (1993).

**55.** Z. Chu, T.D. Wilkerson, and U.N. Singh, “Water-vapor absorption line measurements in the 940-nm band by using a Raman-shifted dye laser,” *Appl.Opt.* **32**, 992-998 (1993).

**56.** J.T. Bradley, PhD thesis, University of New York (1970).

**57.** Q. Zou and P. Varanasi, “Laboratory measurement of the spectroscopic line parameters of water vapor in the 610-2100 and 3000-4050  $\text{cm}^{-1}$  regions at lower-tropospheric temperatures,” *JQSRT* **82**, 45-98 (2003).

**58.** R. Schermaul, R.C.M. Learner, D.A. Newnham, R.G. Williams, J. Ballard, N.F. Zobov, D. Belmiloud, and J. Tennyson, “The water vapor spectrum in the region 8600-15000  $\text{cm}^{-1}$ : experimental and theoretical studies to a new spectral line database,” *J.Mol.Spectrosc.* **208**, 32-42 (2001).

**59.** P.L. Ponsardin and E.V. Browell, “Measurements of  $\text{H}_2^{16}\text{O}$  linestrengths and air-induced broadenings and shifts in the 815-nm spectral region,” *J.Mol.Spectrosc.* **185**, 58-70 (1997).

**60.** J.-Y. Mandin, V. Dana, M. Badaoui, A. Barbe, A. Hamdouni, and J.J. Plateaux, “Measurements of pressure-broadening and pressure-shifting coefficients from FT spectra,” *J.Mol.Spectrosc.* **164**, 328-337 (1994).

**61.** EUMETSAT  $\text{H}_2\text{O}$  database, ESA ESTEC contract No. 13312/99/NL/SF

**62.** M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, C., Clerbaux, P.-F. Coheur, R. Colin, S. Fally, and M. Bach, “Water vapor line parameters in the 13000-9250  $\text{cm}^{-1}$  region,” *JQSRT* **82**, 99-117 (2003).

**63.** S. Fally, P.-F. Coheur, M. Carleer, C. Clerbaux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, “Water vapor line broadening and shifting by air in the 26000-13000  $\text{cm}^{-1}$  region,” *JQSRT* **82**, 119-131 (2003).

**64.** A. Lucchesini, S. Gozzini, and C. Gabbanini, “Water vapor overtones pressure line broadening and shifting measurements, *Eur.Phys.J.* **D 8**, 223-226 (2000).

**65.** M.Yu. Tretyakov, V.V. Parshin, M.A. Koshelev, V.N. Shanin, S.E. Myasnikova, and A.F. Krupnov, “Studies of 183GHz water line: broadening and shifting by air,  $\text{N}_2$  and  $\text{O}_2$  and integral intensity measurements,” *J.Mol.Spectrosc.* **218**, 239-245 (2003).

**67.** R.R. Gamache and J.-M. Hartmann, “An intercomparison of measured pressure-broadening and pressure-shifting parameters of water vapor,” *Can.J.Chem.* **82**, 1013-1027 (2004).

**68.** R.R. Gamache, private communication; calculation using the complex Robert-Bonamy formalism (2004).

**69.** Smoothed values from R.A. Toth, “Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ,” see <http://mark4sun.jpl.nasa.gov/h2o.html>.

**70.** S.D. Gasster, C.H. Townes, D. Goorvitch, and F.P.J. Valero, “Foreign-gas collision

broadening of the far-infrared spectrum of water vapor,” *JOSA B* **5**, 593-601 (1988).

71. D.W. Steyert, W.F. Wang, J.M. Sirota, N.M. Donahue, and D.C. Reuter, “Pressure broadening coefficients for rotational transitions of water in the 380-600  $\text{cm}^{-1}$  range,” *JQSRT* **72**, 775-782 (2002).
72. V.G. Avetisov, A.I. Nadezhdinskii, A.N. Khusnutdinov, P.M. Omarova, and M.V. Zyrianov, “Diode laser spectroscopy of water vapor in 1.8  $\mu\text{m}$ : line profile measurements,” *J.Mol.Spectrosc.* **160**, 326-334 (1993).
73. R.A. Toth, “Strengths and air-broadened widths of  $\text{H}_2\text{O}$  lines in the 2950-3400  $\text{cm}^{-1}$  region,” *JQSRT* **13**, 1127-1142 (1973).
74. R.A. Toth, “Air- and  $\text{N}_2$ -Broadening parameters of water vapor: 604 to 2271  $\text{cm}^{-1}$ ,” *J.Mol.Spectrosc.* **201**, 218-243 (2000).
75. S.J. Davis, W.J. Kessler, and M. Bachmann, “Collisional broadening of absorption lines in water vapor and atomic iodine relevant to COIL diagnostics,” *Proceedings SPIE* **3612**, 157-166 (1999).
76. G. Cazzoli, C. Puzzarini, G. Buffa, and O. Tarrini, “Experimental and theoretical investigation on pressure-broadening and pressure-shifting of the 22.2 GHz line of water,” *JQSRT* **105**, 438-449 (2007).
77. A. Jenouvrier, L. Daumont, L. Régalia-Jarlot, V.G. Tyuterev, M. Carleer, A.C. Vandaele, S. Mikhailenko, and S. Fally, “Fourier transform measurements of water vapor line parameters in the 4200-6600  $\text{cm}^{-1}$  region,” *JQSRT* **105**, 326-355 (2007).
78. G. Durry, V. Zeninari, B. Parvitte, T. Le Barbu, F. Lefevre, J. Ovarlez, and R.R. Gamache, “Pressure-broadening coefficients and line strengths of  $\text{H}_2\text{O}$  near 1.39  $\mu\text{m}$ : application to the in situ sensing of the middle atmosphere with balloonborne diode lasers,” *JQSRT* **94**, 387-403 (2005).
79. X. Liu, X. Zhou, J.B. Jeffries, and R.K. Hanson, “Experimental study of  $\text{H}_2\text{O}$  spectroscopic parameters in the near-IR (6940-7440  $\text{cm}^{-1}$ ) for gas sensing applications at elevated temperature,” *JQSRT* **103**, 565-577 (2007).
80. X. Liu, J.B. Jeffries, and R.K. Hanson, “Measurements of spectral parameters of water-vapour transitions near 1388 and 1345 nm for accurate simulation of high-pressure absorption spectra,” *Meas.Sci.Technol.* **18**, 1185-1194 (2007).
81. T. Seta, H. Hoshina, Y. Kasai, I. Hosako, C. Otani, S. Loßow, J. Urban, M. Ekström, P. Eriksson, and D. Murtagh, “Pressure broadening coefficients of the water vapor lines at 556.936 and 752.033 GHz,” *JQSRT* **109**, 144-150 (2008).
82. R.A. Toth, “Measurements and analysis (using empirical functions for widths) of air- and self-broadening parameters of  $\text{H}_2\text{O}$ ,” *JQSRT* **94**, 1-50 (2005).
83. V.H. Payne, J.S. Delamere, K.E. Cady-Pereira, R.R. Gamache, J.-L. Moncet, E.J. Mlawer, and S.A. Clough, “Air-Broadened Half-Widths of the 22- and 183-GHz Water-Vapor Lines,” *IEEE Trans.Geosci.Remote Sensing* **46**, 3601-3617 (2008).
84. R.R. Gamache, “Lineshape parameters for water vapor in the 3.2-17.76  $\mu\text{m}$  region for atmospheric applications,” *J.Mol.Spectrosc.* **229**, 9-18 (2005).
85. R.R. Gamache and A.L. Laraia, “ $\text{N}_2$ -,  $\text{O}_2$ -, and air-broadened half-widths, their temperature dependence, and line shifts for the rotation band of  $\text{H}_2^{16}\text{O}$ ,” *J.Mol.Spectrosc.* **257**, 116-127 (2009).
86. R.R. Gamache, “ $\text{N}_2$ -,  $\text{O}_2$ -, and air-broadened half-widths, their temperature dependence, and line shifts for the  $3\nu_1 + \nu_3$  and  $2\nu_1 + 2\nu_2 + \nu_3$  bands of  $\text{H}_2^{16}\text{O}$ ,” unpublished data, 2008.
87. R.A. Toth, L.R. Brown, M.A.H. Smith, V. Malathy Devi, D. Chris Benner, and M. Dulick, “Air-broadening of  $\text{H}_2\text{O}$  as a function of temperature: 696-2163  $\text{cm}^{-1}$ ,” *JQSRT* **101**, 339-366

(2006).

**88.** G. Cazzoli, C. Puzzarini, G. Buffa, and O. Tarrini, “Pressure-broadening of water lines in the THz frequency region: Improvements and confirmations for spectroscopic databases: Part I,” *JQSRT* **109**, 2820-2831 (2008).

**89.** A. Bruno, G. Pesce, G. Rusciano, and A. Sasso, “Self-, Nitrogen-, and Oxygen-Broadening Coefficient Measurements in the  $\nu_1$  Band of  $\text{H}_2\text{O}$  Using a Difference Frequency Generation Spectrometer at  $3\text{ }\mu\text{m}$ ,” *J.Mol.Spectrosc.* **215**, 244-250 (2002).

**90.** N. Ibrahim, P. Chelin, J. Orphal, and Y.I. Baranov, “Line parameters of  $\text{H}_2\text{O}$  around  $0.8\text{ }\mu\text{m}$  studied by tuneable diode laser spectroscopy,” *JQSRT* **109**, 2523-2536 (2008).

**91.** Polynomial fit of the values from Ref. [85] averaged as a function of  $J''$  and asymptotic value of  $\gamma_{\text{air}}(J'' = 50) = 0.00839\text{ cm}^{-1}\text{atm}^{-1}$ .

**92.** Approximation of Ref. 25 with estimated exchange of vibrational quanta.

**93.** Approximation of Ref. 28 with estimated exchange of vibrational quanta.

**94.** Approximation of Ref. 29 with estimated exchange of vibrational quanta.

**95.** Approximation of Ref. 30 with estimated exchange of vibrational quanta.

**96.** Approximation of Ref. 31 with estimated exchange of vibrational quanta.

**97.** Approximation of Ref. 32 with estimated exchange of vibrational quanta.

#### Half-widths (self)

**1.** For perpendicular bands derived from R.A. Toth, L.R. Brown, and C. Plymate, “Self-broadened widths and frequency shifts of water vapor lines between  $590$  and  $2400\text{ cm}^{-1}$ ,” *JQSRT* **59**, 529-562 (1998), for parallel bands from R.A. Toth, JPL, unpublished.

**2.** Unassigned lines using default value  $0.444\text{ cm}^{-1}/\text{atm}$ , L.R. Brown, JPL, private communication (2000).

**3.** R.A. Toth, “Linelist of water vapor parameters from  $500$  to  $8000\text{ cm}^{-1}$ ,” measured values, see <http://mark4sun.jpl.nasa.gov/data/spec/H2O>.

**4.** Use of self-widths of  $\text{H}_2^{16}\text{O}$  from Ref. 3 assuming no vibrational dependence.

**5.** Use of self-widths of  $\text{HD}^{16}\text{O}$  from Ref. 3 assuming no vibrational dependence.

**6.** Default value of  $0.35\text{ cm}^{-1}/\text{atm}$  used for unassigned lines, D. Jacquemart, private communication (2004).

**7.** B.E. Grossmann and E.V. Browell, “Spectroscopy of Water Vapor in the  $720\text{-nm}$  Wavelength Region: Line Strengths, Self-Induced Pressure Broadenings and Shifts, and Temperature Dependence of Linewidths and Shifts,” *J.Mol.Spectrosc.* **136**, 264-294 (1989).

**8.** L.P. Giver, B. Gentry, G. Schwemmer, and T.D. Wilkerson, “Water absorption lines,  $931\text{-}961\text{ nm}$ : selected intensities,  $\text{N}_2$ -collision-broadening coefficients, self-broadening coefficients, and pressure shifts in air,” *JQSRT* **27**, 423-436 (1982).

**9.** J.-Y. Mandin, J.-M. Flaud, and C. Camy-Peyret, “Measurements and calculations of self broadening coefficients of lines belonging to the  $\nu_2$  band of  $\text{H}_2^{16}\text{O}$ ,” *JQSRT* **23**, 351-370 (1980).

**10.** F.M. Nicolaisen, 1990 ASA workshop, paper 5.8, Moscow June 6-8, (1990).

**11.** V. Malathy Devi, B. Fridovich, G.D. Jones, and D.G.S. Snyder, “Intensities and half-widths for several  $\text{H}_2\text{O}$   $\nu_2$  lines in the region  $1500\text{-}1523\text{ cm}^{-1}$ ,” *J.Mol.Spectrosc.* **111**, 114-118 (1985).

**12.** R.S. Eng, P.L. Kelley, A. Mooradian, A.R. Calawa, and T.C. Harman, “Tunable laser measurements of water vapor transitions in the vicinity of  $5\text{ }\mu\text{m}$ ,” *Chem.Phys.Lett.* **19**, 524-528 (1973).

**13.** R.S. Eng, and A.W. Mantz, “Tunable diode laser measurement of water vapor line parameters in the  $10\text{- to }15\text{-}\mu\text{m}$  spectral region,” *J.Mol.Spectrosc.* **74**, 388-399 (1979).

**14.** Y. Ben Aryeh, “Line widths and intensities in the wings of the  $\nu_2$  water vapor band at  $400^\circ\text{K}$

and 540°K,” *JQSRT* **7**, 211-224 (1967).

**15.** J.R. Izatt, H. Sakai, H., and W.S. Benedict, “Positions, intensities, and widths of water-vapor lines between 475 and 692  $\text{cm}^{-1}$ ,” *JOSA* **59**, 19-26 (1969).

**16.** M.A. Guerra, M. Ketabi, A. Sanchez, M.S. Feld, and A. Javan, “Water vapor spectroscopy at 5  $\mu\text{m}$  using a tunable SFR laser,” *J.Chem.Phys.* **63**, 1317-1319 (1975).

**17.** A. Bauer, M. Godon, and B. Duterage, “Self- and air-broadened linewidth of the 183 GHz absorption in water vapour,” *JQSRT* **33**, 167-175 (1985).

**18.** D. Mrowinski, “Refraction and absorption in atmospheric gases near the 22 GHz water vapour rotational line,” *Z.Angew.Phys.* **29**, 323-330 (1970).

**19.** J.A. Mucha, “Tunable diode laser measurements of water vapor line parameters in the 6- $\mu\text{m}$  spectral region,” *Appl.Spectrosc.* **36**, 141-147 (1982).

**20.** R.S. Eng, P.L. Kelley, A.R. Calawa, T.C. Harman, and K.W. Nill, “Tunable diode laser measurements of water vapour absorption line parameters,” *Mol.Phys.* **28**, 653-664 (1974).

**21.** J.-Y. Mandin, C. Camy-Peyret, J.-M. Flaud, and G. Guelachvili, “Measurements and calculations of self-broadening coefficients of lines belonging to the  $2\nu_2$ ,  $\nu_1$ , and  $\nu_3$  bands of  $\text{H}_2^{16}\text{O}$ ,” *Can.J.Phys.* **60**, 94-101 (1982).

**22.** L. Frenkel and D. Woods, “Microwave absorption by  $\text{H}_2\text{O}$  vapor and its mixtures with other gases between 100 and 300 Gc/s,” *Proc IEEE* **54**, 498-505 (1966).

**23.** V.N. Markov, “Temperature dependence of self-induced pressure broadening and shift of the 643-550 line of the water molecule,” *J.Molec.Spectrosc.* **164**, 233-238 (1994).

**24.** J.-M. Hartmann, J. Taine, J. Bonamy, B. Labani, and D. Robert, “Collisional broadening of rotation-vibration lines for asymmetric-top molecules. II.  $\text{H}_2\text{O}$  diode laser measurements in the 400-900K range; calculations in the 300-2000K range,” *J.Chem.Phys.* **86**, 144-156 (1987).

**25.** A. Bauer, M. Godon, M. Kheddar, J.-M. Hartmann, J. Bonamy, and D. Robert, “Temperature and perturber dependences of water-vapor 380 GHz-line broadening,” *JQSRT* **37**, 531-539 (1987).

**26.** H.J. Liebe, M.C. Thompson, and T.A. Dillon, “Dispersion studies of the 22 GHz water vapor line shape I. The Lorentzian behavior,” *JQSRT* **9**, 31-47 (1969).

**27.** J.R. Rusk, “Line-Breadth Study of the 1.64-mm Absorption in Water Vapor,” *J.Chem.Phys.* **42**, 493-500 (1965).

**28.** A. Bauer, M. Godon, M. Kheddar, and J.-M. Hartmann, “Temperature and perturber dependences of water vapor line-broadening. Experiments at 183 GHz; calculations below 1000 GHz” *JQSRT* **41**, 49-54 (1989).

**29.** T. Kasuga, H. Kuze, and T. Shimizu, “Determinations of relaxation rate constants on the 22 GHz rotational transition of  $\text{H}_2\text{O}$  by coherent transient spectroscopy,” *J.Chem.Phys.* **69**, 5195-5198 (1978).

**30.** R. Emery, “Atmospheric Absorption Measurements in the Region of 1 mm Wavelength,” *Infrared Phys.* **12**, 65-79 (1972).

**31.** R.B. Sanderson, and N. Ginsburg, “Line widths and line strengths in the rotational spectrum of water vapor,” *JQSRT* **3**, 435-444 (1963).

**32.** A.F. Aushev, N.F. Borisova, E.S. Bykova, V.M. Osipov, and V.V. Tsukanov, “On the temperature dependence of the half-widths of the spectral lines of  $\text{CO}_2$  and  $\text{H}_2\text{O}$ ,” *Opt.Spectrosc.* **68**, 700-701 (1990).

**33.** S. Adler-Golden, J. Lee, and N. Goldstein, “Diode laser measurements of temperature dependent line parameters for water vapor near 820 nm,” *JQSRT* **48**, 527-535 (1992).

**34.** A.P. Godlevskii, and V.A. Kapitanov, “Changes in the line shapes of water vapor due to broadening by foreign gases,” *J.Appl.Spectrosc.* **28**, 142-146 (1978).



35. J.J. Remedios, D.Phil.thesis, Oxford University (1990).
36. C.H. Townes and F.R. Merritt, *Phys.Rev.* **70**, 558-559 (1946).
37. M.P. Arroyo and R.K. Hanson, "Absorption measurements of water-vapor concentration, temperature, and line-shape parameters using a tunable InGaAsP diode laser," *Appl.Opt.* **32**, 6104-6116 (1993).
38. Q. Zou and P. Varanasi, "Laboratory measurement of the spectroscopic line parameters of water vapor in the 610-2100 and 3000-4050  $\text{cm}^{-1}$  regions at lower-tropospheric temperatures," *JQSRT* **82**, 45-98 (2003).
39. D.W. Steyert, W.F. Wang, J.M. Sirota, N.M. Donahue, and D.C. Reuter, "Pressure broadening coefficients for rotational transitions of water in the 380-600  $\text{cm}^{-1}$  range," *JQSRT* **72**, 775-782 (2002).
40. P.-F. Coheur, S. Fally, M. Carleer, C. Clerbaux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, "New water vapor line parameters in the 26000-13000  $\text{cm}^{-1}$  region," *JQSRT* **74**, 493-510 (2002).
41. K. Singh and J.J. O'Brien, "Intensities and self-broadening coefficients of weak water vapor lines in the 720-nm region determined by intracavity laser absorption spectroscopy," *J.Mol.Spectrosc.* **167**, 99-108 (1994).
42. B.L. Upschulte and M.G. Allen, "Diode laser measurements of line strengths and self-broadening parameters of water vapor between 300 and 1000 K near 1.31  $\mu\text{m}$ ," *JQSRT* **59**, 653-670 (1998).
43. S. Langlois, T.P. Birbeck, and R.K. Hanson, "Diode laser measurements of  $\text{H}_2\text{O}$  line intensities and self-broadening coefficients in the 1.4- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **163**, 27-42 (1994).
44. V. Nagali, S.I. Chou, D.S. Baer, and R.K. Hanson, "Diode laser measurements of temperature dependent half-widths of  $\text{H}_2\text{O}$  transitions in the 1.4  $\mu\text{m}$  region," *JQSRT* **57**, 795-809 (1997).
45. K.V. Chance, K. Park, and K.M. Evenson, "Pressure broadening of far infrared rotational transitions: 88.65  $\text{cm}^{-1}$   $\text{H}_2\text{O}$  and 114.47  $\text{cm}^{-1}$   $\text{O}_3$ ," *JQSRT* **59**, 687-688 (1998).
46. S.J. Davis, W.J. Kessler, and M. Bachmann, "Collisional broadening of absorption lines in water vapor and atomic iodine relevant to COIL diagnostics," Proceedings-of-the-SPIE --The-International-Society-for-Optical-Engineering. **3612**, 157-166 (1999).
47. S. Fally, P.-F. Coheur, M. Carleer, C. Clerbaux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, "Water vapor line broadening and shifting by air in the 26000-13000  $\text{cm}^{-1}$  region," *JQSRT* **82**, 119-131 (2003).
48. M. Lepère, A. Henry, A. Valentin, and C. Camy-Peyret, "Diode-Laser Spectroscopy: Line Profiles of  $\text{H}_2\text{O}$  in the Region of 1.39  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **208**, 25-31 (2001).
49. L. Moretti, A. Sasso, L. Gianfrani, and R. Ciurylo, "Collisional-Broadened and Dicke-Narrowed Lineshapes of  $\text{H}_2^{16}\text{O}$  and  $\text{H}_2^{18}$  Transitions at 1.39  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **205**, 20-27 (2001).
50. Smoothed values from R.A. Toth, "Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ," see <http://mark4sun.jpl.nasa.gov/data/spec/H2O>.
51. R.R. Gamache, unpublished data, average values of experimental data as a function of  $J'$  (2000).
52. R.R. Gamache, default values, unpublished data (2000).
53. M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, C., Clerbaux, P.-F. Coheur, R. Colin, S. Fally, and M. Bach, "Water vapor line parameters in the 13000-9250  $\text{cm}^{-1}$  region," *JQSRT* **82**, 99-117 (2003).

54. V.G. Avetisov, A.I. Nadezhdinskii, A.N. Khusnutdinov, P.M. Omarova, and M.V. Zyrianov, "Diode laser spectroscopy of water vapor in 1.8  $\mu\text{m}$ : line profile measurements," *J.Mol.Spectrosc.* **160**, 326-334 (1993).
55. N. Goldstein, S. Adler-Golden, J. Lee, and F. Bien, "Measurement of molecular concentrations and line parameters using line-locked second harmonic spectroscopy with an AlGaAs diode laser," *Appl.Opt.* **31**, 3409-3415 (1992).
56. G. Cazzoli, C. Puzzarini, G. Buffa, O. Tarrini, "Experimental and theoretical investigation on pressure-broadening and pressure-shifting of the 22.2 GHz line of water," *JQSRT* **105**, 438-449 (2007).
57. A. Jenouvrier, L. Daumont, L. Régalia-Jarlot, V.G. Tyuterev, M. Carleer, A.C. Vandaele, S. Mikhailenko, and S. Fally, "Fourier transform measurements of water vapor line parameters in the 4200-6600  $\text{cm}^{-1}$  region," *JQSRT* **105**, 326-355 (2007).
58. G. Cazzoli, C. Puzzarini, G. Buffa, and O. Tarrini, "Pressure-broadening in the THz frequency region: The 1.113 THz line of water," *JQSRT* **109**, 1563-1574 (2008).
59. M.A. Koshelev, M.Y. Tretyakov, G.Y. Golubiatnikov, V.V. Parshin, V.N. Markov, and I.A. Koval, "Broadening and shifting of the 321-, 325- and 380-GHz lines of water vapor by pressure of atmospheric gases," *J.Mol.Spectrosc.* **241**, 101-108 (2007).
60. G.Y. Golubiatnikov, M.A. Koshelev, and A.F. Krupnov, "Pressure shift and broadening of 110-101 water vapor lines by atmosphere gases," *JQSRT* **109**, 1828-1833 (2008).
61. N. Ibrahim, P. Chelin, J. Orphal, and Y.I. Baranov, "Line parameters of  $\text{H}_2\text{O}$  around 0.8  $\mu\text{m}$  studied by tuneable diode laser spectroscopy," *JQSRT* **109**, 2523-2536 (2008).
62. R.A. Toth, "Measurements and analysis (using empirical functions for widths) of air- and self-broadening parameters of  $\text{H}_2\text{O}$ ," *JQSRT* **94**, 1-50 (2005).
63. D. Lisak, G. Rusciano, and A. Sasso, "An accurate comparison of lineshape models on  $\text{H}_2\text{O}$  lines in the spectral region around 3  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **227**, 162-171 (2004).
64. G. Cazzoli, C. Puzzarini, G. Buffa, and O. Tarrini, "Pressure-broadening of water lines in the THz frequency region: Improvements and confirmations for spectroscopic databases: Part I," *JQSRT* **109**, 2820-2831 (2008).
65. A. Bruno, G. Pesce, G. Rusciano, and A. Sasso, "Self-, Nitrogen-, and Oxygen-Broadening Coefficient Measurements in the  $\nu_1$  Band of  $\text{H}_2\text{O}$  Using a Difference Frequency Generation Spectrometer at 3  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **215**, 244-250 (2002).
66. R.R. Gamache and J.-M. Hartmann, "An intercomparison of measured pressure-broadening and pressure-shifting parameters of water vapor," *Can.J.Chem.* **82**, 1013-1027 (2004).
67. B.K. Antony and R.R. Gamache, "Self-broadened half-widths and self-induced line shifts for water vapor transitions in the 3.2-17.76  $\mu\text{m}$  spectral region via complex Robert-Bonamy theory," *J.Mol.Spectrosc.* **243**, 113-123 (2007).
68. B.K. Antony, S. Neshyba, and R.R. Gamache, "Self-broadening of water vapor transitions via the complex Robert-Bonamy theory," *JQSRT* **105**, 148-163 (2007).
69. V.B. Podobedov, D.F. Plusquellic, and G.T. Fraser, "THz laser study of self-pressure and temperature broadening and shifts of water vapor lines for pressures up to 1:4 kPa," *JQSRT* **87**, 377-385 (2004).
70. R. Tolchenov and J. Tennyson, "Water Line Parameters from Refitted Spectra constrained by empirical upper state levels: study of the 9500 - 14500  $\text{cm}^{-1}$  region," *JQSRT* **109**, 559-568 (2008).
71. Polynomial fit of the values from Ref. [85] averaged as a function of  $J''$  and asymptotic value of  $\gamma_{\text{self}}(J'' = 50) = 0.0400 \text{ cm}^{-1} \text{ atm}^{-1}$ .

Temperature dependence of air-broadened half-width

1. Unassigned lines using default value 0.68, R.R. Gamache and L.R. Brown, private communication (2000).
2. R.A. Toth, "Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ," see <http://mark4sun.jpl.nasa.gov/data/spec/H2O>.
3. Unassigned lines using default value of 0.5, R.R. Gamache, B.K. Antony, P.R. Gamache, G. Wagner, and M. Birk, "Temperature Dependence of  $\text{N}_2$ -,  $\text{O}_2$ - and Air-broadened Half-widths of Water Vapor Transitions: Insight from Theory and Comparison with Measurement," The 9<sup>th</sup> HITRAN Database Conference, Harvard-Smithsonian Center for Astrophysics, Cambridge MA, USA (2006).
4.  $n$  as a function of the rotational quantum numbers (vibrationally independent) from CRB calculations of rotation and  $\nu_2$  band.
5.  $n$  as a function of  $J''$  from Table 7 of the 2004 HITRAN paper.
6. T.M Goyette and F.C. DeLucia, "The pressure broadening of the 31,3-22,0 transition of Water between 80 and 600 K," *J.Mol.Spectrosc.* **143**, 346-358, (1990).
7. B.E. Grossmann and E.V. Browell, "Spectroscopy of water vapor in the 720-nm wavelength region - Line strengths, self-induced pressure broadenings and shifts, and temperature dependence of linewidths and shifts," *J.Mol.Spectrosc.* **136**, 264-294 (1989).
8. A. Bauer, M. Godon, and B. Duterage, "Self- and air-broadened linewidth of the 183 GHz absorption in water vapor," *JQSRT* **33**, 167-175 (1985).
9. A. Bauer, M. Godon, M. Kheddar, J.-M. Hartmann, J. Bonamy, and D. Robert, "Temperature and perturber dependences of water-vapor 380 GHz-line broadening," *JQSRT* **37**, 531-539 (1987).
10. A. Bauer, M. Godon, M. Kheddar, and J.-M. Hartmann, "Temperature and perturber dependences of water vapor line-broadening. Experiments at 183 GHz; calculations below 1000 GHz," *JQSRT* **41**, 49-54 (1989).
11. S. Adler-Golden, J. Lee, and N. Goldstein, "Diode laser measurements of temperature dependent line parameters for water vapor near 820 nm," *JQSRT* **48**, 527-535, (1992).
12. J.J. Remedios, PhD thesis University of Oxford (1990).
13. Q. Zou and P. Varanasi, "Laboratory measurement of the spectroscopic line parameters of water vapor in the 950-2100 and 3000-4050  $\text{cm}^{-1}$  regions at lower-tropospheric temperatures," *JQSRT* **82**, 45-98 (2003).
14. P.L. Ponsardin and E.V. Browell, "Measurements of  $\text{H}_2^{16}\text{O}$  linestrengths and air-induced broadenings and shifts in the 815-nm spectral region," *J.Mol.Spectrosc.* **185**, 58-70 (1997).
15. X. Liu, X. Zhou, J.B. Jeffries, and R.K. Hanson, "Experimental study of  $\text{H}_2\text{O}$  spectroscopic parameters in the near-IR (6940-7440  $\text{cm}^{-1}$ ) for gas sensing applications at elevated temperature," *JQSRT* **103**, 565-577 (2007).
16. X. Liu, J.B. Jeffries, and R.K. Hanson, "Measurements of spectral parameters of water-vapour transitions near 1388 and 1345 nm for accurate simulation of high-pressure absorption spectra," *Meas.Sci.Technol.* **18**, 1185-1194 (2007).
17. R.R. Gamache, "Line Shape parameters for water vapor in the 3.2 to 17.76  $\mu\text{m}$  region for Atmospheric Applications," *J.Mol.Spectrosc.* **229**, 9-18 (2005).
18. R.R. Gamache and A.L. Laraia, " $\text{N}_2$ -,  $\text{O}_2$ -, and air-broadened half-widths, their temperature dependence, and line shifts for the rotation band of  $\text{H}_2^{16}\text{O}$ ," *J.Mol.Spectrosc.* **257**, 116-127 (2009).
19. R.R. Gamache, " $\text{N}_2$ -,  $\text{O}_2$ -, and air-broadened half-widths, their temperature dependence, and line shifts for the  $3\nu_1 + \nu_3$  and  $2\nu_1 + 2\nu_2 + \nu_3$  bands of  $\text{H}_2^{16}\text{O}$ ," unpublished data, 2008.

Pressure shift (air)

1. Set to constant  $-0.0111 \text{ cm}^{-1}/\text{atm}$ , L.R. Brown, JPL, private communication (2000).
2. Determined from average of many bands, L.R. Brown, JPL, private communication (2000).
3. L.R. Brown, R.A. Toth, and M. Dulick, "Empirical Line Parameters of  $\text{H}_2^{16}\text{O}$  near  $0.94 \mu\text{m}$ : Positions, Intensities and Air-Broadening Coefficients," *J.Mol.Spectrosc.* **212**, 57-82 (2002).
4. R.R. Gamache and J. Fischer, "Calculated Halfwidths and Lineshifts of Water-vapor transitions in the  $0.7 \mu\text{m}$  Region and a Comparison with Published Data," *J.Mol.Spectrosc.* **207**, 254-262 (2001).
5. B.E. Grossmann and E.V. Browell, "Water-Vapor Line Broadening and Shifting by Air, Nitrogen, Oxygen, and Argon in the 720-nm Wavelength Region," *J.Mol.Spectrosc.* **138**, 562-595 (1989).
6. R.A. Toth, "Linelist of water vapor parameters from 500 to  $8000 \text{ cm}^{-1}$ ," measured values, see <http://mark4sun.jpl.nasa.gov/data/spec/H2O>.
7. Use of the semi-empirical coefficients of section 4.1 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, "Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines," *JQSRT* **96**, 205-239 (2005).
8. Use of the semi-empirical coefficients of section 4.2.1 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, "Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines," *JQSRT* **96**, 205-239 (2005).
9. Use of the semi-empirical coefficients of section 4.2.2 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, "Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines," *JQSRT* **96**, 205-239 (2005).
10. Use of the semi-empirical coefficients of section 4.2.3 corresponding to Table 4 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, "Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines," *JQSRT* **96**, 205-239 (2005).
11. Use of the semi-empirical coefficients of section 4.2.3 corresponding to Table 9 of D. Jacquemart, R.R. Gamache, and L.S. Rothman, "Semi-empirical calculation of air-broadened half-widths and air pressure-induced frequency shifts of water-vapor absorption lines," *JQSRT* **96**, 205-239 (2005).
12. B.E. Grossmann and E.V. Browell, "Water-Vapor Line Broadening and Shifting by Air, Nitrogen, Oxygen, and Argon in the 720-nm Wavelength Region," *J.Mol.Spectrosc.* **138**, 562-595 (1989).
13. L.P. Giver, B. Gentry, G. Schwemmer, and T.D. Wilkerson, "Water absorption lines, 931-961 nm: selected intensities,  $\text{N}_2$ -collision-broadening coefficients, self-broadening coefficients, and pressure shifts in air," *JQSRT* **27**, 423-436 (1982).
14. T. Giesen, R. Schieder, G. Winnewisser, and K.M.T. Yamada, "Precise measurements of pressure broadening and shift for several  $\text{H}_2\text{O}$  lines in the  $\nu_2$  band by argon, nitrogen, oxygen, and air," *J.Mol.Spectrosc.* **153**, 406-418 (1992).
15. V.G. Avetisov, A.I. Nadezhdinskii, A.N. Khusnutdinov, P.M. Omarova, and M.V. Zyrianov, "Diode laser spectroscopy of water vapor in  $1.8 \mu\text{m}$ : line profile measurements," *J.Mol.Spectrosc.* **160**, 326-334 (1993).
16. K.M.T. Yamada, M. Harter, and T. Giesen, "Survey study of air-broadened water vapor lines in the  $\nu_2$  band by high-resolution FTIR spectroscopy," *J.Mol.Spectrosc.* **157**, 84-94 (1993).
17. P.L. Ponsardin and E.V. Browell, "Measurements of  $\text{H}_2^{16}\text{O}$  linestrengths and air-induced broadenings and shifts in the 815-nm spectral region," *J.Mol.Spectrosc.* **185**, 58-70 (1997).
18. A. Lucchesini, S. Gozzini, and C. Gabbanini, "Water vapor overtones pressure broadening



and shifting measurements,” *Eur.Phys.J.* **D8**, 223-226 (2000).

**19.** J.-Y. Mandin, V. Dana, M. Badaoui, A. Barbe, A. Hamdouni, and J.J. Plateaux, “Measurements of pressure-broadening and pressure-shifting coefficients from FT spectra,” *J.Mol.Spectrosc.* **164**, 328-337 (1994).

**20.** M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, C., Clerbaux, P.-F. Coheur, R. Colin, S. Fally, and M. Bach, “Water vapor line parameters in the 13000-9250  $\text{cm}^{-1}$  region,” *JQSRT* **82**, 99-117 (2003).

**21.** S. Fally, P.-F. Coheur, M. Carleer, C. Clerbaux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, and A.C. Vandaele, “Water vapor line broadening and shifting by air in the 26000-13000  $\text{cm}^{-1}$  region,” *JQSRT* **82**, 119-131 (2003).

**22.** M.Yu. Tretyakov, V.V. Parshin, M.A. Koshelev, V.N. Shanin, S.E. Myasnikova, and A.F. Krupnov, “Studies of 183GHz water line: broadening and shifting by air,  $\text{N}_2$  and  $\text{O}_2$  and integral intensity measurements,” *J.Mol.Spectrosc.* **218**, 239-245 (2003).

**23.** R.R. Gamache and J.-M. Hartmann, “An intercomparison of measured pressure-broadening and pressure-shifting parameters of water vapor,” *Can.J.Chem.* **82**, 1013-1027 (2004)..

**24.** R.R. Gamache, private communication; calculation using the complex Robert-Bonamy formalism (2004).

**25.** Smoothed values from R.A. Toth, “Linelist of water vapor parameters from 500 to 8000  $\text{cm}^{-1}$ ,” see <http://mark4sun.jpl.nasa.gov/data/spec/H2O>.

**26.** Q. Zou and P. Varanasi, “Laboratory measurement of the spectroscopic line parameters of water vapor in the 610-2100 and 3000-4050  $\text{cm}^{-1}$  regions at lower-tropospheric temperatures,” *JQSRT* **82**, 45-98 (2003).

**27.** R.S. Eng, P.L. Kelley, A. Mooradian, A.R. Calawa, and T.C. Harman, “Tunable laser measurements of water vapor transitions in the vicinity of 5  $\mu\text{m}$ ,” *Chem.Phys.Lett.* **19**, 524-528 (1973).

**28.** V.B. Podobedov, D.F. Plusquellic, and G.T. Fraser, “THz laser study of self-pressure and temperature broadening and shifts of water vapor lines for pressures up to 1:4 kPa,” *JQSRT* **87**, 377-385 (2004).

**29.** R.A. Toth, “Air- and  $\text{N}_2$ -Broadening parameters of water vapor: 604 to 2271  $\text{cm}^{-1}$ ,” *J.Mol.Spectrosc.* **201**, 218-243 (2000).

**30.** S.J. Davis, W.J. Kessler, and M. Bachmann, “Collisional broadening of absorption lines in water vapor and atomic iodine relevant to COIL diagnostics,” *Proceedings SPIE* **3612**, 157-166 (1999).

**31.** G. Cazzoli, C. Puzzarini, G. Buffa, and O. Tarrini, “Experimental and theoretical investigation on pressure-broadening and pressure-shifting of the 22.2 GHz line of water,” *JQSRT* **105**, 438-449 (2007).

**32.** X. Liu, J.B. Jeffries, and R.K. Hanson, “Measurements of spectral parameters of water-vapour transitions near 1388 and 1345 nm for accurate simulation of high-pressure absorption spectra,” *Meas.Sci.Technol.* **18**, 1185-1194 (2007).

**33.** M.A. Koshelev, M.Y. Tretyakov, G.Y. Golubiatnikov, V.V. Parshin, V.N. Markov, and I.A. Koval, “Broadening and shifting of the 321-, 325- and 380-GHz lines of water vapor by pressure of atmospheric gases,” *J.Mol.Spectrosc.* **241**, 101-108 (2007).

**34.** R.A. Toth, “Measurements and analysis (using empirical functions for widths) of air- and self-broadening parameters of  $\text{H}_2\text{O}$ ,” *JQSRT* **94**, 1-50 (2005).

**35.** R.R. Gamache, “ $\text{N}_2$ -,  $\text{O}_2$ -, and air-broadened half-widths, their temperature dependence, and line shifts for the  $3\nu_1 + \nu_3$  and  $2\nu_1 + 2\nu_2 + \nu_3$  bands of  $\text{H}_2^{16}\text{O}$ ,” unpublished data, 2008.

**36.** R.R. Gamache and J.-M. Hartmann, “An intercomparison of measured pressure-broadening

and pressure-shifting parameters of water vapor,” *Can.J.Chem.* **82**, 1013-1027 (2004).

**37.** R.R. Gamache and A.L. Laraia, “N<sub>2</sub>-, O<sub>2</sub>-, and air-broadened half-widths, their temperature dependence, and line shifts for the rotation band of H<sub>2</sub><sup>16</sup>O,” *J.Mol.Spectrosc.* **257**, 116-127 (2009).

**38.** A. Jenouvrier, L. Daumont, L. Régalia-Jarlot, V.G. Tyuterev, M. Carleer, A.C. Vandaele, S. Mikhailenko, and S. Fally, “Fourier transform measurements of water vapor line parameters in the 4200-6600 cm<sup>-1</sup> region,” *JQSRT* **105**, 326-355 (2007).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. L.S. Rothman, R.L. Hawkins, R.B. Wattson, and R.R. Gamache, "Energy Levels, Intensities, and Linewidths of Atmospheric Carbon Dioxide Bands," *JQSRT* **48**, 537-566 (1992).
2. Update to Ref. 1 (1994).
3. D.Chris Benner, College of William and Mary, private communication (1994).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
5. D.Chris Benner, College of William and Mary, private communication (2003).
6. C.E. Miller and L.R. Brown, "Near Infrared Spectroscopy of Carbon Dioxide I. <sup>16</sup>O<sup>12</sup>C<sup>16</sup>O Line Positions," *J. Molec. Spectrosc.* **228**, 329-354 (2004).
7. S.A.Tashkun, V.I.Perevalov, J.-L. Teffo, A.D. Bykov, and N.N. Lavrentieva, "CDSD-296, the carbon dioxide spectroscopic databank: version for atmospheric applications," XIV symposium on High Resolution Molecular Spectroscopy, Krasnoyarsk, Russia, July 6-11, 2003.
8. Y. Ding, E. Bertseva, and A. Campargue, "The 2v<sub>1</sub> + 2v<sub>3</sub> Triad of <sup>12</sup>CO<sub>2</sub>," *J.Molec.Spectrosc.* **212**, 219-222 (2002).
9. C. Claveau, J.-L. Teffo, D. Hurtmans, A. Valentin, and R.R. Gamache, "Line Positions and Absolute Intensities in the Laser Bands of Carbon-12 Oxygen-17 Isotopic Species of Carbon Dioxide," *J. Molec. Spectrosc.* **193**, 15-32 (1999).
10. A. Campargue, A. Charvat, and D. Permogorov, "Absolute intensity measurement of CO<sub>2</sub> overtone transitions in the near-infrared," *Chem.Phys.Letters* **223**, 567-572 (1994).
11. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, "Spectroscopic database of CO<sub>2</sub> line parameters: 4300-7000 cm<sup>-1</sup>," *JQSRT* **109**, 906-921 (2008).
12. V.I. Perevalov and S.A. Tashkun, "CDSD-296 (Carbon Dioxide Spectroscopic Databank): Updated and Enlarged Version for Atmospheric Applications," 10<sup>th</sup> HITRAN Database Conference, Cambridge MA, USA (2008).
13. B.V. Perevalov, V.I. Perevalov, and A. Campargue, "A (nearly) complete experimental linelist for <sup>13</sup>C<sup>16</sup>O<sub>2</sub>, <sup>16</sup>O<sup>13</sup>C<sup>18</sup>O, <sup>16</sup>O<sup>13</sup>C<sup>17</sup>O, <sup>13</sup>C<sup>18</sup>O<sub>2</sub> and <sup>17</sup>O<sup>13</sup>C<sup>18</sup>O by high-sensitivity CW-CRDS spectroscopy between 5851 and 7045 cm<sup>-1</sup>," *JQSRT* **109**, 2437-2462 (2008).
14. B.V. Perevalov, A. Campargue, B. Gao, S. Kassi, S.A. Tashkun, and V.I. Perevalov, "New CW-CRDS measurements and global modeling of <sup>12</sup>C<sup>16</sup>O<sub>2</sub> absolute line intensities in the 1.6 μm region," *J.Mol.Spectrosc.* **252**, 190-197 (2008).
15. V.I. Perevalov, Institute of Atmospheric Optics, private communication (2008).
16. Updated and enlarged (in 2008), CDSD-2010 database described in S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva, "CDSD-1000, the high-temperature carbon dioxide spectroscopic databank," *JQSRT* **82**, 165-196 (2003). See <ftp://ftp.iao.ru/pub/CDSD-2008/1000/>
17. S.A. Tashkun and V.I. Perevalov, "CDSD-Venus database, adapted for Venus conditions (750 K)," <ftp://ftp.iao.ru/pub/CDSD-2008/Venus/>

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith,

“The HITRAN database: 1986 Edition,” *Appl. Opt.* **26**, 4058-4097 (1987).

1. L.S. Rothman, R.L. Hawkins, R.B. Wattson, and R.R. Gamache, “Energy Levels, Intensities, and Linewidths of Atmospheric Carbon Dioxide Bands,” *JQSRT* **48**, 537-566 (1992).
2. Update to Ref. 1 (1994).
3. D.Chris Benner, College of William and Mary, private communication (1994).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, “Submillimeter, Millimeter, and Microwave Spectral Line Catalog,” *JQSRT* **60**, 883-890 (1998).
5. D.Chris Benner, College of William and Mary, private communication (2003).
6. V. Malathy Devi, D.C. Benner, C.P. Rinsland, and M.A.H. Smith, “Absolute Rovibrational Intensities of  $^{12}\text{C}^{16}\text{O}_2$  Absorption Bands in the 3090-3850  $\text{cm}^{-1}$  Spectral Region,” *JQSRT* **60**, 741-770 (1998).
7. J. Henningsen and H. Simonsen, “The  $(22^0_1-00^0_0)$  Band of  $\text{CO}_2$  at 6348  $\text{cm}^{-1}$ : Linestrengths, Broadening Parameters, and Pressure Shifts,” *J. Molec. Spectrosc.* **203**, 16-27 (2000).
8. L.P. Giver, NASA Ames Research Center, private communication (1994).
9. L.P. Giver, C. Chackerian, Jr., M.N. Spencer, L.R. Brown, and R.B. Wattson, “The Rovibrational Intensities of the  $(40^0_1) \leftarrow (00^0_0)$  Pentad Absorption Bands of  $^{12}\text{C}^{16}\text{O}_2$  between 7284 and 7921  $\text{cm}^{-1}$ ,” *J.Mol.Spectrosc.* **175**, 104-111 (1996).
10. R.J. Kshirsagar, L.P. Giver, and C. Chackerian Jr, “Rovibrational Intensities of the  $(00^0_3) \leftarrow (10^0_0)$  Dyad Absorption Bands of  $^{12}\text{C}^{16}\text{O}_2$ ,” *J.Molec.Spectrosc.* **199**, 230-235 (2000).
11. R.J. Kshirsagar, L.P. Giver, C. Chackerian Jr, and L.R. Brown, “The Rovibrational Intensities of the  $2\nu_3$  Band of  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  at 4639  $\text{cm}^{-1}$ ,” *JQSRT* **61**, 695-701 (1999).
12. L.P. Giver, L.R. Brown, C. Chackerian Jr, and R.S. Freedman, “The rovibrational intensities of five bands of  $^{12}\text{C}^{16}\text{O}_2$  between 5218 and 5349  $\text{cm}^{-1}$ ,” *JQSRT* **78**, 417-436 (2003).
13. J.-Y. Mandin, V. Dana, J.-Y. Allout, L. Régalia, A. Barbe, and J.-J. Plateaux, “Line Intensities and Self-Broadening Coefficients in the 10012-10001 Band of  $^{12}\text{C}^{16}\text{O}_2$  Centered at 2224.657  $\text{cm}^{-1}$ ,” *J.Molec.Spectrosc.* **170**, 604-607 (1995).
14. J.-L. Teffo, C. Claveau, and A. Valentin, “Infrared Fundamental Bands of  $\text{O}^{13}\text{C}^{17}\text{O}$  Isotopic Variants of Carbon Dioxide,” *JQSRT* **59**, 151-164 (1998).
15. J.-L. Teffo, C. Claveau, Q. Kou, G. Guelachvili, A. Ubelmann, V.I. Perevalov, and S.A. Tashkun, “Line Intensities of  $^{12}\text{C}^{16}\text{O}_2$  in the 1.2-1.4  $\mu\text{m}$  Spectral Region,” *J.Molec.Spectrosc.* **201**, 249-255 (2000).
16. C. Claveau, J.-L. Teffo, D. Hurtmans, A. Valentin, and R.R. Gamache, “Line Positions and Absolute Intensities in the Laser Bands of Carbon-12 Oxygen-17 Isotopic Species of Carbon Dioxide,” *J.Molec.Spectrosc.* **193**, 15-32 (1999).
17. C. Claveau, J.-L. Teffo, D. Hurtmans, and A. Valentin, “Infrared Fundamental and First Hot Bands of  $\text{O}^{12}\text{C}^{17}\text{O}$  Isotopic Variants of Carbon Dioxide,” *J.Molec.Spectrosc.* **189**, 153-195 (1998).
18. S.A.Tashkun, V.I.Perevalov, J.-L. Teffo, A.D. Bykov, and N.N. Lavrentieva, “CDSD-296, the carbon dioxide spectroscopic databank: version for atmospheric applications,” XIV symposium on High Resolution Molecular Spectroscopy, Krasnoyarsk, Russia, July 6-11, 2003.
19. A. Campargue, D. Bailly, J.-L. Teffo, S. A. Tashkun, and V.I. Perevalov, “The  $\nu_1+\nu_3$  Dyad of  $^{12}\text{CO}_2$  and  $^{13}\text{CO}_2$ ,” *J.Mol.Spec.* **193**, 204-212 (1999).
20. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, “Spectroscopic database of  $\text{CO}_2$  line parameters: 4300-7000  $\text{cm}^{-1}$ ,” *JQSRT* **109**, 906-921 (2008).
21. V.I. Perevalov and S.A. Tashkun, “CDSD-296 (Carbon Dioxide Spectroscopic Databank): Updated and Enlarged Version for Atmospheric Applications,” 10th HITRAN Database Conference, Cambridge MA, USA (2008).



22. B.V. Perevalov, V.I. Perevalov, and A. Campargue, “A (nearly) complete experimental linelist for  $^{13}\text{C}^{16}\text{O}_2$ ,  $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ ,  $^{16}\text{O}^{13}\text{C}^{17}\text{O}$ ,  $^{13}\text{C}^{18}\text{O}_2$  and  $^{17}\text{O}^{13}\text{C}^{18}\text{O}$  by high-sensitivity CW-CRDS spectroscopy between 5851 and 7045  $\text{cm}^{-1}$ ,” *JQSRT* **109**, 2437-2462 (2008).
23. Experimental intensities from: B.V. Perevalov, A. Campargue, B. Gao, S. Kassi, S.A. Tashkun, and V.I. Perevalov, “New CW-CRDS measurements and global modeling of  $^{12}\text{C}^{16}\text{O}_2$  absolute line intensities in the 1.6  $\mu\text{m}$  region,” *J.Mol.Spectrosc.* **252**, 190-197 (2008).
24. Theoretical intensities from: B.V. Perevalov, A. Campargue, B. Gao, S. Kassi, S.A. Tashkun, and V.I. Perevalov, “New CW-CRDS measurements and global modeling of  $^{12}\text{C}^{16}\text{O}_2$  absolute line intensities in the 1.6  $\mu\text{m}$  region,” *J.Mol.Spectrosc.* **252**, 190-197 (2008).
25. Updated and enlarged (in 2008), CDSD-2010 database described in S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva, “CDSD-1000, the high-temperature carbon dioxide spectroscopic databank,” *JQSRT* **82**, 165-196 (2003). See <ftp://ftp.iao.ru/pub/CDSD-2008/1000/>
26. S.A. Tashkun and V.I. Perevalov, “CDSD-Venus database, adapted for Venus conditions (750 K),” <ftp://ftp.iao.ru/pub/CDSD-2008/Venus/>

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, “The HITRAN database: 1986 Edition,” *Appl.Opt.* **26**, 4058-4097 (1987).
1. L.S. Rothman, R.L. Hawkins, R.B. Wattson, and R.R. Gamache, “Energy Levels, Intensities, and Linewidths of Atmospheric Carbon Dioxide Bands,” *JQSRT* **48**, 537-566 (1992).
2. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, “Spectroscopic database of  $\text{CO}_2$  line parameters: 4300-7000  $\text{cm}^{-1}$ ,” *JQSRT* **109**, 906-921 (2008). Supplemented with results of A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013 $\leftarrow$ 00001 and 30012 $\leftarrow$ 00001 bands of  $\text{CO}_2$  near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
3. A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013 $\leftarrow$ 00001 and 30012 $\leftarrow$ 00001 bands of  $\text{CO}_2$  near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
4. Values are calculated based on the semi-empirical approach described in A.D. Bykov, N.N. Lavrentieva, and L.N. Sinitsa, “Calculation of  $\text{CO}_2$  broadening and shift coefficients for high-temperature databases,” *Atmos.OceanicOpt.* **13**, 1015-1019 (2000) and S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva “CDSD-1000, the high-temperature carbon dioxide spectroscopic databank,” *JQSRT* **82**, 165-196 (2003).

#### Half-widths (self)

1. L.S. Rothman, R.L. Hawkins, R.B. Wattson, and R.R. Gamache, “Energy Levels, Intensities, and Linewidths of Atmospheric Carbon Dioxide Bands,” *JQSRT* **48**, 537-566 (1992).
2. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, “Spectroscopic database of  $\text{CO}_2$  line parameters: 4300-7000  $\text{cm}^{-1}$ ,” *JQSRT* **109**, 906-921 (2008).
3. Values are calculated based on the semi-empirical approach described in A.D. Bykov, N.N. Lavrentieva, and L.N. Sinitsa, “Calculation of  $\text{CO}_2$  broadening and shift coefficients for high-temperature databases,” *Atmos.OceanicOpt.* **13**, 1015-1019 (2000) and S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva “CDSD-1000, the high-temperature

carbon dioxide spectroscopic databank,” *JQSRT* **82**, 165-196 (2003).

Temperature dependence of air-broadened half-width

1. L.S. Rothman, R.L. Hawkins, R.B. Wattson, and R.R. Gamache, “Energy Levels, Intensities, and Linewidths of Atmospheric Carbon Dioxide Bands,” *JQSRT* **48**, 537-566 (1992).
2. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, “Spectroscopic database of CO<sub>2</sub> line parameters: 4300-7000 cm<sup>-1</sup>,” *JQSRT* **109**, 906-921 (2008). Supplemented with results of A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013←00001 and 30012←00001 bands of CO<sub>2</sub> near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
3. A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013←00001 and 30012←00001 bands of CO<sub>2</sub> near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
4. Values are calculated based on the semi-empirical approach described in A.D. Bykov, N.N. Lavrentieva, and L.N. Sinitsa, “Calculation of CO<sub>2</sub> broadening and shift coefficients for high-temperature databases,” *Atmos.OceanicOpt.* **13**, 1015-1019 (2000) and S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva “CDSD-1000, the high-temperature carbon dioxide spectroscopic databank,” *JQSRT* **82**, 165-196 (2003).

Pressure shift (air)

1. V.M. Devi, D.C. Benner, C.P. Rinsland, and M.A.H. Smith, “Measurements of Pressure Broadening and Pressure Shifting by Nitrogen in the 4.3-μm Band of <sup>12</sup>C<sup>16</sup>O<sub>2</sub>,” *JQSRT* **48**, 581-589 (1992).
2. V.M. Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, “Air- and N<sub>2</sub>-Broadening Coefficients and Pressure-shift Coefficients in the <sup>12</sup>C<sup>16</sup>O<sub>2</sub> laser bands,” *JQSRT* **59**, 137-149 (1998).
3. R.A. Toth, L.R. Brown, C.E. Miller, V. Malathy Devi, and D.C. Benner, “Spectroscopic database of CO<sub>2</sub> line parameters: 4300-7000 cm<sup>-1</sup>,” *JQSRT* **109**, 906-921 (2008). Supplemented with results of A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013←00001 and 30012←00001 bands of CO<sub>2</sub> near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
4. A. Predoi-Cross, A.R.W. McKellar, D. Chris Benner, V. Malathy Devi, R.R. Gamache, C.E. Miller, et al, “Temperature dependences for air-broadened Lorentz half width and pressure-shift coefficients in the 30013←00001 and 30012←00001 bands of CO<sub>2</sub> near 1600 nm,” *Can.J.Phys.* **87**, 517-535 (2009).
6. J.-M. Hartmann, “A simple empirical model for the collisional spectral shift of air-broadened CO<sub>2</sub> lines,” *JQSRT* **110**, 2019-2026 (2009).

Positions

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
- 1.** J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, and V. Malathy Devi, "Atlas of Ozone Spectral Parameters from Microwave to Medium Infrared," Academic Press, Inc. (1990).
- 2.** J.-M. Flaud, C. Camy-Peyret, A. Perrin, V. Malathy Devi, A. Barbe, S. Bouazza, J.J. Plateaux, C.P. Rinsland, M.A.H. Smith, and A. Goldman, "Line Parameters for Ozone Hot Bands in the 3.3- $\mu$ m Spectral Region," *J. Mol. Spectrosc.* **160**, 378-386 (1993).
- 3.** V. Malathy Devi, A. Perrin, J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, and M.A.H. Smith, "Line positions and intensities for the  $\nu_2 + 3\nu_3$  band of  $^{16}\text{O}_3$  around 2.7  $\mu$ m," *J. Mol. Spectrosc.* **143**, 381-388 (1990).
- 4.** S. Bouazza, A. Barbe, J.J. Plateaux, J.-M. Flaud, and C. Camy-Peyret, "The  $3\nu_1$  and  $\nu_1 + 3\nu_3 - \nu_2$  Absorption Bands of  $^{16}\text{O}_3$ ," *J. Mol. Spectrosc.* **160**, 371-377 (1993).
- 5.** C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, A. Perrin, J.-M. Flaud, and C. Camy-Peyret, "The  $\nu_2$  bands of  $^{16}\text{O}^{17}\text{O}^{16}\text{O}$  and  $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ : Line positions and intensities," *J. Mol. Spectrosc.* **149**, 474-480 (1991).
- 6.** K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
- 7.** H.M. Pickett and E.A. Cohen, Jet Propulsion Laboratory, private communication (1995).
- 9.** Calculated using Direct Numerical Diagonalization method, R.B. Wattson, Utah State University (Bedford), private communication (1995).
- 10.** A. Perrin, Université Pierre et Marie Curie, private communication (1995).
- 11.** A. Barbe, M.R. De Backer-Barilly, V.I.G. Tyuterev, and S.A. Tashkun, "Observations of infrared bands of asymmetrical ozone isotopologues  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$  and  $^{16}\text{O}^{18}\text{O}^{18}\text{O}$ ," *Appl. Opt.* **42**, 5136-5139 (2003).
- 12.** G. Wagner, M. Birk, F. Schreier, and J.-M. Flaud, "Spectroscopic database for ozone in the fundamental spectral regions," *J. Geophys. Res.* **D107**, 4626 (2002).
- 13.** S. Mikhailenko, private communication (2002), using calculation based on S. Mikhailenko, A. Barbe, J. J. Plateaux and V.I. G. Tyuterev, "New Analysis of  $2\nu_1 + \nu_2$ ,  $\nu_1 + \nu_2 + \nu_3$ , and  $\nu_2 + 2\nu_3$  Bands of Ozone in the 2600–2900  $\text{cm}^{-1}$  Region," *J. Mol. Spectrosc.* **196**, 93-101 (1999); J.-M. Flaud, C. Camy-Peyret, V.M. Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$  line positions and intensities," *J. Mol. Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V.M. Devi, "Line parameters of  $^{16}\text{O}_3$  in the 7- $\mu$ m region," *J. Mol. Spectrosc.* **134**, 106-112 (1989).
- 14.** J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L. Coudert, J.-L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment," *Atmos. Oceanic Opt.* **16**, 172-182 (2003); J.-M. Flaud, private communication (2004).
- 15.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
- 16.** S. Mikhailenko and A. Barbe, private communication, (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities," *J. Mol. Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland,

- M.A.H. Smith, V. Malathy Devi, "Line parameters for  $^{16}\text{O}_3$  bands in the 7- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **134**, 106-112 (1989); A. Barbe, A. Chichery, V.I.G. Tyuterev, S.A. Tashkun, S.N. Mikhailenko, "The  $2\nu_2$  and  $3\nu_2-\nu_2$  bands of ozone," *Spectrochimica Acta Part A* **54**, 1935-1945 (1998); A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, V.I.G. Tyuterev, "First study of the  $\nu_2=3$  dyad  $\{(130), (031)\}$  of ozone through the analysis of hot bands in the 2300-2600  $\text{cm}^{-1}$  region," *J.Mol.Spectrosc.* **187**, 70-74 (1998).
- 17.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities," *J.Mol.Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, "Line parameters for  $^{16}\text{O}_3$  bands in the 7- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **134**, 106-112 (1989); A. Barbe, A. Chichery, V.I.G. Tyuterev, S.A. Tashkun, S.N. Mikhailenko, "The  $2\nu_2$  and  $3\nu_2-\nu_2$  bands of ozone," *Spectrochimica Acta Part A* **54**, 1935-1945 (1998); S. Bouazza, A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, "Line positions and intensities of the  $\nu_1+2\nu_2+\nu_3$  and  $2\nu_2+2\nu_3$  bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **166**, 365-371 (1994).
- 18.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities," *J.Mol.Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, "Line parameters for  $^{16}\text{O}_3$  bands in the 7- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **134**, 106-112 (1989); S.N. Mikhailenko, A. Barbe, V.I.G. Tyuterev, L. Régalia, J.-J. Plateaux, "Line positions and intensities of the  $\nu_1+\nu_2+3\nu_3$ ,  $\nu_2+4\nu_3$ , and  $3\nu_1+2\nu_2$  bands of ozone," *J.Mol.Spectrosc.* **180**, 227-235 (1996).
- 19.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities," *J.Mol.Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, "Line parameters for  $^{16}\text{O}_3$  bands in the 7- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **134**, 106-112 (1989); A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, "First observation of the  $\nu_2=3$  state of ozone: The (131) state through analysis of cold and hot bands. Study of  $\nu_2$  behavior," *J.Mol.Spectrosc.* **184**, 448-453 (1997).
- 20.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from A. Barbe, J.-J. Plateaux, Analysis of the  $2\nu_1+2\nu_3$  band of ozone: Line positions and intensities," *JQSRT* **55**, 449-455 (1996); A. Barbe, O.N. Sulakshina, J.-J. Plateaux, V.I.G. Tyuterev, S. Bouazza, Line positions and intensities of the  $3\nu_1+\nu_3$  band of ozone," *J.Mol.Spectrosc.* **175**, 296-302 (1996); A. Barbe, S.N. Mikhailenko, V.I.G. Tyuterev, A. Hamdouni, J.-J. Plateaux, "Analysis of the  $2\nu_1+2\nu_2+\nu_3$  band of ozone," *J.Mol.Spectrosc.* **171**, 583-588 (1995); A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, V.I.G. Tyuterev, "Analysis of the  $2\nu_1+\nu_2+2\nu_3$  band of ozone," *J.Mol.Spectrosc.* **182**, 333-341 (1997).
- 21.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$ : Line positions and intensities," *J.Mol.Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, "Line parameters for  $^{16}\text{O}_3$  bands in the 7- $\mu\text{m}$  region," *J.Mol.Spectrosc.* **134**, 106-112 (1989); S. Mikhailenko, A. Barbe, V.I.G. Tyuterev, "Extended analysis of line positions and intensities of ozone bands in the 2900-3400  $\text{cm}^{-1}$  region,"



*J.Mol.Spectrosc.* **215**, 29-41 (2002).

- 22.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, A. N'Gom, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_2$  bands of  $^{16}\text{O}^{18}\text{O}^{16}\text{O}$  and  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ : Line positions and intensities," *J.Mol.Spectrosc.* **133**, 217-223 (1989); A. Chichery, A. Barbe, V.I.G. Tyuterev, S.A. Tashkun, "High resolution IR spectra of  $^{18}\text{O}$ -enriched ozone: Band centers of  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ ,  $^{16}\text{O}^{18}\text{O}^{18}\text{O}$ ,  $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ , and  $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ ," *J.Mol.Spectrosc.* **205**, 347-349 (2001).
- 23.** S. Mikhailenko and A. Barbe, private communication (2008). Calculation of the line positions was made by using Hamiltonian parameters from J.-M. Flaud, C. Camy-Peyret, A. N'Gom, V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_2$  bands of  $^{16}\text{O}^{18}\text{O}^{16}\text{O}$  and  $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ : Line positions and intensities," *J.Mol.Spectrosc.* **133**, 217-223 (1989); M.-R. De Backer-Barilly, A. Barbe, V.I.G. Tyuterev, A. Chichery, M.-T. Bourgeois, "High-resolution infrared spectra of the  $^{16}\text{O}^{18}\text{O}^{16}\text{O}$  ozone isotopomer in the range 900-5000  $\text{cm}^{-1}$ : Line positions," *J.Mol.Spectrosc.* **216**, 454-464 (2002).
- 24.** Data taken from the Spectroscopy & Molecular Properties of Ozone (SMPO) database, <http://smmpo.iao.ru/en/>, in July 2008. This ozone database is developed by researchers at the Université de Reims, Reims, France and at the Institute of Atmospheric Optics in Tomsk, Russia.

### Intensities

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
- 1.** J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, and V. Malathy Devi, "Atlas of Ozone Spectral Parameters from Microwave to Medium Infrared," Academic Press, Inc. (1990).
- 2.** J.-M. Flaud, C. Camy-Peyret, A. Perrin, V. Malathy Devi, A. Barbe, S. Bouazza, J.J. Plateaux, C.P. Rinsland, M.A.H. Smith, and A. Goldman, "Line Parameters for Ozone Hot Bands in the 3.3- $\mu\text{m}$  Spectral Region," *J.Mol.Spectrosc.* **160**, 378-386 (1993).
- 3.** V. Malathy Devi, A. Perrin, J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, and M.A.H. Smith, "Line positions and intensities for the  $\nu_2 + 3\nu_3$  band of  $^{16}\text{O}_3$  around 2.7  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **143**, 381-388 (1990).
- 4.** S. Bouazza, A. Barbe, J.J. Plateaux, J.-M. Flaud, and C. Camy-Peyret, "The  $3\nu_1$  and  $\nu_1 + 3\nu_3 - \nu_2$  Absorption Bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **160**, 371-377 (1993).
- 5.** C.P. Rinsland, M.A.H. Smith, V. Malathy Devi, A. Perrin, J.-M. Flaud, and C. Camy-Peyret, "The  $\nu_2$  bands of  $^{16}\text{O}^{17}\text{O}^{16}\text{O}$  and  $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ : Line positions and intensities," *J.Mol.Spectrosc.* **149**, 474-480 (1991).
- 6.** H.M. Pickett and E.A. Cohen, Jet Propulsion Laboratory, private communication (1995).
- 9.** Calculated using Direct Numerical Diagonalization method, R.B. Wattson, Utah State University (Bedford), private communication (1995).
- 10.** G. Wagner, M. Birk, F. Schreier, and J.-M. Flaud, "Spectroscopic database for ozone in the fundamental spectral regions," *J.Geophys.Res.* **D107**, 4626 (2002).
- 11.** S. Mikhailenko, private communication (2002), using calculation based on S. Mikhailenko, A. Barbe, J. J. Plateaux and V.I. G. Tyuterev, "New Analysis of  $2\nu_1 + \nu_2$ ,  $\nu_1 + \nu_2 + \nu_3$ , and  $\nu_2 + 2\nu_3$  Bands of Ozone in the 2600–2900  $\text{cm}^{-1}$  Region," *J.Mol.Spectrosc.* **196**, 93-101 (1999); J.-M. Flaud, C. Camy-Peyret, V.M. Devi, C.P. Rinsland, M.A.H. Smith, "The  $\nu_1$  and  $\nu_3$  bands of  $^{16}\text{O}_3$  line positions and intensities," *J.Mol.Spectrosc.* **124**, 209-217 (1987); J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, V.M. Devi, "Line parameters of  $^{16}\text{O}_3$  in the 7- $\mu\text{m}$  region,"

*J.Mol.Spectrosc.* **134**, 106-112 (1989).

**12.** J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L. Coudert, J.-L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment," *Atmos.Oceanic Opt.* **16**, 172-182 (2003); J.-M. Flaud, private communication (2004).

**13.** Rescale by dividing J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, and V.Malathy Devi, "Atlas of Ozone Spectral Parameters from Microwave to Medium Infrared," Academic Press, Inc. (1990) by the factor 1.04.

**14.** Rescale by dividing J.-M. Flaud, C. Camy-Peyret, A. Perrin, V.Malathy Devi, A. Barbe, S. Bouazza, J.J. Plateaux, C.P. Rinsland, M.A.H. Smith, and A. Goldman, *J.Mol.Spectrosc.* **160**, 378-386 (1993) by the factor 1.04.

**15.** Rescale by dividing V.Malathy Devi, A. Perrin, J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, and M.A.H. Smith, *J.Mol.Spectrosc.* **143**, 381-388 (1990) by the factor 1.04.

**16.** Rescale by dividing S. Bouazza, A. Barbe, J.J. Plateaux, J.-M. Flaud, and C. Camy-Peyret, *J.Mol.Spectrosc.* **160**, 371-377 (1993) by the factor 1.04.

**17.** Rescale by dividing C.P. Rinsland, M.A.H. Smith, V.Malathy Devi, A. Perrin, J.-M. Flaud, and C. Camy-Peyret, *J.Mol.Spectrosc.* **149**, 474-480 (1991) by the factor 1.04.

**18.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

**19.** S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, V.I.G. Tyuterev, "First study of the  $\nu_2=3$  dyad  $\{(130), (031)\}$  of ozone through the analysis of hot bands in the  $2300-2600\text{ cm}^{-1}$  region," *J.Mol.Spectrosc.* **187**, 70-74 (1998).

**20.** S.N. Mikhailenko and A. Barbe, private communication (2008). Transition moment parameters of the  $\nu_2+\nu_3$  band from V. Malathy Devi, J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, M.A.H. Smith, "Line positions and intensities for the  $\nu_1+\nu_2$  and  $\nu_2+\nu_3$  bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **125**, 174-183 (1987) were used for calculation of line intensities for the  $3\nu_2+\nu_3-2\nu_2$  band.

**21.** S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S. Bouazza, A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, "Line positions and intensities of the  $\nu_1+2\nu_2+\nu_3$  and  $2\nu_2+2\nu_3$  bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **166**, 365-371 (1994).

**22.** S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S.N. Mikhailenko, A. Barbe, J.-J. Plateaux, V.I.G. Tyuterev, "New analysis of  $2\nu_1+\nu_2$ ,  $\nu_1+\nu_2+\nu_3$ , and  $\nu_2+2\nu_3$  bands of ozone in the  $2600-2900\text{ cm}^{-1}$  region," *J.Mol.Spectrosc.* **196**, 93-101 (1999).

**23.** S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S.N. Mikhailenko, A. Barbe, J.-J. Plateaux, V.I.G. Tyuterev, "New analysis of  $2\nu_1+\nu_2$ ,  $\nu_1+\nu_2+\nu_3$ , and  $\nu_2+2\nu_3$  bands of ozone in the  $2600-2900\text{ cm}^{-1}$  region," *J.Mol.Spectrosc.* **196**, 93-101 (1999) and S. Bouazza, A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, "Line positions and intensities of the  $\nu_1+2\nu_2+\nu_3$  and  $2\nu_2+2\nu_3$  bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **166**, 365-371 (1994).

**24.** S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Barbe, J.-J. Plateaux, S. Bouazza, O.N. Sulakshina, S.N. Mikhailenko, V.I.G. Tyuterev, S.A. Tashkun, "Experimental and theoretical study of absolute intensities of ozone spectral lines in the range  $1850-2300\text{ cm}^{-1}$ ," *JQSRT* **52**, 341-355 (1994).

25. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S.N. Mikhailenko, A. Barbe, V.I.G. Tyuterev, L. Régalia, J.-J. Plateaux, "Line positions and intensities of the  $\nu_1+\nu_2+3\nu_3$ ,  $\nu_2+4\nu_3$ , and  $3\nu_1+2\nu_2$  bands of ozone," *J.Mol.Spectrosc.* **180**, 227-235 (1996).
26. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Perrin, A.M. Vasserot, J.M. Flaud, C. Camy-Peyret, V. Malathy Devi, M.A.H. Smith, C.P. Rinsland, A. Barbe, S. Bouazza, J.-J. Plateaux, "The 2.5- $\mu\text{m}$  bands of ozone: Line positions and intensities," *J.Mol.Spectrosc.* **149**, 519-529 (1991).
27. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S. Bouazza, S.N. Mikhailenko, A. Barbe, L. Régalia, V.I.G. Tyuterev, J.-J. Plateaux, "The  $\nu_1+\nu_2+2\nu_3$  and  $\nu_2+3\nu_3$  bands of  $^{16}\text{O}_3$ ," *J.Mol.Spectrosc.* **174**, 510-519 (1995).
28. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, "First observation of the  $\nu_2=3$  state of ozone: The (131) state through analysis of cold and hot bands. Study of  $\nu_2$  behavior," *J.Mol.Spectrosc.* **184**, 448-453 (1997).
29. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Barbe, J.-J. Plateaux, "Analysis of the  $2\nu_1+2\nu_3$  band of ozone: Line positions and intensities," *JQSRT* **55**, 449-455 (1996); A. Barbe, O.N. Sulakshina, J.-J. Plateaux, V.I.G. Tyuterev, S. Bouazza, "Line positions and intensities of the  $3\nu_1+\nu_3$  band of ozone," *J.Mol.Spectrosc.* **175**, 296-302 (1996); A. Barbe, S.N. Mikhailenko, V.I.G. Tyuterev, A. Hamdouni, J.-J. Plateaux, "Analysis of the  $2\nu_1+2\nu_2+\nu_3$  band of ozone," *J.Mol.Spectrosc.* **171**, 583-588 (1995); A. Barbe, S.N. Mikhailenko, J.-J. Plateaux, V.I.G. Tyuterev, "Analysis of the  $2\nu_1+\nu_2+2\nu_3$  band of ozone," *J.Mol.Spectrosc.* **182**, 333-341 (1997).
30. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S. Mikhailenko, A. Barbe, V.I.G. Tyuterev, "Extended analysis of line positions and intensities of ozone bands in the 2900-3400  $\text{cm}^{-1}$  region," *J.Mol.Spectrosc.* **215**, 29-41 (2002).
31. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from A. Barbe, O.N. Sulakshina, J.-J. Plateaux, A. Hamdouni, S. Bouazza, "High-resolution infrared spectra of ozone in the 2300-2600  $\text{cm}^{-1}$  region," *J.Mol.Spectrosc.* **170**, 244-250 (1995); A. Barbe, J.-J. Plateaux, S. Bouazza, O.N. Sulakshina, S.N. Mikhailenko, V.I.G. Tyuterev, S.A. Tashkun, "Experimental and theoretical study of absolute intensities of ozone spectral lines in the range 1850-2300  $\text{cm}^{-1}$ ," *JQSRT* **52**, 341-355 (1994).
32. A. Barbe and M.-R. De Backer-Barilly, private communication (2007).
33. Data taken from the Spectroscopy & Molecular Properties of Ozone (SMPO) database, <http://smpo.iao.ru/en/>, in July 2008. This ozone database is developed by researchers at the Université de Reims, Reims, France and at the Institute of Atmospheric Optics in Tomsk, Russia.

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. R.R. Gamache and L.S. Rothman, "Theoretical  $\text{N}_2$ -broadened halfwidths of  $^{16}\text{O}_3$ ," *Appl.Opt.*

- 24**, 1651-1655 (1985) scaled by 0.90 (N<sub>2</sub>/air) ratio and increased by 9% as recommended by M.A.H. Smith, NASA Langley Research Center, private communication (1990).
- 2**. Second order polynomial fit in  $J$  (used for  $J > 35$ ) by C.P. Rinsland, NASA Langley Research Center, private communication (1990).
- 3**. Average values from Ref. 1 as a function of  $J$  ( $J \leq 35$ ) used for lines not in database of Ref. 1.
- 4**. G. Wagner, M. Birk, F. Schreier, and J.-M. Flaud, "Spectroscopic database for ozone in the fundamental spectral regions," *J. Geophys. Res.* **D107**, 4626 (2002).
- 5**. Use of values obtained for the  $\nu_3$  band from Ref. 4.
- 6**. Use of values obtained for the  $\nu_1/\nu_2$  bands from Ref. 4.
- 7**. Third order polynomial fit in  $J$  for transitions where  $J = K_a$  by I.E. Gordon (2008).
- 8**. J.-M. Flaud, C. Camy-Peyret, C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, A. Goldman, "Improved line parameters for ozone bands in the 10- $\mu$ m spectral region," *Appl. Opt.* **29**, 3667-3671 (1990). The polynomial expression in  $J''$  from this article has been multiplied by a factor of 1.05 (I. Gordon, private communication, 2008).

#### Half-widths (self)

- 1**. C.P. Rinsland, J.-M. Flaud, A. Goldman, A. Perrin, C. Camy-Peyret, M.A.H. Smith, V. Malathy Devi, D. Chris Benner, A. Barbe, T.M. Stephen, and F.J. Murcray, "Spectroscopic Parameters for Ozone and Its Isotopes: Current Status, Prospects for Improvement, and the Identification of <sup>16</sup>O<sup>16</sup>O<sup>17</sup>O and <sup>16</sup>O<sup>17</sup>O<sup>16</sup>O Lines in Infrared Ground-based and Stratospheric Solar Absorption Spectra," *JQSRT* **60**, 803-814 (1998).
- 2**. M.A.H. Smith, NASA Langley Research Center, private communication (2004).

#### Temperature dependence of air-broadened half-width

- 1**. Mean value of R.R. Gamache, "Temperature dependence of N<sub>2</sub>-broadened halfwidths of ozone," *J. Mol. Spectrosc.* **114**, 31-41 (1985).
- 2**. G. Wagner, M. Birk, F. Schreier, and J.-M. Flaud, "Spectroscopic database for ozone in the fundamental spectral regions," *J. Geophys. Res.* **D107**, 4626 (2002).
- 3**. Use of values obtained for the  $\nu_3$  band from Ref. 2.
- 4**. Use of values obtained for the  $\nu_1/\nu_2$  bands from Ref. 2.

#### Pressure shift (air)

- 1**. Mean values of M.A.H. Smith, private communication (2004) based on V. Malathy Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, "Air-broadening and shift coefficients of O<sub>3</sub> lines in the  $\nu_2$  band and their temperature dependence," *J. Mol. Spectrosc.* **182**, 221-238 (1997); M.A.H. Smith, V. Malathy Devi, D.C. Benner, and C.P. Rinsland, "Temperature dependence of air-broadening and shift coefficients of O<sub>3</sub> lines in the  $\nu_1$  band," *J. Mol. Spectrosc.* **182**, 239-259 (1997); M.A.H. Smith, C.P. Rinsland, V. Malathy Devi, and E.S. Prochaska, "Measurements of pressure broadening and shifts of O<sub>3</sub> lines in the 3- $\mu$ m region," *J. Mol. Spectrosc.* **164**, 239-259 (1994); M.A.H. Smith, C.P. Rinsland, V. Malathy Devi, and E.S. Prochaska, "Erratum: Measurements of pressure broadening and shifts of O<sub>3</sub> lines in the 3- $\mu$ m region" by M.A.H. Smith, C.P. Rinsland, V. Malathy Devi, and E.S. Prochaska," *J. Mol. Spectrosc.* **165**, 596 (1994).

## **N<sub>2</sub>O** [4] 446, 456, 546, 448, 447

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. G. Guelachvili, *Can.J.Phys.* **60**, 1334 (1982).
2. R.A. Toth, "Line-frequency measurements and analysis of N<sub>2</sub>O between 900 and 4700 cm<sup>-1</sup>," *Appl. Opt.* **30**, 5289-5315 (1991).
3. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
4. J.W.C. Johns, Z. Lu, M. Weber, J.M. Sirota, and D.C. Reuter, "Absolute Intensities in the  $\nu_2$  fundamental of N<sub>2</sub>O at 17  $\mu$ m," *J.Mol.Spectrosc.* **177**, 203-210 (1996).
5. L. Daumont, C. Claveau, M.R Debacker-Barrilly, A. Hamdouni, L. Régalia-Jarlot, J.-L. Teffo, S. Tashkun, and V.I. Perevalov, "Line intensities of <sup>14</sup>N<sub>2</sub><sup>16</sup>O: the 10 micrometers region revisited," *JQSRT* **72**, 37-55 (2002).
6. R.A. Toth, "Linelist of N<sub>2</sub>O parameters from 500 to 7500 cm<sup>-1</sup>," see <http://mark4sun.jpl.nasa.gov/n2o.html>.
7. L. Daumont, J. Vander Auwera, J.-L. Teffo, V.I. Perevalov, and S.A. Tashkun, "Line Intensity Measurements in <sup>14</sup>N<sub>2</sub><sup>16</sup>O and their Treatment using the Effective Dipole Moment Approach," *J.Mol.Spectrosc.* **208**, 281-291 (2001).
8. Line originally missing from R.A. Toth linelist (see Ref. 6 above).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. J.W.C. Johns, Z. Lu, M. Weber, J.M. Sirota, and D.C. Reuter, "Absolute Intensities in the  $\nu_2$  fundamental of N<sub>2</sub>O at 17  $\mu$ m," *J.Mol.Spectrosc.* **177**, 203-210 (1996).
3. L. Daumont, C. Claveau, M.R Debacker-Barrilly, A. Hamdouni, L. Régalia-Jarlot, J.-L. Teffo, S. Tashkun, and V.I. Perevalov, "Line intensities of <sup>14</sup>N<sub>2</sub><sup>16</sup>O: the 10 micrometers region revisited," *JQSRT* **72**, 37-55 (2002).
4. L. Daumont, J. Vander Auwera, J.-L. Teffo, V.I. Perevalov, and S.A. Tashkun, "Line Intensity Measurements in <sup>14</sup>N<sub>2</sub><sup>16</sup>O and their Treatment using the Effective Dipole Moment Approach," *J.Mol.Spectrosc.* **208**, 281-291 (2001).
5. R.A. Toth, "Linelist of N<sub>2</sub>O parameters from 500 to 7500 cm<sup>-1</sup>," see <http://mark4sun.jpl.nasa.gov/n2o.html>.

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. N. Lacome, A. Levy, and G. Guelachvili, "Fourier transform measurement of self-, N<sub>2</sub>-, and O<sub>2</sub>-broadening of N<sub>2</sub>O lines: temperature dependence of linewidths," *Appl. Opt.* **23**, 425-434



(1984).

3. Third-order polynomial fit of experimental results based on the three works: N. Lacome, A. Levy, and G. Guelachvili, “Fourier transform measurement of self-, N<sub>2</sub>-, and O<sub>2</sub>-broadening of N<sub>2</sub>O lines: temperature dependence of linewidths,” *Appl.Opt.* **23**, 425-434 (1984); R.A. Toth, “N<sub>2</sub>- and air-broadened linewidths and frequency-shifts of N<sub>2</sub>O,” *JQSRT* **66**, 285-304 (2000); and V. Nemtchinov, C. Sun, and P. Varanasi, “Measurements of Line Intensities and Line Widths in the  $\nu_3$ -fundamental Band of Nitrous Oxide at Atmospheric Temperatures,” *JQSRT* **83**, 267-284 (2004).

#### Half-widths (self)

1. Third-order polynomial fit of experimental results based on: R.A. Toth, “Line strengths (900-3600 cm<sup>-1</sup>), self-broadened linewidths, and frequency shifts (1800-2660 cm<sup>-1</sup>) of N<sub>2</sub>O,” *Appl.Opt.* **32**, 7326-7365 (1993).

#### Temperature dependence of air-broadened half-width

1. Fixed to a constant value of 0.75 based on the two works: N. Lacome, A. Levy, and G. Guelachvili, “Fourier transform measurement of self-, N<sub>2</sub>-, and O<sub>2</sub>-broadening of N<sub>2</sub>O lines: temperature dependence of linewidths,” *Appl.Opt.* **23**, 425-434 (1984); V. Nemtchinov, C. Sun, and P. Varanasi, “Measurements of Line Intensities and Line Widths in the  $\nu_3$ -fundamental Band of Nitrous Oxide at Atmospheric Temperatures,” *JQSRT* **83**, 267-284 (2004).

#### Pressure shift (air)

1. R.A. Toth, “Linelist of N<sub>2</sub>O parameters from 500 to 7500 cm<sup>-1</sup>,” see <http://mark4sun.jpl.nasa.gov/n2o.html>.

## CO [5] 26, 36, 28, 27, 38, 37

### Positions

1. G. Guelachvili, D. De Villeneuve, R. Farrenq, W. Urban, and J. Verges, “Dunham Coefficients for Seven Isotopic Species of CO,” *J.Mol.Spectrosc.* **98**, 64-79 (1983); C.R. Pollock, F.R. Petersen, D.A. Jennings, and J.S. Wells “Absolute Frequency Measurements of the 2-0 Band of CO at 2.3  $\mu\text{m}$ ; Calibration Standard Frequencies from High Resolution Color Center Laser Spectroscopy,” *J.Mol.Spectrosc.* **99**, 357-368 (1983).
2. R. Farrenq, G. Guelachvili, A.J. Sauval, N. Grevesse, and C.B. Farmer, “Improved Dunham Coefficients for CO from Infrared Solar Lines of High Rotational Excitation,” *J.Mol.Spectrosc.* **149**, 375-390 (1991).
3. T.D. Varberg and K.M. Evenson, “Accurate far-infrared rotational frequencies of carbon monoxide,” *Astrophys.J.* **385**, 763-765 (1992).
4. H.S.P. Müller, F. Schloder, J. Stutzki, and G Winnewisser, “The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists,” *J.Mol.Struct.* **742**, 215-227 (2005). Data adopted in June 2010.

### Intensities

1. C. Chackerian and R.H. Tipping, “Vibration-Rotational and Rotational Intensities for CO Isotopes,” *J.Mol.Spectrosc.* **99**, 431-449 (1983).
2. D. Goorvitch, “Infrared CO Linelist for the  $X^1\Sigma^+$  State,” *Astrophys.J.Suppl.Ser.* **95**, 535-552 (1994).
3. J.W. Brault, L.R. Brown, C. Chackerian, Jr, R. Freedman, A. Predoi-Cross, and A.S. Pine, “Self-broadened  $^{12}\text{C}^{16}\text{O}$  line shapes in the  $v = 2 \leftarrow 0$  band,” *J.Mol.Spectrosc.* **222**, 220-239 (2003).
4. K. Sung and P. Varanasi, “Intensities, collision-broadened half-widths, and collision-induced line shifts in the second overtone band of  $^{12}\text{C}^{16}\text{O}$ ” *JQSRT* **83**, 445-458 (2004).
5. H.S.P. Müller, F. Schloder, J. Stutzki, and G Winnewisser, “The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists,” *J.Mol.Struct.* **742**, 215-227 (2005). Data adopted in June 2010.

### Half-widths (air)

1. T. Nakazawa and M. Tanaka, “Measurements of Intensities and Self- and Foreign gas broadened halfwidths of spectral Lines in the CO fundamental Band,” *JQSRT* **28**, 409-416 (1982); values for transitions having  $20 < |m| \leq 33$  are extrapolated, while those for  $|m| > 34$  are assumed to be constant ( $0.0400 \text{ cm}^{-1}/\text{atm}$ ).
2. Polynomial fit of several measurements (M.A.H. Smith, private communication, 2004). For details, see L.S. Rothman, D. Jacquemart, A. Barbe, D.C. Benner, M. Birk, L.R. Brown, M. Carleer, C. Chackerian Jr, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, “The HITRAN 2004 Molecular Spectroscopic Database,” *JQSRT* **96**, 139-204 (2005).

### Half-widths (self)

1. T. Nakazawa and M. Tanaka, “Measurements of Intensities and Self- and Foreign gas broadened halfwidths of spectral Lines in the CO fundamental Band,” *JQSRT* **28**, 409-416 (1982); values for transitions having  $20 < |m| \leq 33$  are extrapolated, while those for  $|m| > 34$  are

assumed to be constant ( $0.0460 \text{ cm}^{-1}/\text{atm}$ ).

2. Polynomial fit of several measurements (M.A.H. Smith, private communication, 2004). For details, see L.S. Rothman, D. Jacquemart, A. Barbe, D.C. Benner, M. Birk, L.R. Brown, M. Carleer, C. Chackerian Jr, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, "The *HITRAN* 2004 Molecular Spectroscopic Database," *JQSRT* **96**, 139-204 (2005).

#### Temperature dependence of air-broadened half-width

1. Polynomial fit of several measurements (M.A.H. Smith, private communication, 2004). For details, see L.S. Rothman, D. Jacquemart, A. Barbe, D.C. Benner, M. Birk, L.R. Brown, M. Carleer, C. Chackerian Jr, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, "The *HITRAN* 2004 Molecular Spectroscopic Database," *JQSRT* **96**, 139-204 (2005).

#### Pressure shift (air)

1. Q. Zou and P. Varanasi, "New laboratory data on the spectral line parameters in the 1-0 and 2-0 bands of  $^{12}\text{C}^{16}\text{O}$  relevant to atmospheric remote sensing," *JQSRT* **75**, 63-92 (2002); for the 1-0 band, values for transitions having  $-24 \geq m \geq 25$  are assumed to be constant ( $-0.003 \text{ cm}^{-1}/\text{atm}$ ). For the 2-0 band, values for transitions having  $-23 \geq m \geq 24$  are assumed to be constant ( $-0.0055 \text{ cm}^{-1}/\text{atm}$ ).

2. K. Sung and P. Varanasi, "Intensities, collision-broadened half-widths, and collision-induced line shifts in the second overtone band of  $^{12}\text{C}^{16}\text{O}$ ," *JQSRT* **83**, 445-458 (2004); for the 3-0 band, values for transitions having  $-24 \geq m \geq 26$  are assumed to be constant ( $-0.0075 \text{ cm}^{-1}/\text{atm}$ ).

## CH<sub>4</sub> [6] 211, 311, 212, 312

### Positions

0. The 1986 HITRAN article: Refs. numbers 46-52 therein are needed to document the 1991 methane linelist completely.
7. J.P. Champion, J.C. Hilico, C. Wenger, and L.R. Brown, "Analysis of the  $\nu_2/\nu_4$  dyad of  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ ," *J.Mol.Spectrosc.* **133**, 256-272 (1989).
9. L.R. Brown, "Methane line parameters from 3700 to 4136  $\text{cm}^{-1}$ ," *Appl.Opt.* **27**, 3275-3279 (1988).
10. J.S. Margolis, "Measured line positions and strengths of methane between 5500 and 6180  $\text{cm}^{-1}$ ," *Appl.Opt.* **27**, 4038-4051 (1988); J.S. Margolis, "Empirical values of the ground state energies for methane transitions between 5500 and 6150  $\text{cm}^{-1}$ ," *Appl.Opt.* **29**, 2295-2302 (1990).
11. M. Oldani, A. Bauder, J.C. Hilico, M. Loëte, and J.P. Champion, "Microwave Fourier Transform Spectroscopy of Rovibrational Transitions in the  $\nu_2 - \nu_4$  Dyads of Methane- $\text{C}^{12}$  and Methane- $\text{C}^{13}$ ," *Europhys.Lett.* **4**, 29-33 (1987).
12. J.C. Hilico, M. Loëte, J.P. Champion, J.L. Destomes, and M. Bogey, "The millimeter-wave spectrum of methane," *J.Mol.Spectrosc.* **122**, 381-389 (1987).
13. O. Ouardi, "Intensités des bandes chaudes du methane dans la région de 8 microns," thesis, Université de Bourgogne (1988).
15. G. Tarrago, M. Delaveau, L. Fusina, and G. Guelachvili, "Absorption of  $^{12}\text{CH}_3\text{D}$  at 6-10  $\mu\text{m}$ : triad  $\nu_3, \nu_5, \nu_6$ ," *J.Mol.Spectrosc.* **126**, 149-158 (1987); for  $\nu_2$ , C. Chackerian, NASA Ames Research Center, unpublished (1990).
18. L.R. Brown and L.S. Rothman, "Methane line parameters for the 2.3- $\mu\text{m}$  region," *Appl.Opt.* **21**, 2425-2427 (1982).
19. L.R. Brown, "Empirical Lower State Energies of Methane at 2.5- $\mu\text{m}$ ," 3<sup>rd</sup> International Conference on Laboratory Research for Planetary Atmospheres (1991).
20. G.S. Orton and A.G. Robiette, "A Line Parameter List for the  $\nu_2$  and  $\nu_4$  Bands of  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ , Extended to  $J' = 25$  and its Application to Planetary Atmospheres," *JQSRT* **24**, 81-95 (1980).
21. R.A. Toth, L.R. Brown, R.H. Hunt, and L.S. Rothman, "Line parameters of methane from 2385 to 3200  $\text{cm}^{-1}$ ," *Appl.Opt.* **20**, 932-935 (1981).
22. B. Bobin and K. Fox, "New analysis of  $\nu_3$  of  $^{12}\text{CH}_4$ ," *J.Chem.Phys.* **58**, 1771-1773 (1973).
23. N. Husson, G. Poussigue, A. Valentin, and C. Amiot, "Study of  $\nu_1 + \nu_4$  band of  $^{12}\text{CH}_4$  from 4,136  $\text{cm}^{-1}$  to 4,288  $\text{cm}^{-1}$ ," *Rev.Phys.Appl.* **7**, 267-278 (1972).
24. L.R. Brown, Jet Propulsion Laboratory, private communication (1981).
25. B. Bobin, "Interpretation de la Bande Harmonique  $2\nu_3$  du Methane  $^{12}\text{CH}_4$  (de 5890 à 6107  $\text{cm}^{-1}$ )," *J.Phys.* **33**, 345-352 (1972).
26. M. Dang-Nhu, G. Poussigue, G. Tarrago, A. Valentin, and P. Cardinet, "Etude de la Bande  $\nu_3$  de  $^{13}\text{CH}_4$  entre 2863 et 3132  $\text{cm}^{-1}$ ," *J.Phys.* **34**, 389-401 (1973).
28. C. Chackerian, Jr. and G. Guelachvili, "Ground-State Rotational Constants of  $^{12}\text{CH}_3\text{D}$ ," *J.Mol.Spectrosc.* **84**, 447-456 (1980).
29. Estimated.
30. O. Ouardi, J.C. Hilico, M., Loëte, and L.R. Brown, "The hot bands of methane between 5 and 10  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **180**, 311-322 (1996).
31. J.C. Hilico, J.-P. Champion, S. Toumi, V.I.G. Tyuterev, and S.A. Tashkun, "New Analysis of the Pentad System of Methane and Prediction of the (Pentad-pentad) Spectrum," *J.Mol.Spectrosc.* **168**, 455-476 (1994); J.C. Hilico, G.S. Baronov, D.K. Bronnikov, S.A.

- Gavrikov, I.I. Nikolaev, V.D. Rusanov, and Y.G. Filimonov, "High-resolution Spectroscopy of (Pentad Dyad) and (Octad Pentad) Hot Bands of Methane in a Supersonic Jet," *J.Mol.Spectrosc.* **161**, 435-444 (1993).
- 32.** D.C. Benner, College of William and Mary, Unpublished data.
- 33.** J.C. Hilico, O. Robert, M. Loëte, S. Toumi, S.A. Pine, and L.R. Brown, "Analysis of the interacting octad system of  $^{12}\text{CH}_4$ ," *J.Mol.Spectrosc.* **208**, 1-13 (2001).
- 34.** A. Predoi Cross, M. Brawley-Tremblay, L.R. Brown, V.M. Devi, and D.C. Benner, "Multispectrum analysis of  $^{12}\text{CH}_4$  from 4100 to 4635  $\text{cm}^{-1}$ : II. Air-broadening coefficients (widths and shifts)," *J.Mol.Spectrosc.* **236**, 201-215 (2006).
- 35.** J.M. Jouvard, B. Lavorel, J.-P. Champion, and L.R. Brown, "Preliminary analysis of the pentad of  $^{13}\text{CH}_4$  from Raman and infrared spectra," *J.Mol.Spectrosc.* **150**, 201-217 (1991).
- 36.** L.R. Brown, A. Nikitin, D.C. Benner, V.M. Devi, M.A.H. Smith, L. Fejard, J.-P. Champion, V.G. Tyuterev, and R.L. Sams, "Line intensities of  $\text{CH}_3\text{D}$  in the triad region: 6-10  $\mu\text{m}$ ," *J.Mol.Struct.* **695**, 181-188 (2004).
- 37.** A. Nikitin, J.-P. Champion, V.G. Tyuterev, L.R. Brown, G. Mellau, and M. Lock, "The infrared spectrum of  $\text{CH}_3\text{D}$  between 900 and 3200  $\text{cm}^{-1}$ : extended assignment and modeling," *J.Mol.Struct.* **517**, 1-24 (2000); A. Nikitin, L.R. Brown, J.-P. Champion, L. Fejard, and V.G. Tyuterev, "Analysis of the  $\text{CH}_3\text{D}$  nonad from 2000 to 3300  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **216**, 225-251 (2002).
- 38.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
- 39.** L.R. Brown, JPL, private communication (2004).
- 40.** S. Albert, A. Bauerecker, V. Boudon, L.R. Brown, J.-P. Champion, M. Loëte, A. Nikitin, and M. Quack, "Global Frequency and Intensity Analysis of  $^{12}\text{CH}_4$  in the 0-4800  $\text{cm}^{-1}$  region," *Chem.Phys.* **356**, 131-146 (2009).
- 41.** V. Lattanzi, A. Walters, J.C. Pearson, and B.J. Drouin, "THz spectrum of monodeuterated methane," *JQSRT* **109**, 580-586 (2008).
- 42.** O.N. Ulenikov, G.A. Onopenko, N.E. Tyabaeva, R. Anttila, S. Alanko, and J. Schroderus, "Rotational Analysis of the Ground State and the Lowest Fundamentals  $\nu_3$ ,  $\nu_5$ , and  $\nu_6$  of  $^{13}\text{CH}_3\text{D}$ ," *J.Mol.Spectrosc.* **201**, 9-17 (2000).
- 43.** A.V. Nikitin, J.-P. Champion, and L.R. Brown, "Preliminary analysis of  $\text{CH}_3\text{D}$  from 3250 to 3700  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **240**, 14-25 (2006).
- 44.** C. Boussin, B.L. Lutz, C. de Bergh, and A. Hamdouni, "Line intensities and self-broadening coefficients for the  $3\nu_2$  band of monodeuterated methane," *JQSRT* **60**, 501-514 (1998).

### Intensities

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
- 8.** L.R. Brown, M. Loëte, and J.C. Hilico, "Linestrengths of the  $\nu_2$  and  $\nu_4$  bands of  $^{12}\text{CH}_4$  and  $^{13}\text{CH}_4$ ," *J.Mol.Spectrosc.* **133**, 273-311 (1989).
- 9.** L.R. Brown, "Methane line parameters from 3700 to 4136  $\text{cm}^{-1}$ ," *Appl.Opt.* **27**, 3275-3279 (1988).
- 10.** J.S. Margolis, "Measured line positions and strengths of methane between 5500 and 6180  $\text{cm}^{-1}$ ," *Appl.Opt.* **27**, 4038-4051 (1988); J.S. Margolis, "Empirical values of the ground state energies for methane transitions between 5500 and 6150  $\text{cm}^{-1}$ ," *Appl.Opt.* **29**, 2295-2302 (1990).
- 11.** M. Oldani, A. Bauder, J.C. Hilico, M. Loëte, and J.P. Champion, "Microwave Fourier



Transform Spectroscopy of Rovibrational Transitions in the  $\nu_2 - \nu_4$  Dyads of Methane- $C^{12}$  and Methane- $C^{13}$ ,” *Europhys.Lett.* **4**, 29-33 (1987).

**12.** J.C. Hilico, M. Loëte, J.P. Champion, J.L. Destomes, and M. Bogey, “The millimeter-wave spectrum of methane,” *J.Mol.Spectrosc.* **122**, 381-389 (1987).

**13.** O. Ouardi, “Intensités des bandes chaudes du methane dans la région de 8 microns,” thesis, Université de Bourgogne, (1988).

**16.** L.R. Brown, A. Nikitin, D.C. Benner, V.M. Devi, M.A.H. Smith, L. Fejard, J.-P. Champion, V.G. Tyuterev, and R.L. Sams, “Line intensities of  $CH_3D$  in the triad region: 6-10  $\mu m$ ,” *J.Mol.Struct.* **695**, 181-188 (2004).

**18.** L.R. Brown and L.S. Rothman, “Methane line parameters for the 2.3- $\mu m$  region,” *Appl.Opt.* **21**, 2425-2427 (1982).

**19.** L.R. Brown, “Empirical Lower State Energies of Methane at 2.5- $\mu m$ ,” 3<sup>rd</sup> International Conference on Laboratory Research for Planetary Atmospheres (1991).

**20.** O. Ouardi, J.C. Hilico, M., Loete, and L.R. Brown, “The hot bands of methane between 5 and 10  $\mu m$ ,” *J.Mol.Spectrosc.* **180**, 311-322 (1996).

**21.** L. Fejard, J.-P. Champion, J.M. Jouvard, L.R. Brown, and A.S. Pine, “The intensities of methane in the 3-5  $\mu m$  region revisited,” *J.Mol.Spectrosc.* **201**, 83-94 (2000).

**22.** D.C. Benner, College of William and Mary, Unpublished data.

**23.** J.C. Hilico, J.-P. Champion, S. Toumi, V.I.G. Tyuterev, and S.A. Tashkun, “New Analysis of the Pentad System of Methane and Prediction of the (Pentad-pentad) Spectrum,”

*J.Mol.Spectrosc.* **168**, 455-476 (1994); J.C. Hilico, G.S. Baronov, D.K. Bronnikov, S.A. Gavrikov, I.I. Nikolaev, V.D. Rusanov, and Y.G. Filimonov, “High-resolution Spectroscopy of (Pentad Dyad) and (Octad Pentad) Hot Bands of Methane in a Supersonic Jet,” *J.Mol.Spectrosc.* **161**, 435-444 (1993); J.C. Hilico, O. Robert, M. Loëte, S. Toumi, S.A. Pine, and L.R. Brown, “Analysis of the interacting octad system of  $^{12}CH_4$ ,” *J.Mol.Spectrosc.* **208**, 1-13 (2001).

**24.** L.R. Brown, A. Nikitin, D.C. Benner, V.M. Devi, M.A.H. Smith, L. Fejard, J.-P. Champion, V.G. Tyuterev, and R.L. Sams, “Line intensities of  $CH_3D$  in the triad region: 6-10  $\mu m$ ,” *J.Mol.Struct.* **695**, 181-188 (2004).

**25.** L.R. Brown, A. Nikitin, D.C. Benner, V.M. Devi, M.A.H. Smith, L. Fejard, J.-P. Champion, V.G. Tyuterev, and R.L. Sams, “Line intensities of  $CH_3D$  in the triad region: 6-10  $\mu m$ ,” *J.Mol.Struct.* **695**, 181-188 (2004).

**26.** A. Nikitin, J.-P. Champion, V.I.G. Tyuterev, L.R. Brown, G. Mellau, and M. Lock, “The infrared spectrum of  $CH_3D$  between 900 and 3200  $cm^{-1}$ : extended assignment and modeling,” *J.Mol.Struct.* **517**, 1-24 (2000); A. Nikitin, L.R. Brown, J.-P. Champion, L. Fejard, and V.I.G. Tyuterev, “Analysis of the  $CH_3D$  nonad from 2000 to 3300  $cm^{-1}$ ,” *J.Mol.Spectrosc.* **216**, 225-251 (2002).

**27.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, “Submillimeter, Millimeter, and Microwave Spectral Line Catalog,” *JQSRT* **60**, 883-890 (1998).

**28.** L.R. Brown, JPL, private communication (2004).

**29.** S. Albert, A. Bauerecker, V. Boudon, L.R. Brown, J.-P. Champion, M. Loëte, A. Nikitin, and M. Quack, “Global Frequency and Intensity Analysis of  $^{12}CH_4$  in the 0-4800  $cm^{-1}$  region,” *Chem.Phys.* **356**, 131-146 (2009).

**30.** V. Lattanzi, A. Walters, J.C. Pearson, and B.J. Drouin, “THz spectrum of monodeuterated methane,” *JQSRT* **109**, 580-586 (2008).

**31.** L.R. Brown, A. Nikitin, D.C. Benner, V.M. Devi, M.A.H. Smith, L. Fejard, J.-P. Champion, V.G. Tyuterev, and R.L. Sams, “Line intensities of  $CH_3D$  in the Triad region: 6-10  $\mu m$ ,” *J.Mol.Struct.* **695-696**, 181-188 (2004).

32. A.V. Nikitin, J.-P. Champion, and L.R. Brown, "Preliminary analysis of CH<sub>3</sub>D from 3250 to 3700 cm<sup>-1</sup>," *J.Mol.Spectrosc.* **240**, 14-25 (2006).
33. C. Boussin, B.L. Lutz, C. de Bergh, and A. Hamdouni, "Line intensities and self-broadening coefficients for the 3ν<sub>2</sub> band of monodeuterated methane," *JQSRT* **60**, 501-514 (1998).

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. C.P. Rinsland, V.Malathy Devi, M.A.H. Smith, and D.C. Benner, "Measurements of air-broadened and nitrogen-broadened Lorentz width coefficients and pressure shift coefficients in the ν<sub>4</sub> and ν<sub>2</sub> bands of <sup>12</sup>CH<sub>4</sub>," *Appl.Opt.* **27**, 631-651 (1988).
2. Table IV of Ref. 1.
3. V.Malathy Devi, C.P. Rinsland, M.A.H. Smith, and D.C.Benner, "Air-broadened Lorentz halfwidths and pressure induced line shifts in the ν<sub>4</sub> band of <sup>13</sup>CH<sub>4</sub>," *Appl.Opt.* **27**, 2296-2308 (1988).
4. Table IV of Ref. 1, scaled by 0.95.
5. V.Malathy Devi, C.P. Rinsland, D.C. Benner, M.A.H. Smith, and K.B. Thakur, "Absolute intensities and self-, N<sub>2</sub>, and air-broadened Lorentz halfwidths for selected lines in the ν<sub>3</sub> band of <sup>12</sup>CH<sub>3</sub>D from measurements with a tunable diode laser spectrometer," *Appl.Opt.* **25**, 1848-1853 (1986).
6. V.Malathy Devi, D.C. Benner, C.P. Rinsland, M.A.H. Smith, and K.B. Thakur, "Diode-Laser Measurements of Intensities and Halfwidths in the ν<sub>6</sub> Band of <sup>12</sup>CH<sub>3</sub>D," *J.Mol.Spectrosc.* **122**, 182-189 (1987).
19. D.C. Benner, V.Malathy Devi, C.P. Rinsland, and M.A.H. Smith, "Halfwidth and pressure-induced lineshift coefficients in the ν<sub>3</sub>, ν<sub>2</sub>+ ν<sub>4</sub>, ν<sub>3</sub>+ ν<sub>4</sub> and ν<sub>1</sub>+ν<sub>4</sub> bands of <sup>12</sup>CH<sub>4</sub>," 45<sup>th</sup> Ohio State University Symposium on Molecular Spectroscopy, p.105 (1990); D.C. Benner, C.P. Rinsland, and V.Malathy Devi, "Air-broadened halfwidths in the ν<sub>3</sub> band of <sup>12</sup>CH<sub>4</sub>," 41<sup>st</sup> Symposium on Molecular Spectroscopy, p.63 (1986); D.C. Benner, V.Malathy Devi, M.A.H. Smith, and C.P. Rinsland, "Air-broadened and nitrogen-broadened halfwidth coefficients and pressure shifts in the ν<sub>3</sub> band spectral region of <sup>12</sup>CH<sub>4</sub>," 43<sup>rd</sup> Symposium on Molecular Spectroscopy, p.171 (1988).
20. V.Malathy Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, "Measurements of air-, N<sub>2</sub>-, and O<sub>2</sub>-broadened halfwidths and pressure-induced line shifts in the ν<sub>3</sub> band of <sup>13</sup>CH<sub>4</sub>," *Appl.Opt.* **30**, 287-304 (1991); V.Malathy Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, "Measurements of air-, N<sub>2</sub>-, and O<sub>2</sub>-broadened halfwidths and pressure-induced line shifts in the ν<sub>3</sub> band of <sup>13</sup>CH<sub>4</sub>: errata," *Appl.Opt.* **30**, 2928 (1991).
21. M.A.H. Smith, C.P. Rinsland, V.M. Devi, and D.C. Benner, "Temperature-dependence of Broadening and Shifts of Methane Lines in the ν<sub>4</sub> Band," *Spectrochimica Acta* **48A**, 1257-1272 (1992).
22. V.M. Devi, C.P. Rinsland, M.A.H. Smith, and D.C. Benner, "Air-broadened Lorentz Halfwidths And Pressure-induced Line Shifts in the ν<sub>4</sub> Band of <sup>13</sup>CH<sub>4</sub>," *Appl.Opt.* **27**, 2296-2308 (1988).
23. D.C. Benner et al. unpublished data 2800 - 3000 cm<sup>-1</sup>; D.C. Benner, V.M. Devi, M.A.H. Smith, and C.P. Rinsland, "Air-broadening, N<sub>2</sub>-broadening, and O<sub>2</sub>-broadening and Shift Coefficients in the ν<sub>3</sub> Spectral Region of <sup>12</sup>CH<sub>4</sub>," *JQSRT* **50**, 65-89 (1993); V.M. Devi, D.C. Benner, M.A.H. Smith, et al. Measurements of Air-broadened, N<sub>2</sub>-broadened, and O<sub>2</sub>-broadened

Half-widths and Pressure-induced Line Shifts in the  $\nu_3$  Band of  $^{13}\text{CH}_4$ ,” *Appl. Opt.* **30**, 287-304 (1991).

**24.** A.S. Pine, “Self-broadening,  $\text{N}_2$ -broadening,  $\text{O}_2$ -broadening,  $\text{H}_2$ -broadening, Ar-broadening, and He-broadening in the  $\nu_3$  Band Q-branch of  $\text{CH}_4$ ,” *J.Chem.Phys.* **97**, 773-785 (1992).

**25.** V.M. Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, “Temperature-dependence of Lorentz Air-broadening and Pressure-shift Coefficients of  $^{12}\text{CH}_4$  Lines in the 2.3- $\mu\text{m}$  Spectral Region,” *JQSRT* **51**, 439-465 (1994).

**26.** V.M. Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, “Measurements of Air-broadening and Pressure-shifting of Methane Lines in the 2.3- $\mu\text{m}$  Region,” *J.Mol.Spectrosc.* **157**, 95-111 (1993).

**27.** A. Predoi Cross, M. Brawley-Tremblay, L.R. Brown, V.M. Devi, and D.C. Benner, “Multispectrum analysis of  $^{12}\text{CH}_4$  from 4100 to 4635  $\text{cm}^{-1}$ : II. Air-broadening coefficients (widths and shifts),” *J.Mol.Spectrosc.* **236**, 201-215 (2006).

**28.**  $\text{CH}_3\text{D}$  empirical fit of measurements reported in Ref. 30.

**29.** L.R. Brown, J.S. Margolis, J.P. Champion, J.C. Hilico, J.M. Jouvard, M. Loëte, C. Chackerian, Jr, G. Tarrago, and D.C. Benner, “Methane and its Isotopes: Current Status and Prospects for Improvement,” *JQSRT* **48**, 617-639 (1992).

**30.** V.M. Devi, D.C. Benner, M.A.H. Smith, and C.P. Rinsland, “Measurements of air broadened width and air induced shift coefficients and line mixing in the  $\nu_5$  band of  $^{12}\text{CH}_3\text{D}$ ,” *JQSRT* **68**, 135-161 (2001); V.M. Devi, D.C. Benner, M.A.H. Smith, C.P. Rinsland, and L.R. Brown, “Measurements of air-broadened width and air-induced shift coefficients and line mixing in the  $\nu_6$  band of  $^{12}\text{CH}_3\text{D}$ ,” *JQSRT* **68**, 1-41 (2001); V.M. Devi, D.C. Benner, M.A.H. Smith, C.P. Rinsland, and L.R. Brown, “Measurements of air broadening, pressure shifting and off diagonal relaxation matrix coefficients in the  $\nu_3$  band of  $^{12}\text{CH}_3\text{D}$ ,” *J.Mol.Struct.* **517**, 455-475 (2000); V.M. Devi et al. (in preparation).

**31.** L.R. Brown, JPL, private communication (2004).

**32.** Estimated broadening parameters described in L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, “Methane line parameters in HITRAN,” *JQSRT* **82**, 219-238 (2003) and L.R. Brown, “Empirical line parameters of methane from 1.1 to 2.1  $\mu\text{m}$ ,” *JQSRT* **96**, 251-270 (2005).

**33.** B.K. Antony, D.L. Niles, S.B. Wroblewski, C.M. Humphrey, T. Gabard, and R.R. Gamache, “ $\text{N}_2$ -,  $\text{O}_2$ - and air-broadened half-widths and line shifts for transitions in the  $\nu_3$  band of methane in the 2726- to 3200- $\text{cm}^{-1}$  spectral region,” *J.Mol.Spectrosc.* **251**, 268-281 (2008).

**34.** V. Malathy Devi, D. Chris Benner, M.A.H. Smith, C.P. Rinsland, and L.R. Brown, “Self- and  $\text{N}_2$ -broadening, pressure induced shift and line mixing in the  $\nu_5$  band of  $^{12}\text{CH}_3\text{D}$  using a multispectrum fitting technique,” *JQSRT* **74**, 1-41 (2002).

**35.** C. Boussin, B.L. Lutz, C. de Bergh, and A. Hamdouni, “Line intensities and self-broadening coefficients for the  $3\nu_2$  band of monodeuterated methane,” *JQSRT* **60**, 501-514 (1998).

**36.** M.A.H. Smith, D. C. Benner, A. Predoi-Cross, and V. Malathy Devi, “Multispectrum analysis of  $^{12}\text{CH}_4$  in the  $\nu_4$  band: I. Air-broadened half widths, pressure-induced shifts, temperature dependences and line mixing,” *JQSRT* **110**, 639-653 (2009).

#### Half-widths (self)

**1.** L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P.

- Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane Line Parameters in HITRAN," *JQSRT* **82**, 219-238 (2003).
2. L.R. Brown, JPL, private communication (2004); A. Predoi Cross, L.R. Brown, V.M. Devi, M. Brawley-Tremblay, and D.C. Benner, "Multispectrum analysis of  $^{12}\text{CH}_4$  from 4100 to 4635  $\text{cm}^{-1}$ : 1. Self-broadening coefficients (widths and shifts)," *J.Mol.Spectrosc.* **232**, 231-246 (2005).
  3. Estimated broadening parameters described in L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane line parameters in HITRAN," *JQSRT* **82**, 219-238 (2003) and L.R. Brown, "Empirical line parameters of methane from 1.1 to 2.1  $\mu\text{m}$ ," *JQSRT* **96**, 251-270 (2005).
  4. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, C.P. Rinsland, and L.R. Brown, "Self- and  $\text{N}_2$ -broadening, pressure induced shift and line mixing in the  $\nu_5$  band of  $^{12}\text{CH}_3\text{D}$  using a multispectrum fitting technique," *JQSRT* **74**, 1-41 (2002).
  5. C. Boussin, B.L. Lutz, C. de Bergh, and A. Hamdouni, "Line intensities and self-broadening coefficients for the  $3\nu_2$  band of monodeuterated methane," *JQSRT* **60**, 501-514 (1998).
  6. M.A.H. Smith, D. C. Benner, A. Predoi-Cross, and V. Malathy Devi, "Multispectrum analysis of  $^{12}\text{CH}_4$  in the  $\nu_4$  band: I. Air-broadened half widths, pressure-induced shifts, temperature dependences and line mixing," *JQSRT* **110**, 639-653 (2009).

#### Temperature dependence of air-broadened half-width

1. L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane Line Parameters in HITRAN," *JQSRT* **82**, 219-238 (2003).
2. L.R. Brown, JPL, private communication (2004).
3. Estimated broadening parameters described in L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane line parameters in HITRAN," *JQSRT* **82**, 219-238 (2003) and L.R. Brown, "Empirical line parameters of methane from 1.1 to 2.1  $\mu\text{m}$ ," *JQSRT* **96**, 251-270 (2005).
4. B.K. Antony, D.L. Niles, S.B. Wroblewski, C.M. Humphrey, T. Gabard, and R.R. Gamache, " $\text{N}_2$ -,  $\text{O}_2$ - and air-broadened half-widths and line shifts for transitions in the  $\nu_3$  band of methane in the 2726- to 3200- $\text{cm}^{-1}$  spectral region," *J.Mol.Spectrosc.* **251**, 268-281 (2008).
5. M.A.H. Smith, D. C. Benner, A. Predoi-Cross, and V. Malathy Devi, "Multispectrum analysis of  $^{12}\text{CH}_4$  in the  $\nu_4$  band: I. Air-broadened half widths, pressure-induced shifts, temperature dependences and line mixing," *JQSRT* **110**, 639-653 (2009).

#### Pressure shift (air)

1. L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane Line Parameters in HITRAN," *JQSRT* **82**, 219-238 (2003).
2. L.R. Brown, JPL, private communication (2004).
3. Estimated broadening parameters described in L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard, J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau,

- A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane line parameters in HITRAN," *JQSRT* **82**, 219-238 (2003) and L.R. Brown, "Empirical line parameters of methane from 1.1 to 2.1  $\mu\text{m}$ ," *JQSRT* **96**, 251-270 (2005).
4. B.K. Antony, D.L. Niles, S.B. Wroblewski, C.M. Humphrey, T. Gabard, and R.R. Gamache, "N<sub>2</sub>-, O<sub>2</sub>- and air-broadened half-widths and line shifts for transitions in the  $\nu_3$  band of methane in the 2726- to 3200-cm<sup>-1</sup> spectral region," *J.Mol.Spectrosc.* **251**, 268-281 (2008).
5. C. Boussin, B.L. Lutz, C. de Bergh, and A. Hamdouni, "Line intensities and self-broadening coefficients for the  $3\nu_2$  band of monodeuterated methane," *JQSRT* **60**, 501-514 (1998).
6. M.A.H. Smith, D. C. Benner, A. Predoi-Cross, and V. Malathy Devi, "Multispectrum analysis of <sup>12</sup>CH<sub>4</sub> in the  $\nu_4$  band: I. Air-broadened half widths, pressure-induced shifts, temperature dependences and line mixing," *JQSRT* **110**, 639-653 (2009).



## O<sub>2</sub> [7] 66, 68, 67

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. G. Rouillé, G. Millot, R. Saint-Loup, and H. Berger, "High-Resolution Stimulated Raman Spectroscopy of O<sub>2</sub>," *J.Mol.Spectrosc.* **154**, 372-382 (1992).
2. P.H. Krupenie, "The Spectrum of Molecular Oxygen," *J.Phys.Chem.Ref.Dat.* **1**, 423-534 (1972).
3. Molecular Hamiltonian constants for the  $v''=0$  and  $v'=0$  of the  $X\Sigma$  state are from G. Rouillé et al (Ref. 1).
4. Molecular Hamiltonian constants for the  $v''=0$  and  $v'=1$  of the  $X\Sigma$  state are from G. Rouillé et al (Ref. 1). Vibrational term values are from Krupenie (Ref. 2), upper vibrational state energy shifted to agree with band center of G. Rouillé et al for (1 $\leftarrow$ 0) band.
5. Molecular Hamiltonian constants for the  $v''=1$  and  $v'=1$  of the  $X\Sigma$  state are from G. Rouillé et al (Ref. 1). Vibrational term values are from P.H. Krupenie (Ref. 2), upper vibrational state energy shifted to agree with band center of G. Rouillé et al for (1 $\leftarrow$ 0) band.
6. M. Mizushima and S. Yamamoto, "Microwave Absorption Lines of <sup>16</sup>O<sup>18</sup>O in its ( $X\Sigma_g$ ,  $v=0$ ) State," *J.Mol.Spectrosc.* **148**, 447-452 (1991).
7. Molecular Hamiltonian constants for the  $v''=0$  and  $v'=0$  of the  $X\Sigma$  state are from M. Mizushima and S. Yamamoto (Ref. 6). Vibrational term values are from P.H. Krupenie (Ref. 2).
8. K.W. Hillig II, C.C.W. Chiu, W.G. Read, and E.A. Cohen, "The Pure Rotation Spectrum of  $a^1\Delta_g$  O<sub>2</sub>," *J.Mol.Spectrosc.* **109**, 205-206 (1985).
9. T. Scalabrin, R.J. Saykally, K.M. Evenson, H.E. Radford, and M. Mizushima, "Laser Magnetic Resonance Measurement of Rotational transitions in the Metastable  $a^1\Delta_g$  State of Oxygen," *J.Mol.Spectrosc.* **89**, 344-351 (1981).
10. J. Brault, Kitt Peak National Solar Observatory, private communication (1982).
11. Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=0$  of the  $a\Delta$  state, the constants of K.W. Hillig et al (Ref. 8) are used in the formalism of T. Scalabrin et al (Ref. 9). Vibrational term values are from Krupenie (Ref. 2). Upper vibrational state energy shifted by  $-0.002788\text{ cm}^{-1}$  to agree with data of J. Brault (Ref. 10).
12. Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=1$  of the  $a\Delta_g$  state the constants of J. Brault (Ref. 10) are used. Vibrational term values are from P.H. Krupenie (Ref. 2). Upper vibrational state energy shifted by  $-0.050385\text{ cm}^{-1}$  to agree with data of J. Brault (Ref. 10).
13. Molecular Hamiltonian constants for the  $v'=1$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=0$  of the  $a\Delta_g$  state, the constants of K.W. Hillig et al (Ref. 8) are used in the formalism of T. Scalabrin et al (Ref. 9). Vibrational term values are from Krupenie (Ref. 2). Upper vibrational state energy shifted by  $-0.002788\text{ cm}^{-1}$  to be consistent with the (0 $\leftarrow$ 0) transitions.
14. L. Herzberg and G. Herzberg, "Fine Structure of the Infrared Atmospheric Oxygen Bands," *Astrophys.J.* **105**, 353 (1947).
15. Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima and S. Yamamoto (Ref. 6). For the  $v'=0$  of the  $a\Delta_g$  state, the constants of Herzberg and Herzberg (Ref. 14) are used. Vibrational term values are from P.H. Krupenie (Ref. 2). Upper vibrational state energy shifted by  $+0.29573\text{ cm}^{-1}$  to agree with data of J. Brault (Ref. 10).
16. M. Mizushima, L.R. Zink, and K.M. Evenson, "Rotational Structure of <sup>16</sup>O<sub>2</sub>, <sup>16</sup>O<sup>17</sup>O, and

- $^{16}\text{O}^{18}\text{O} (X\Sigma_g^-)$  from Laser Magnetic Resonance Spectra,” *J.Mol.Spectrosc.* **107**, 395-404 (1984).
- 17.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima et al (Ref. 16). For the  $v'=0$  of the  $a\Delta_g$  state, the constants of L. Herzberg and G. Herzberg (Ref. 14) are used. Vibrational term values are from Krupenie (Ref. 2). Upper vibrational state energy shifted by  $+0.15634\text{ cm}^{-1}$  to agree with data of J. Brault (Ref. 10).
- 18.** D.L. Albritton, W.J. Harrop, A.L. Schmeltekopf, and R.N. Zare, “Resolution of the Discrepancies Concerning the Optical and Microwave values for  $B_0$  and  $D_0$  of the  $X\Sigma_g^-$  State of  $\text{O}_2$ ,” *J.Mol.Spectrosc.* **46**, 103-118 (1973).
- 19.** H. Babcock and L. Herzberg, “Fine Structure of the Red System of Atmospheric Oxygen Bands,” *Astrophys.J.* **108**, 167-190 (1948).
- 20.** W.S. Benedict, University of Maryland, private communication, 8/27/76.
- 21.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=0$  of the  $b\Sigma$  state, the constants of D.L. Albritton (Ref. 18) are used. Vibrational and electronic term values are from Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
- 22.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=1$  of the  $b\Sigma$  state, the constants of D.L. Albritton (Ref. 18) are used. Vibrational and electronic term values are from P.H. Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
- 23.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=2$  of the  $b\Sigma$  state, the constants of D.L. Albritton (Ref. 18) are used. Vibrational and electronic term values are from Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
- 24.** Molecular Hamiltonian constants for the  $v''=1$  state of  $X\Sigma$  are from G. Rouillé et al (Ref. 1). For the  $v'=1$  of the  $b\Sigma$  state, the constants of D.L. Albritton (Ref. 18) are used. Vibrational and electronic term values are from Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
- 25.** Molecular Hamiltonian constants for the  $v''=1$  state of  $X\Sigma$  are from Rouillé et al. (Ref. 1). For the  $v'=0$  of the  $b\Sigma$  state, the constants of D.L. Albritton (Ref. 18) are used. Vibrational and electronic term values are from Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
- 26.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima and S. Yamamoto (Ref. 6). For the  $v'=0$  of the  $b\Sigma$  state, the constants of H. Babcock and L. Herzberg (Ref. 19) are used. Vibrational and electronic term values are from Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state. Electronic term value is shifted by  $(-0.041-0.014)\text{ cm}^{-1}$ , unknown reference.
- 27.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima and S. Yamamoto (Ref. 6). For the  $v'=1$  of the  $b\Sigma$  state, the constants of W.S. Benedict (Ref. 20) are used. Vibrational and electronic term values are from P.H. Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state. Electronic term value is shifted by  $(-0.041-0.014)\text{ cm}^{-1}$ , unknown reference.
- 28.** Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima and S. Yamamoto (Ref. 6). For the  $v'=2$  of the  $b\Sigma$  state, the constants from W.S. Benedict, University of Maryland (private communication) are used. Vibrational and electronic term values are from P.H. Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state. Electronic term value is shifted by  $(-0.041-0.014)\text{ cm}^{-1}$ , unknown reference.

29. Molecular Hamiltonian constants for the  $v''=0$  state of  $X\Sigma$  are from M. Mizushima and S. Yamamoto (Ref. 6). For the  $v'=1$  of the  $b\Sigma$  state, the constants of H. Babcock and L. Herzberg (Ref. 19) are used. Vibrational and electronic term values are from P.H. Krupenie (Ref. 2). Dunham zero point energy correction applied to zero point energy of upper vibrational state.
30. R.L. Poynter and H.M. Pickett, "Submillimeter, Millimeter, and Microwave Spectral Line Catalogue," JPL Publication 80-23, Revision 1, (1981).
31. Data from J. Brault and W.S. Benedict, analysis of Kitt Peak observations, private communication (1978).
32. K. Minschwaner, G.P. Anderson, L.A. Hall, and K. Yoshino, "Polynomial Coefficients for Calculating  $O_2$  Schumann-Runge Cross Sections at  $0.5\text{ cm}^{-1}$  Resolution," *J.Geophys.Res.* **97**, 10103-10108 (1992).
33. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
34. K. Yoshino and J.R. Esmond, Harvard-Smithsonian Center for Astrophysics, private communication (1994).
35. L.R. Brown and C. Plymate, "Experimental Line Parameters of the Oxygen A Band at 760 nm," *J.Mol.Spectrosc.* **199**, 166-179 (2000).
36. C. Camy-Peyret, private communication based on "High resolution balloon-borne spectroscopy within the  $O_2$  A-band: observations and radiative transfer modeling," C. Camy-Peyret, S. Payan, P. Jeseck, Y. Té, and T. Hawat, Paper E4, Proceedings of the International Radiation Symposium, (2000).
37. M.-F. Mérienne, A. Jenouvrier, B. Coquart, M. Carleer, S. Fally, R. Colin, A.C. Vandaele, and C. Hermans, "Improved dataset for the Herzberg band system of  $^{16}O_2$ ," *J.Mol.Spectrosc.* **207**, 120 (2001).
38. Blended lines from M.-F. Mérienne, A. Jenouvrier, B. Coquart, M. Carleer, S. Fally, R. Colin, A.C. Vandaele, and C. Hermans, "Improved dataset for the Herzberg band system of  $^{16}O_2$ ," *J.Mol.Spectrosc.* **207**, 120 (2001).
39. D.J. Robichaud, J.T. Hodges, P. Maslowski, L.Y. Yeung, M. Okumura, C.E. Miller, and L.R. Brown, "High-accuracy transition frequencies for the  $O_2$  A-band," *J.Mol.Spectrosc.* **251**, 27-37 (2008).
40. D.J. Robichaud, L.Y. Yeung, D.A. Long, D.K. Havey, J.T. Hodges, D. Lisak, C.E. Miller, M. Okumura, and L.R. Brown, "Experimental Line Parameters of the  $b^1\Sigma_g^+ - X^3\Sigma_g^-$  Band of Oxygen Isotopologues at 760 nm Using Frequency-Stabilized Cavity Ring-Down Spectroscopy," *J. Phys. Chem. A*, **113**, 13089-99 (2009).
41. The Q2Q2 and Q2R1 lines that were missing from reference 40 above were calculated in 2009 using input parameters of Ref. 1 above.

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. R.R. Gamache, A. Goldman, and L.S. Rothman, "Improved Spectral Parameters for the Three Most Abundant Isotopomers of the Oxygen Molecule," *JQSRT* **59**, 495-509 (1998).
2. K.J. Ritter and T.D. Wilkerson, "High Resolution Spectroscopy of the Oxygen A Band," *J.Mol.Spectrosc.* **121**, 1-19 (1987).
3. L.P. Giver, R.W. Boese, and J.H. Miller, "Intensity Measurements, Self-Broadening Coefficients, and Rotational Intensity Distribution for Lines of the Oxygen B Band at  $6880\text{ Å}$ ,"

*JQSRT* **14**, 793-802 (1974).

4. M.A. Mélières, M. Chenevier, and F. Stoeckel, "Intensity Measurements and Self-broadening coefficients in the  $\gamma$  Band of  $O_2$  at 628 nm using Intracavity Laser-absorption Spectroscopy (ICLAS)," *JQSRT* **33**, 337-345 (1985).

5. V.D. Galkin, "Electronic moment of the  $b^1\Sigma_g^- - X^3\Sigma_g^-$  transition of the oxygen band system," *Opt.Spektrosk. (USSR)* **47**, 266-271 (1979).

6. Y.T. Hsu, Y.-P. Lee, and J.F. Ogilvie, "Linestrengths of the Band  $a^1\Delta_g (v'=0) - X^3\Sigma_g^- (v''=0)$  of  $^{16}O_2$ ," *Spectrochim.Acta* **48A**, 1227-1230 (1992).

7. K. Minschwaner, G.P. Anderson, L.A. Hall, and K. Yoshino, "Polynomial Coefficients for Calculating  $O_2$  Schumann-Runge Cross Sections at  $0.5\text{ cm}^{-1}$  Resolution," *J.Geophys.Res.* **97**, 10103-10108 (1992).

8. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

9. R.L. Poynter and H.M. Pickett, "Submillimeter, Millimeter, and Microwave Spectral Line Catalogue," JPL Publication 80-23, Revision 1, (1981).

10. Data from J. Brault and W.S. Benedict, analysis of Kitt Peak observations, private communication (1978).

11. W.J. Lafferty, A.M. Solodov, C.L. Lugez, and G.T. Fraser, "Rotational line strengths and self-pressure-broadening coefficients for the  $1.27\text{-}\mu\text{m}$ ,  $a^1\Delta_g - X^3\Sigma_g^-$ ,  $v = 0 - 0$  band of  $O_2$ ," *Appl.Opt.* **37**, 2264-2270 (1998).

12. Intensity reduced by 15% from HITRAN96 values (Ref. 6 above), private communication, G.T. Fraser, NIST (2000).

13. C. Camy-Peyret, private communication based on "High resolution balloon-borne spectroscopy within the  $O_2$  A-band: observations and radiative transfer modeling," C. Camy-Peyret, S. Payan, P. Jeseck, Y. Té, and T. Hawat, Paper E4, Proceedings of the International Radiation Symposium, (2000).

14. M.-F. Mérienne, A. Jenouvrier, B. Coquart, M. Carleer, S. Fally, R. Colin, A.C. Vandaele, C. Hermans "Improved dataset for the Herzberg band system of  $^{16}O_2$ ," *J.Mol.Spectrosc.* **207**, 120 (2001).

15. Blended lines, from M.-F. Mérienne, A. Jenouvrier, B. Coquart, M. Carleer, S. Fally, R. Colin, A.C. Vandaele, C. Hermans "Improved dataset for the Herzberg band system of  $^{16}O_2$ ," *J.Mol.Spectrosc.* **207**, 120 (2001).

16. D.J. Robichaud, J.T. Hodges, L.R. Brown, D. Lisak, P. Maslowski, L.Y. Yeung, M. Okumura, and C.E. Miller, "Experimental intensity and lineshape parameters of the oxygen A-band using frequency-stabilized cavity ring-down spectroscopy," *J.Mol.Spectrosc.* **248**, 1-13 (2008).

17. D.J. Robichaud, L.Y. Yeung, D.A. Long, D.K. Havey, J.T. Hodges, D. Lisak, C.E. Miller, M. Okumura, and L.R. Brown, "Experimental Line Parameters of the  $b^1\Sigma_g^+ - X^3\Sigma_g^-$  Band of Oxygen Isotopologues at 760 nm Using Frequency-Stabilized Cavity Ring-Down Spectroscopy," *J. Phys. Chem. A*, **113**, 13089-99 (2009).

18. Intensities calculated by Prof. Andrew Orr-Ewing based on the intensities measured in S.M. Newman, A.J. Orr-Ewing, D.A. Newnham, and J. Ballard, "Temperature and pressure dependence of line widths and integrated absorption intensities for the  $O_2\ a^1\Delta_g - X^3\Sigma_g^- (0,0)$  transition," *J.Phys.Chem.A*. **104**, 9467 (2000).

19. Q2Q2 and Q2R1 lines missing from either reference 1 or 18 above were calculated in 2009 using input parameters of Ref. 1.

**20.** Intensities from Ref. 1 scaled according to S. Kassi, D. Romanini, A. Campargue, and B. Bussery-Honvault, “Very high sensitivity CW-cavity ring down spectroscopy: Application to the  $a^1\Delta_g(0)-X^3\Sigma_g^-(1)$  O<sub>2</sub> band near 1.58  $\mu\text{m}$ ,” *Chem.Phys.Lett.* **409**, 281-287 (2005).

#### Half-widths (air)

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, “The HITRAN database: 1986 Edition,” *Appl.Opt.* **26**, 4058-4097 (1987).
- 1.** P.H. Krupenie, “The Spectrum of Molecular Oxygen,” *J.Phys.Chem.Ref.Dat.* **1**, 423-534 (1972).
- 2.** L.P. Giver, R.W. Boese, and J.H. Miller, “Intensity Measurements, Self-Broadening Coefficients, and Rotational Intensity Distribution for Lines of the Oxygen B Band at 6880 Å,” *JQSRT* **14**, 793-802 (1974).
- 3.** K.J. Ritter and T.D. Wilkerson, “High Resolution Spectroscopy of the Oxygen A Band,” *J.Mol.Spectrosc.* **121**, 1-19 (1987).
- 4.** K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, “The Smithsonian Astrophysical Observatory Database SAO92,” *JQSRT* **52**, 447-457 (1994).
- 5.** L.R. Brown and C. Plymate, “Experimental Line Parameters of the Oxygen A Band at 760 nm,” *J.Mol.Spectrosc.* **199**, 166-179 (2000).
- 6.** C. Camy-Peyret, private communication based on “High resolution balloon-borne spectroscopy within the O<sub>2</sub> A-band: observations and radiative transfer modeling,” C. Camy-Peyret, S. Payan, P. Jeseck, Y. Té, and T. Hawat, Paper E4, Proceedings of the International Radiation Symposium, (2000).
- 7.** D.J. Robichaud, J.T. Hodges, L.R. Brown, D. Lisak, P. Maslowski, L.Y. Yeung, M. Okumura, and C.E. Miller, “Experimental intensity and lineshape parameters of the oxygen A-band using frequency-stabilized cavity ring-down spectroscopy,” *J.Mol.Spectrosc.* **248**, 1-13 (2008).
- 8.** R.A. Washenfelder, G.C. Toon, J.-F. Blavier, Z. Yang, N.T. Allen, P.O. Wennberg, S.A. Vay, D.M. Matross, and B.C. Daube, “Carbon dioxide column abundances at the Wisconsin Tall Tower site,” *J.Geophys.Res.* **111**, D22305 (2006).

#### Half-widths (self)

- 1.** W.J. Lafferty, A.M. Solodov, C.L. Lugez, and G.T. Fraser, “Rotational line strengths and self-pressure-broadening coefficients for the 1.27- $\mu\text{m}$ ,  $a^1\Delta_g - X^3\Sigma_g^-$ ,  $v = 0-0$  band of O<sub>2</sub>,” *Appl.Opt.* **37**, 2264-2270 (1998).
- 2.** K. Minschwaner, G.P. Anderson, L.A. Hall, and K. Yoshino, “Polynomial Coefficients for Calculating O<sub>2</sub> Schumann-Runge Cross Sections at 0.5  $\text{cm}^{-1}$  Resolution,” *J.Geophys.Res.* **97**, 10103-10108 (1992).
- 3.** L.R. Brown and C. Plymate, “Experimental Line Parameters of the Oxygen A Band at 760 nm,” *J.Mol.Spectrosc.* **199**, 166-179 (2000).
- 4.** D.J. Robichaud, J.T. Hodges, L.R. Brown, D. Lisak, P. Maslowski, L.Y. Yeung, M. Okumura, and C.E. Miller, “Experimental intensity and lineshape parameters of the oxygen A-band using frequency-stabilized cavity ring-down spectroscopy,” *J.Mol.Spectrosc.* **248**, 1-13 (2008).
- 5.** R.A. Washenfelder, G.C. Toon, J.-F. Blavier, Z. Yang, N.T. Allen, P.O. Wennberg, S.A. Vay, D.M. Matross, and B.C. Daube, “Carbon dioxide column abundances at the Wisconsin Tall Tower site,” *J.Geophys.Res.* **111**, D22305 (2006).



Temperature dependence of air-broadened half-width

1. L.R. Brown and C. Plymate, "Experimental Line Parameters of the Oxygen *A* Band at 760 nm," *J.Mol.Spectrosc.* **199**, 166-179 (2000).
2. R.A. Washenfelder, G.C. Toon, J.-F. Blavier, Z. Yang, N.T. Allen, P.O. Wennberg, S.A. Vay, D.M. Matross, and B.C. Daube, "Carbon dioxide column abundances at the Wisconsin Tall Tower site," *J.Geophys.Res.* **111**, D22305 (2006).

Pressure shift (air)

1. L.R. Brown and C. Plymate, "Experimental Line Parameters of the Oxygen *A* Band at 760 nm," *J.Mol.Spectrosc.* **199**, 166-179 (2000).
2. D.J. Robichaud, J.T. Hodges, P. Maslowski, L.Y. Yeung, M. Okumura, C.E. Miller, and L.R. Brown, "High-accuracy transition frequencies for the O<sub>2</sub> A-band," *J.Mol.Spectrosc.* **251**, 27-37 (2008).
3. R.A. Washenfelder, G.C. Toon, J.-F. Blavier, Z. Yang, N.T. Allen, P.O. Wennberg, S.A. Vay, D.M. Matross, and B.C. Daube, "Carbon dioxide column abundances at the Wisconsin Tall Tower site," *J.Geophys.Res.* **111**, D22305 (2006).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. Same as Ref. 0.
2. M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, "The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines," *J.Mol.Spectrosc.* **165**, 506-524 (1994).
3. V. Dana, J.-Y. Mandin, L.H. Coudert, M. Badaoui, F. LeRoy, G. Guelachvili, and L.S. Rothman, " $\lambda$ -Splittings and Line Intensities in the 2 - 1 Hot Band of Nitric Oxide," *J.Mol.Spectrosc.* **165**, 525-540 (1994).
4. L.H. Coudert, V. Dana, J.-Y. Mandin, M. Morillon-Chapey, R. Farrenq, and G. Guelachvili, "The Spectrum of Nitric Oxide between 1700 and 2100  $\text{cm}^{-1}$ ," *J.Mol.Spectrosc.* **172**, 435-448 (1995).
5. J.-Y. Mandin, V. Dana, L. Régalia, A. Barbe, and X. Thomas, " $\Lambda$ -Splittings and Line Intensities in the First Overtone of Nitric Oxide," *J.Mol.Spectrosc.* **185**, 347-355 (1997); J.-Y. Mandin, V. Dana, L. Régalia, A. Barbe, and P. Von der Heyden, "Lambda-Splittings and Line Intensities in the 3  $\leftarrow$  1 Hot Band of  $^{14}\text{N}^{16}\text{O}$ : The Spectrum of Nitric Oxide in the First Overtone Region," *J.Mol.Spectrosc.* **187**, 200-205 (1998).
6. J.R. Gillis and A. Goldman, "Nitric oxide IR line parameters for the upper atmosphere," *Appl.Opt.* **21**, 1161-1163 (1982).
7. A. Goldman, private communication (2004), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana and J.-Y. Mandin "Nitric oxide line parameters: review of 1996 HITRAN update and new results," *JQSRT* **60**, 825-838 (1998).
8. A. Goldman, private communication (2006), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin "Nitric oxide line parameters: review of 1996 HITRAN update and new results," *JQSRT* **60**, 825-838 (1998).
9. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. J. Ballard, W.B. Johnston, B.J. Kerridge, and J.J. Remedios, "Experimental Spectral Line Parameters in the 1-0 Band of Nitric Oxide," *J.Mol.Spectrosc.* **127**, 70-82 (1988).
2. M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, "The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines," *J.Mol.Spectrosc.* **165**, 506-524 (1994).
3. V. Dana, J.-Y. Mandin, L.H. Coudert, M. Badaoui, F. LeRoy, G. Guelachvili, and L.S. Rothman, " $\lambda$ -Splittings and Line Intensities in the 2 - 1 Hot Band of Nitric Oxide," *J.Mol.Spectrosc.* **165**, 525-540 (1994).
4. L.H. Coudert, V. Dana, J.-Y. Mandin, M. Morillon-Chapey, R. Farrenq, and G. Guelachvili,

“The Spectrum of Nitric Oxide between 1700 and 2100  $\text{cm}^{-1}$ ,” *J.Mol.Spectrosc.* **172**, 435-448 (1995).

5. J.-Y. Mandin, V. Dana, L. Régalia, A. Barbe, and X. Thomas, “ $\Lambda$ -Splittings and Line Intensities in the First Overtone of Nitric Oxide,” *J.Mol.Spectrosc.* **185**, 347-355 (1997); J.-Y. Mandin, V. Dana, L. Régalia, A. Barbe, and P. Von der Heyden, “Lambda-Splittings and Line Intensities in the  $3 \leftarrow 1$  Hot Band of  $^{14}\text{N}^{16}\text{O}$ : The Spectrum of Nitric Oxide in the First Overtone Region,” *J.Mol.Spectrosc.* **187**, 200-205 (1998).

6. J.R. Gillis and A. Goldman, “Nitric oxide IR line parameters for the upper atmosphere,” *Appl.Opt.* **21**, 1161-1163 (1982).

7. A. Goldman, private communication (2004), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana and J.-Y. Mandin “Nitric oxide line parameters: review of 1996 HITRAN update and new results,” *JQSRT* **60**, 825-838 (1998).

8. A. Goldman, private communication (2006), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin “Nitric oxide line parameters: review of 1996 HITRAN update and new results,” *JQSRT* **60**, 825-838 (1998).

9. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, “Submillimeter, Millimeter, and Microwave Spectral Line Catalog,” *JQSRT* **60**, 883-890 (1998).

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, “The HITRAN database: 1986 Edition,” *Appl.Opt.* **26**, 4058-4097 (1987).

1. J. Ballard, Rutherford Appleton Laboratory, private communication (1990).

2. M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, “The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines,” *J.Mol.Spectrosc.* **165**, 506-524 (1994).

3. M.-Y. Allout, V. Dana, J.-Y. Mandin, P. Von der Heyden, D. Décatoire, and J.-J. Plateaux, “Oxygen-Broadening Coefficients of First Overtone Nitric Oxide Lines,” *JQSRT* **61**, 759-765 (1999); J.-Y. Mandin, V. Dana, L. Régalia, X. Thomas, and A. Barbe, “Nitrogen-Broadening in the Nitric Oxide First Overtone Band,” *JQSRT* **66**, 93-100 (2000).

4. Assumption of validity of J.-Y. Mandin, V. Dana, L. Régalia, X. Thomas, and A. Barbe, “Nitrogen-Broadening in the Nitric Oxide First Overtone Band,” *JQSRT* **66**, 93-100 (2000) for other  $\Delta v = 2$  transitions including forbidden sub-bands.

5. C. Chackerian, Jr., R.S. Freedman, L.P. Giver, and L.R. Brown, “The NO Vibrational Fundamental Band:  $\text{O}_2$ -Broadening Coefficients,” *J.Mol.Spectrosc.* **192**, 215-219 (1998); M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, “The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines,” *J.Mol.Spectrosc.* **165**, 506-524 (1994).

6. Assumption of validity of C. Chackerian, Jr., R.S. Freedman, L.P. Giver, and L.R. Brown, “The NO Vibrational Fundamental Band:  $\text{O}_2$ -Broadening Coefficients,” *J.Mol.Spectrosc.* **192**, 215-219 (1998); M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, “The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines,” *J.Mol.Spectrosc.* **165**, 506-524 (1994) for other  $\Delta v$  transitions (except  $\Delta v = 2$ ) including forbidden sub-bands.

7. A. Goldman, private communication (2006), based on A. Goldman, L.R. Brown, W.G.

Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin “Nitric oxide line parameters: review of 1996 HITRAN update and new results,” *JQSRT* **60**, 825-838 (1998).

#### Half-widths (self)

1. Polynomial fit of measurements from A. Pine, A.G. Maki, N.-Y. Chou, “Pressure broadening, lineshapes and intensity measurements in the 2 from 0 band of NO,” *J.Mol.Spectrosc.* **114**, 132-147 (1985).

2. A. Goldman, private communication (2006), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin “Nitric oxide line parameters: review of 1996 HITRAN update and new results,” *JQSRT* **60**, 825-838 (1998).

#### Temperature dependence of air-broadened half-width

1. A. Goldman, private communication (2004), based on M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, “Temperature Dependence of Nitrogen Broadening of the NO Fundamental Vibrational Band,” *J.Mol.Spectrosc.* **181**, 307-315 (1997).

2. A. Goldman, private communication (2006), based on A. Goldman, L.R. Brown, W.G. Schoenfeld, M.N. Spencer, C. Chackerian, L.P. Giver, H. Dothe, C.P. Rinsland, L.H. Coudert, V. Dana, and J.-Y. Mandin “Nitric oxide line parameters: review of 1996 HITRAN update and new results,” *JQSRT* **60**, 825-838 (1998).

#### Pressure shift (air)

1. M.N. Spencer, C. Chackerian, Jr., L.P. Giver, and L.R. Brown, “The Nitric Oxide Fundamental Band: Frequency and Shape Parameters for Ro-vibrational Lines,” *J.Mol.Spectrosc.* **165**, 506-524 (1994).

2. A.S. Pine, J.W.C. Johns, and A.G. Robiette, “ $\Lambda$ -Doubling in the  $v = 2 \leftarrow 0$  overtone band in the infrared spectrum of NO,” *J.Mol.Spectrosc.* **74**, 52-69 (1979).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. A. Goldman, F.J. Murcray, C.P. Rinsland, R.D. Blatherwick, S.J. David, F.H. Murcray, and D.G. Murcray, "Mt. Pinatubo SO<sub>2</sub> Column Measurements from Mauna Loa," *Geophys.Res.Lett.* **19**, 183-186 (1992).
2. W.G. Mankin, M.T. Coffey, and A. Goldman, "Airborne Observations of SO<sub>2</sub>, HCl, and O<sub>3</sub> in the Stratospheric Plume of the Pinatubo Volcano in July 1991," *Geophys.Res.Lett.* **19**, 179-182 (1991); also Ref.1.
3. R.J. Corice, Jr., K. Fox, and G.D.T. Tejwani, " $\nu_1+\nu_3$  combination band of  $^{32}\text{S}^{16}\text{O}_2$ ," *J.Chem.Phys.* **59**, 672-675 (1973).
4. A. Goldman, University of Denver, private communication (1992).
5. A. Pine, National Bureau of Standards, private communication.
6. W.J. Lafferty, A.S. Pine, J.-M. Flaud, and C. Camy-Peyret, "The  $2\nu_3$  Band of  $^{32}\text{S}^{16}\text{O}_2$ : Line Positions and Intensities," *J.Mol.Spectrosc.* **157**, 499-511 (1993).
7. W.J. Lafferty, G.T. Fraser, A.S. Pine, J.-M. Flaud, and C. Camy-Peyret, V. Dana, J.-Y. Mandin, A. Barbe, J.-J. Plateaux, S. Bouazza, "The  $3\nu_3$  Band of  $^{32}\text{S}^{16}\text{O}_2$  Line Positions and Intensities," *J.Mol.Spectrosc.* **154**, 51-60 (1992); J.-M. Flaud and W.J. Lafferty, " $^{32}\text{S}^{16}\text{O}_2$ : a refined analysis of the  $3\nu_3$  band and determination of equilibrium rotational constants," *J.Mol.Spectrosc.* **161**, 396-402 (1993).
8. W.J. Lafferty, A.S. Pine, G. Hilpert, R.L. Sams, and J.-M. Flaud, "The  $\nu_1+\nu_3$  and  $2\nu_1+\nu_3$  Band Systems of SO<sub>2</sub>: Line Positions and Intensities," *J.Mol.Spectrosc.* **176**, 280-286 (1996).
9. J.-M. Flaud, A. Perrin, L.M. Salah, W.J. Lafferty, and G. Guelachvili, "A reanalysis of the (010), (020), (100) and (001) rotational levels of  $^{32}\text{S}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **160**, 272-278 (1993).
10. J. Henningsen, A. Barbe, and M.-R. De Backer-Barilly, "Revised molecular parameters for  $^{32}\text{SO}_2$  and  $^{34}\text{SO}_2$  from high resolution study of the infrared spectrum in the 7-8  $\mu\text{m}$  wavelength region," *JQSRT* **109**, 2491-2510 (2008).
11. W.J. Lafferty, J.-M. Flaud, E.H.A. Ngom, and R.L. Sams, " $^{34}\text{S}^{16}\text{O}_2$ : High-resolution analysis of the (0 3 0), (1 0 1), (1 1 1), (0 0 2) and (2 0 1) vibrational states; determination of equilibrium rotational constants for sulfur dioxide and anharmonic vibrational constants," *J.Mol.Spectrosc.* **253**, 51-54 (2009). The global fit that was performed in this work included results from W.J. Lafferty, J.-M. Flaud, R.L. Sams, and E.H. Abib Ngom, "High resolution analysis of the rotational levels of the (0 0 0), (0 1 0), (1 0 0), (0 0 1), (0 2 0), (1 1 0) and (0 1 1) vibrational states of  $^{34}\text{S}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **252**, 72-76 (2008).
12. H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists," *J.Mol.Struct.* **742**, 215-227 (2005).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. A. Goldman, F.J. Murcray, C.P. Rinsland, R.D. Blatherwick, S.J. David, F.H. Murcray, and D.G. Murcray, "Mt. Pinatubo SO<sub>2</sub> Column Measurements from Mauna Loa," *Geophys.Res.Lett.*



**19**, 183-186 (1992).

**2.** W.G. Mankin, M.T. Coffey, and A. Goldman, "Airborne Observations of SO<sub>2</sub>, HCl, and O<sub>3</sub> in the Stratospheric Plume of the Pinatubo Volcano in July 1991," *Geophys.Res.Lett.* **19**, 179-182 (1991); also Ref.1.

**3.** W.J. Lafferty, A.S. Pine, J.-M. Flaud, and C. Camy-Peyret, "The 2v<sub>3</sub> Band of <sup>32</sup>S<sup>16</sup>O<sub>2</sub>: Line Positions and Intensities," *J.Mol.Spectrosc.* **157**, 499-511 (1993).

**4.** W.J. Lafferty, G.T. Fraser, A.S. Pine, J.-M. Flaud, and C. Camy-Peyret, "The 3v<sub>3</sub> Band of <sup>32</sup>S<sup>16</sup>O<sub>2</sub> Line Positions and Intensities," *J.Mol.Spectrosc.* **154**, 51-60 (1992); J.-M. Flaud and W.J. Lafferty, *J.Mol.Spectrosc.* **161**, 396-402 (1993).

**5.** W.J. Lafferty, A.S. Pine, G. Hilpert, R.L. Sams, and J.-M. Flaud, "The v<sub>1</sub>+v<sub>3</sub> and 2v<sub>1</sub>+v<sub>3</sub> Band Systems of SO<sub>2</sub>: Line Positions and Intensities," *J.Mol.Spectrosc.* **176**, 280-286 (1996).

**6.** J.R. Spencer, E. Lellouch, M.J. Richter, M.A. López-Valverde, K. Lea Jessup, T.K. Greathouse, and J.-M. Flaud, "Mid-infrared detection of large longitudinal asymmetries in Io's SO<sub>2</sub> atmosphere," *Icarus* **176**, 283-304 (2005).

**7.** P.M. Chu, S.J. Wetzel, W.J. Lafferty, A. Perrin, J.-M. Flaud, P. Arcas, and G. Guelachvili, "Line Intensities for the 8-μm Bands of SO<sub>2</sub>," *J.Mol.Spectrosc.* **189**, 55-63 (1998).

**8.** J. Henningsen, A. Barbe, and M.-R. De Backer-Barilly, "Revised molecular parameters for <sup>32</sup>SO<sub>2</sub> and <sup>34</sup>SO<sub>2</sub> from high resolution study of the infrared spectrum in the wavelength region," *JQSRT* **109**, 2491-2510 (2008).

**9.** J.-M. Flaud, W.J. Lafferty, and R.L. Sams, "Line Intensities for the v<sub>1</sub>, v<sub>3</sub> and v<sub>1</sub> + v<sub>3</sub> bands of <sup>34</sup>SO<sub>2</sub>," *JQSRT*, **110**, 669-674 (2009).

**10.** H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists," *J.Mol.Struct.* **742**, 215-227 (2005).

#### Half-widths (air)

**0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).

**1.** O. Fleischmann, B. Sumpf, J. Waschull, and H.-D. Kronfeldt, "Self- and Air-Broadened Coefficients of Absorption Lines in the v<sub>1</sub> Band of SO<sub>2</sub>," XIII<sup>th</sup> International Conference on High Resolution Spectroscopy, Poznan, Poland, Sept. 1994.

**2.** J.-M. Flaud, private communication (2008).

#### Halfwidths (self)

**1.** J.-M. Flaud, private communication (2008).

#### Temperature dependence of air-broadened half-width

**1.** J.-M. Flaud, private communication (2008).

Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. C. Camy-Peyret, J.-M. Flaud, A. Perrin, and K.Narahari Rao, "Improved Line Parameters for the  $\nu_3$  and  $\nu_2+\nu_3 - \nu_2$  Bands of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **95**, 72-79 (1982).
2. A. Perrin, J.-M. Flaud, C. Camy-Peyret, B. Carli, and M. Carlotti, "The far infrared spectrum of  $^{14}\text{N}^{16}\text{O}_2$  Electron spin-rotation and hyperfine Fermi contact resonances in the ground state," *Mol.Phys.* **63**, 791-810 (1988).
3. A. Perrin, C. Camy-Peyret, J.-M. Flaud, and J. Kauppinen, "The  $\nu_2$  Band of  $^{14}\text{N}^{16}\text{O}_2$  - Spin-Rotation Perturbations in the (010) State," *J.Mol.Spectrosc.* **130**, 168-182 (1988).
4. A. Perrin, J.-M. Flaud, C. Camy-Peyret, A.-M. Vasserot, G. Guelachvili, A. Goldman, F.J. Murcray, and R.D. Blatherwick, "The  $\nu_1$ ,  $2\nu_2$ , and  $\nu_3$  Interacting Bands of  $^{14}\text{N}^{16}\text{O}_2$ : Line Positions and Intensities," *J.Mol.Spectrosc.* **154**, 391-406 (1992).
5. C. Camy-Peyret, J.-M. Flaud, and A. Perrin, "Improved Line Parameters for the  $\nu_3$  and  $\nu_2+\nu_3-\nu_2$  Bands of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **95**, 72-79 (1982).
6. A. Perrin, J.-M. Flaud, C. Camy-Peyret, A. Goldman, F.J. Murcray, R.D. Blatherwick, and C.P. Rinsland, "The  $\nu_2$  and  $2\nu_2-\nu_2$  bands of  $^{14}\text{N}^{16}\text{O}_2$ : Electron Spin-Rotation and Hyperfine Contact Resonances in the (010) Vibration State," *J.Mol.Spectrosc.* **160**, 456-463 (1993).
7. J.-M. Flaud, C. Camy-Peyret, V.Malathy Devi, P.P. Das, and K.Narahari Rao, "Diode Laser Spectra of the  $\nu_2$  Band of  $^{14}\text{N}^{16}\text{O}_2$ : The (010) State of NO<sub>2</sub>," *J.Mol.Spectrosc.* **84**, 234-242 (1980).
8. A. Cabana, M. Lauren, C. Pepin, and W.J. Lafferty, "High-Resolution Infrared Spectrum of the  $\nu_3$  and  $\nu_2+\nu_3-\nu_2$  Bands of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **59**, 13-27 (1976).
9. V. Dana and J.-P. Maillard, "Analysis of the  $\nu_1 + \nu_3$  Band of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **71**, 1-14 (1978).
10. A. Perrin, Université Pierre et Marie Curie, private communication (1995).
11. J.-Y. Mandin, V. Dana, A. Perrin, J.-M. Flaud, C. Camy-Peyret, L. Régalia, and A. Barbe "The  $\{\nu_1+2\nu_2, \nu_1+\nu_3\}$  bands of  $^{14}\text{N}^{16}\text{O}_2$ : line positions and intensities; line intensities in the  $\nu_1+\nu_2+\nu_3 - \nu_2$  hot band," *J.Mol.Spectrosc.* **181**, 379-388 (1997).
12. T.M. Stephen, A. Goldman, A. Perrin, J.-M. Flaud, F. Keller, and C.P. Rinsland, "New High-Resolution Analysis of the  $3\nu_3$  and  $2\nu_1 + \nu_3$  Bands of Nitrogen Dioxide (NO<sub>2</sub>) by Fourier Transform Spectroscopy," *J.Mol.Spectrosc.* **201**, 134-142 (2000).

Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. C. Camy-Peyret, J.-M. Flaud, A. Perrin, and K.Narahari Rao, "Improved Line Parameters for the  $\nu_3$  and  $\nu_2+\nu_3 - \nu_2$  Bands of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **95**, 72-79 (1982).
2. A. Perrin, J.-M. Flaud, C. Camy-Peyret, B. Carli, and M. Carlotti, "The far infrared spectrum of  $^{14}\text{N}^{16}\text{O}_2$  Electron spin-rotation and hyperfine Fermi contact resonances in the ground state," *Mol.Phys.* **63**, 791-810 (1988).
3. A. Perrin, C. Camy-Peyret, J.-M. Flaud, and J. Kauppinen, "The  $\nu_2$  Band of  $^{14}\text{N}^{16}\text{O}_2$  - Spin-Rotation Perturbations in the (010) State," *J.Mol.Spectrosc.* **130**, 168-182 (1988).

4. V. Malathy Devi, Palash P. Das, A. Bano, K. Narahari Rao, J.-M. Flaud, C. Camy-Peyret, and J.-P. Chevillard, "Diode Laser Measurements of Intensities, N<sub>2</sub>-Broadening, and Self-Broadening Coefficients of Lines of the  $\nu_2$  Band of  $^{14}\text{N}^{16}\text{O}_2$ ," *J.Mol.Spectrosc.* **88**, 251-258 (1981).
5. A. Perrin, J.-M. Flaud, C. Camy-Peyret, A.-M. Vasserot, G. Guelachvili, A. Goldman, F.J. Murcray, and R.D. Blatherwick, "The  $\nu_1$ ,  $2\nu_2$ , and  $\nu_3$  Interacting Bands of  $^{14}\text{N}^{16}\text{O}_2$ : Line Positions and Intensities," *J.Mol.Spectrosc.* **154**, 391-406 (1992).
6. A. Perrin, J.-M. Flaud, C. Camy-Peyret, A. Goldman, F.J. Murcray, R.D. Blatherwick, and C.P. Rinsland, "The  $\nu_2$  and  $2\nu_2$ - $\nu_2$  bands of  $^{14}\text{N}^{16}\text{O}_2$ : Electron Spin-Rotation and Hyperfine Contact Resonances in the (010) Vibration State," *J.Mol.Spectrosc.* **160**, 456-463 (1993).
7. J.-Y. Mandin, V. Dana, A. Perrin, J.-M. Flaud, C. Camy-Peyret, L. Régalia, and A. Barbe, "The  $\{\nu_1+2\nu_2, \nu_1+\nu_3\}$  bands of  $^{14}\text{N}^{16}\text{O}_2$ : line positions and intensities; line intensities in the  $\nu_1+\nu_2+\nu_3 - \nu_2$  hot band," *J.Mol.Spectrosc.* **181**, 379-388 (1997).
8. T.M. Stephen, A. Goldman, A. Perrin, J.-M. Flaud, F. Keller, and C.P. Rinsland, "New High-Resolution Analysis of the  $3\nu_3$  and  $2\nu_1 + \nu_3$  Bands of Nitrogen Dioxide (NO<sub>2</sub>) by Fourier Transform Spectroscopy," *J.Mol.Spectrosc.* **201**, 134-142 (2000).

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. C. Camy-Peyret, University of Paris, private communication (1990).
2. V. Dana, J.-Y. Mandin, M.-Y. Allout, A. Perrin, L. Régalia, A. Barbe, J.-J. Plateaux, and X. Thomas, "Broadening parameters of NO<sub>2</sub> lines in the 3.4 micron spectral region," *JQSRT* **57**, 445-457 (1997).
3. L.R. Brown, Jet Propulsion Laboratory, private communication (2004).
4. D.C. Benner, T.A. Blake, L.R. Brown, V.M. Devi, M.A.H. Smith, and R.A. Toth, "Air-broadened parameters in the  $\nu_3$  band of  $^{14}\text{N}^{16}\text{O}_2$  using a multispectrum fitting technique," *J.Mol.Spectrosc.* **228**, 593-619 (2004).

#### Half-widths (self)

1. A. Perrin, J.-M. Flaud, C. Camy-Peyret, D. Hurtmans, M. Herman, and G. Guelachvili, "The  $\nu_2+\nu_3$  and  $\nu_2+\nu_3 - \nu_2$  bands of  $^{14}\text{N}^{16}\text{O}_2$ : line positions and intensities," *J.Mol.Spectrosc.* **168**, 54-66 (1994).

#### Temperature dependence of air-broadened half-width

1. V. Malathy Devi, B. Fridovich, G.D. Jones, D.G.S. Snyder, P.P. Das, J.-M. Flaud, C. Camy-Peyret, and K. Narahari Rao, "Tunable diode laser spectroscopy of NO<sub>2</sub> at 6.2  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **93**, 179-195 (1982); V. Malathy Devi, B. Fridovich, G.D. Jones, D.G.S. Snyder and A. Neuendorffer, "Temperature dependence of the widths of N<sub>2</sub>-broadened lines of the  $\nu_3$  band of  $^{14}\text{N}^{16}\text{O}_2$ ," *Appl.Opt.* **21**, 1537-1538 (1982); R.D. May and C.R. Webster, "Laboratory measurements of NO<sub>2</sub> line parameters near 1600  $\text{cm}^{-1}$  for the interpretation of stratospheric spectra," *Geophys.Res.Let.* **17**, 2157-2160 (1990).
2. L.R. Brown, Jet Propulsion Laboratory, private communication (2004).
3. D.C. Benner, T.A. Blake, L.R. Brown, V.M. Devi, M.A.H. Smith, and R.A. Toth, "Air-broadened parameters in the  $\nu_3$  band of  $^{14}\text{N}^{16}\text{O}_2$  using a multispectrum fitting technique," *J.Mol.Spectrosc.* **228**, 593-619 (2004).

Pressure shift (air)

1. L.R. Brown, Jet Propulsion Laboratory, private communication (2004).
2. D.C. Benner, T.A. Blake, L.R. Brown, V.M. Devi, M.A.H. Smith, and R.A. Toth, “Air-broadened parameters in the  $\nu_3$  band of  $^{14}\text{N}^{16}\text{O}_2$  using a multispectrum fitting technique,” *J.Mol.Spectrosc.* **228**, 593-619 (2004).

## NH<sub>3</sub> [11] 4111, 5111

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. G. Guelachvili, A.H. Abdullah, N. Tu, K. Narahari Rao, Š. Urban, and D. Papoušek, "Analysis of high-resolution Fourier transform spectra of <sup>14</sup>NH<sub>3</sub> at 3.0 μm," *J. Mol. Spectrosc.* **133**, 345-364 (1989).
2. Š. Urban, N. Tu, K. Narahari Rao, and G. Guelachvili, "Analysis of high-resolution Fourier transform spectra of <sup>14</sup>NH<sub>3</sub> at 2.3 μm," *J. Mol. Spectrosc.* **133**, 312-330 (1989).
3. I. Kleiner, G. Tarrago, and L.R. Brown, "Positions and intensities in the 3  $\nu_2/\nu_2 + \nu_4$  vibrational system of <sup>14</sup>NH<sub>3</sub> near 4 micron," *J. Mol. Spectrosc.* **173**, 120-145 (1995).
4. L.R. Brown and J.S. Margolis, "Empirical line parameters of NH<sub>3</sub> from 4791 to 5294 cm<sup>-1</sup>," *JQSRT* **56**, 283-294 (1996).
5. C. Cottaz, I. Kleiner, G. Tarrago, L.R. Brown, J.S. Margolis, P.L. Poynter, H.M. Pickett, T. Fouchet, and P. Drossart, "Line positions and intensities in the 2  $\nu_2/\nu_4$  vibrational system of <sup>14</sup>NH<sub>3</sub> near 5 – 7 μm," *J. Mol. Spectrosc.* **203**, 285-309 (2000).
6. C. Cottaz, G. Tarrago, I. Kleiner, and L.R. Brown, "Assignments and intensities of <sup>14</sup>NH<sub>3</sub> hot bands in the 5-8 μm (3  $\nu_2 - \nu_2$ ,  $\nu_2 + \nu_4 - \nu_2$ ) and 4 μm (4  $\nu_2 - \nu_2$ ,  $\nu_1 - \nu_2$ ,  $\nu_3 - \nu_2$ ) regions," *J. Mol. Spectrosc.* **209**, 30-49 (2001).
7. C. Cottaz, 4-μm hot bands (thesis, U. Paris-Sud).
8. Rotational,  $\nu_2 - \nu_2$ , and  $\nu_2$ -ground state prediction via John Pearson, JPL (private communication, 2000).
9. I. Kleiner, L.R. Brown, G. Tarrago, Q.-L. Kou, N. Picque, G. Guelachvili, V. Dana, and J.-Y. Mandin, "Line positions and intensities in the vibrational system  $\nu_1$ ,  $\nu_3$  and 2  $\nu_4$  of <sup>14</sup>NH<sub>3</sub> near 3 micron," *J. Mol. Spectrosc.* **193**, 46-71 (1999).
10. Same as Ref. 9 above, but upper-state level is unassigned due to mixing from perturbations.
11. Same as Ref. 5 above, but upper-state level is unassigned due to mixing from perturbations.

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. Š. Urban and P. Pracna, unpublished results (1993).
2. Š. Urban, N. Tu, K. Narahari Rao, and G. Guelachvili, "Analysis of high-resolution Fourier transform spectra of <sup>14</sup>NH<sub>3</sub> at 2.3 μm," *J. Mol. Spectrosc.* **133**, 312-330 (1989).
3. I. Kleiner, G. Tarrago, and L.R. Brown, "Positions and intensities in the 3  $\nu_2/\nu_2 + \nu_4$  vibrational system of <sup>14</sup>NH<sub>3</sub> near 4 micron," *J. Mol. Spectrosc.* **173**, 120-145 (1995).
4. L.R. Brown and J.S. Margolis, "Empirical line parameters of NH<sub>3</sub> from 4791 to 5294 cm<sup>-1</sup>," *JQSRT* **56**, 283-294 (1996).
5. C. Cottaz, I. Kleiner, G. Tarrago, L.R. Brown, J.S. Margolis, P.L. Poynter, H.M. Pickett, T. Fouchet, P. Drossart, "Line positions and intensities in the 2 $\nu_2/\nu_4$  vibrational system of <sup>14</sup>NH<sub>3</sub> near 5 – 7 μm," *J. Mol. Spectrosc.* **203**, 285-309 (2000).
6. C. Cottaz, G. Tarrago, I. Kleiner, and L.R. Brown, "Assignments and intensities of <sup>14</sup>NH<sub>3</sub> hot bands in the 5-8 μm (3 $\nu_2 - \nu_2$ ,  $\nu_2 + \nu_4 - \nu_2$ ) and 4 μm (4 $\nu_2 - \nu_2$ ,  $\nu_1 - \nu_2$ ,  $\nu_3 - \nu_2$ ) regions," *J. Mol. Spectrosc.* **209**, 30-49 (2001).



7. C. Cottaz, 4- $\mu\text{m}$  hot bands (thesis, U.Paris-Sud).
8. Rotational,  $\nu_2$ -  $\nu_2$ , and  $\nu_2$ -ground state prediction via John Pearson, JPL (private communication, 2000).
9. I. Kleiner, L.R. Brown, G. Tarrago, Q.-L. Kou, N. Picque, G. Guelachvili, V. Dana, and J.-Y. Mandin, "Line positions and intensities in the vibrational system  $\nu_1$ ,  $\nu_3$  and  $2\nu_4$  of  $^{14}\text{NH}_3$  near 3 micron," *J.Mol.Spectrosc.* **193**, 46-71 (1999).

Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. Polynomial fit by L.R. Brown of data in A.S. Pine, V.N. Markov, G. Buffa, and O. Tarrini, "N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, Ar and He Broadening in the  $\nu_1$  Band of NH<sub>3</sub>," *JQSRT* **50**, 337-348 (1993).
2. V. Nemtchinov (thesis) SUNY, Stonybrook, NY (1998).
3. H. Arou, M. Broquier, A. Picard-Persellini, J.P. Bouanich, M. Chevaliera, and S. Gherissi, "Absorption intensities, pressure-broadening and line mixing parameters of some lines of NH<sub>3</sub> in the  $\nu_4$  band," *JQSRT* **60**, 1011-1023 (1998).

Half-widths (self)

1. L.R. Brown and D.B. Peterson, "An empirical expression for the pressure-broadening of ammonia from far infrared measurements," *J.Mol.Spectrosc.* **168**, 593-606 (1994).

Positions

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
- 1.** A. Goldman and A.G. Maki, private communication (1990): high  $J, K$  extension of A.G. Maki, "High-Resolution Measurements of the  $\nu_2$  Band of HNO<sub>3</sub> and the  $\nu_3$  Band of trans-HONO," *J. Mol. Spectrosc.* **127**, 104-111 (1988); A. Goldman, F.J. Murcray, R.D. Blatherwick, J.J. Kusters, D.G. Murcray, C.P. Rinsland, J.-M. Flaud, and C. Camy-Peyret, "Stratospheric HNO<sub>3</sub> Measurements from 0.002 cm<sup>-1</sup> Resolution Solar Occultation Spectra and Improved Spectroscopic Line Parameters in the 5.8- $\mu$ m Region," *J. Geophys. Res.* **97**, 2561-2567 (1992).
- 2.** A. Goldman,  $\nu_6$  band, private communication (1990): originally generated by A.G. Maki, based on A.G. Maki and W.B. Olson, "Infrared Spectrum of the  $\nu_6$ ,  $\nu_7$ , and  $\nu_8$  Bands of NHO<sub>3</sub>," *J. Mol. Spectrosc.* **133**, 171-181 (1989).
- 3.** A. Goldman,  $\nu_7$  band, private communication (1990): originally generated as in Ref. 2.
- 4.** A. Goldman,  $\nu_8$  band, private communication (1990): originally generated as in Ref. 2.
- 5.** A. Goldman, University of Denver, private communication (1990): based on A. Goldman, J.B. Burkholder, C.J. Howard, R. Escribano, and A.G. Maki, "Spectroscopic Constants for the  $\nu_9$  Infrared Band of HNO<sub>3</sub>," *J. Mol. Spectrosc.* **131**, 195-200 (1988).
- 6.** A. Goldman,  $\nu_8 + \nu_9$  band, private communication (1990): originally generated by A.G. Maki, based on A. Maki, "Infrared Spectrum of the 1205-cm<sup>-1</sup> Band of HNO<sub>3</sub>," *J. Mol. Spectrosc.* **136**, 105-108 (1989).
- 7.** A. Perrin, O. Lado-Bordowsky, and A. Valentin, "The  $\nu_3$  and  $\nu_4$  interacting bands of HNO<sub>3</sub> line positions and line intensities," *Mol. Phys.* **67**, 249-270 (1989).
- 8.** A. Goldman, University of Denver, private communication (1992).
- 9.** J.-C. Fontanella, A. Girard, L. Gramont, and N. Louisnard, "Vertical Distribution of NO, NO<sub>2</sub>, and HNO<sub>3</sub> as Derived from Stratospheric Absorption Infrared Spectra," *Appl. Opt.* **14**, 825-839 (1975).
- 10.** A.G. Maki and J.S. Wells, "High-Resolution Measurement and Analysis of the Infrared Spectrum of Nitric Acid near 1700 cm<sup>-1</sup>," *J. Mol. Spectrosc.* **82**, 427-434 (1980).
- 11.** A. Perrin, V. Jaouen, A. Valentin, J.-M. Flaud, and C. Camy-Peyret, "The  $\nu_5$  and  $2\nu_9$  Bands of Nitric Acid," *J. Mol. Spectrosc.* **157**, 112-121 (1993).
- 12.** A. Goldman, C.P. Rinsland, A. Perrin, and J.-M. Flaud, "HNO<sub>3</sub> Line Parameters: 1996 HITRAN Update and New Results," *JQSRT* **60**, 851-861 (1998).
- 13.** A. Perrin, "Recent Progress in the Analysis of HNO<sub>3</sub> Spectra," *Spectrochimica Acta A* **54**, 375-393 (1998).
- 14.** J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L. Coudert, J.-L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment," *Atmos. Oceanic Opt.* **16**, 172-182 (2003).
- 15.** H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
- 16.** D.T. Petkie, P. Helminger, B.P. Winnewisser, M. Winnewisser, R.A.H. Butlet, K.W. Jucks, and F.C. De Lucia, "The simulation of infrared bands from the analyses of rotational spectra: the  $2\nu_9 - \nu_9$  and  $\nu_5 - \nu_9$  hot bands of HNO<sub>3</sub>," *JQSRT* **92**, 129-141 (2005).
- 17.** J.-M. Flaud, G. Brizzi, M. Carlotti, A. Perrin, and M. Ridolfi, "MIPAS database: Validation of HNO<sub>3</sub> line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6**,

4251-4272 (2006).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A. Goldman and A.G. Maki, private communication (1990): high  $J, K$  extension of A.G. Maki, "High-Resolution Measurements of the  $\nu_2$  Band of  $\text{HNO}_3$  and the  $\nu_3$  Band of trans- $\text{HONO}$ ," *J.Mol.Spectrosc.* **127**, 104-111 (1988); A. Goldman, F.J. Murcray, R.D. Blatherwick, J.J. Kusters, D.G. Murcray, C.P. Rinsland, J.-M. Flaud, and C. Camy-Peyret, "Stratospheric  $\text{HNO}_3$  Measurements from 0.002  $\text{cm}^{-1}$  Resolution Solar Occultation Spectra and Improved Spectroscopic Line Parameters in the 5.8- $\mu\text{m}$  Region," *J.Geophys.Res.* **97**, 2561-2567 (1992).
2. A. Goldman,  $\nu_6$  band, private communication (1990): originally generated by A.G. Maki, based on A.G. Maki and W.B. Olson, "Infrared Spectrum of the  $\nu_6$ ,  $\nu_7$ , and  $\nu_8$  Bands of  $\text{HNO}_3$ ," *J.Mol.Spectrosc.* **133**, 171-181 (1989).
3. A. Goldman,  $\nu_7$  band, private communication (1990): originally generated as in Ref. 2.
4. A. Goldman,  $\nu_8$  band, private communication (1990): originally generated as in Ref. 2.
5. A. Goldman, University of Denver, private communication (1990): based on A. Goldman, J.B. Burkholder, C.J. Howard, R. Escribano, and A.G. Maki, "Spectroscopic Constants for the  $\nu_9$  Infrared Band of  $\text{HNO}_3$ ," *J.Mol.Spectrosc.* **131**, 195-200 (1988).
6. A. Goldman,  $\nu_8 + \nu_9$  band, private communication (1990): originally generated by A.G. Maki, based on A. Maki, "Infrared Spectrum of the 1205- $\text{cm}^{-1}$  Band of  $\text{HNO}_3$ ," *J.Mol.Spectrosc.* **136**, 105-108 (1989).
7. A. Perrin, O. Lado-Bordowsky, and A. Valentin, "The  $\nu_3$  and  $\nu_4$  interacting bands of  $\text{HNO}_3$  line positions and line intensities," *Mol.Phys.* **67**, 249-270 (1989).
8. Blended lines from Ref. 7.
9. A. Perrin, V. Jaouen, A. Valentin, J.-M. Flaud, and C. Camy-Peyret, "The  $\nu_5$  and  $2\nu_9$  Bands of Nitric Acid," *J.Mol.Spectrosc.* **157**, 112-121 (1993).
10. A. Perrin, J.-M. Flaud, C. Camy-Peyret, V. Jaouen, R. Farrenq, G. Guelachvili, Q. Kou, F. LeRoy, M. Morillon-Chapey, J. Orphal, M. Badaoui, J.-Y. Mandin, and V. Dana, "Line Intensities in the 11- and 7.6- $\mu\text{m}$  Bands of  $\text{HNO}_3$ ," *J.Mol.Spectrosc.* **160**, 524-539 (1993).
11. A. Goldman, C.P. Rinsland, A. Perrin, and J.-M. Flaud, " $\text{HNO}_3$  Line Parameters: 1996 HITRAN Update and New Results," *JQSRT* **60**, 851-861 (1998).
12. J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L. Coudert, J.-L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) experiment," *Atmos.Oceanic Opt.* **16**, 172-182 (2003).
13. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
14. D.T. Petkie, P. Helminger, B.P. Winnemisser, M. Winnemisser, R.A.H. Butlet, K.W. Jucks, and F.C. De Lucia, "The simulation of infrared bands from the analyses of rotational spectra: the  $2\nu_9 - \nu_9$  and  $\nu_5 - \nu_9$  hot bands of  $\text{HNO}_3$ ," *JQSRT* **92**, 129-141 (2005).
15. Intensities have been rescaled by multiplying by a factor of 1.067, Ref. 7
16. Intensities have been rescaled by multiplying by a factor of 1.067, Ref. 8
17. J.-M. Flaud, G. Brizzi, M. Carlotti, A. Perrin, and M. Ridolfi, "MIPAS database: Validation of  $\text{HNO}_3$  line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6**, 4251-4272 (2006).

#### Half-widths (air)

1. R.D. May and C.R. Webster, "Measurements of the Line Positions, Intensities, and Collisional Air-broadening Coefficients in the HNO<sub>3</sub> 7.5- $\mu$ m Band Using a Computer-controlled Tunable Diode Laser Spectrometer," *J.Mol.Spectrosc.* **138**, 383-397 (1989).
2. J.-M. Flaud, G. Brizzi, M. Carlotti, A. Perrin, and M. Ridolfi, "MIPAS database: Validation of HNO<sub>3</sub> line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6**, 4251-4272 (2006).

#### Half-widths (self)

1. Set to a constant value of 0.8 cm<sup>-1</sup>/atm based on the works of L. Zu, P.A. Hamilton, and P.B. Davies, "Pressure broadening and frequency measurements of nitric acid lines in the 683 GHz region," *JQSRT* **73**, 545-556 (2002) and P. Brockman, C.H. Bair, and F. Allario, "High resolution spectral measurement of the HNO<sub>3</sub> 11.3- $\mu$ m band using tunable diode lasers," *Appl.Opt.* **17**, 91-99 (1978).
2. J.-M. Flaud, G. Brizzi, M. Carlotti, A. Perrin, and M. Ridolfi, "MIPAS database: Validation of HNO<sub>3</sub> line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6**, 4251-4272 (2006).

#### Temperature dependence of air-broadened half-width

1. J.-M. Flaud, G. Brizzi, M. Carlotti, A. Perrin, and M. Ridolfi, "MIPAS database: Validation of HNO<sub>3</sub> line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6**, 4251-4272 (2006).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. A. Goldman, W.G. Schoenfeld, D. Goorvitch, C. Chackerian, Jr, H. Dothe, F. Mélen, M.C. Abrams, and J.E.A. Selby, "Updated Line Parameters for OH  $X^2\Pi - X^2\Pi$  ( $v'', v'$ ) Transitions," *JQSRT* **59**, 453-469 (1998).
3. J.R. Gillis, A. Goldman, G. Stark, and C.P. Rinsland, "Line Parameters for the  $A^2\Sigma^+ - X^2\Pi$  Bands of OH," *JQSRT* **68**, 225-230 (2000).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
5. Line positions generated by A. Goldman from the term values obtained through analyses of the solar emission spectrum by R. Colin and P. Bernath (2008).
6. Line positions calculated using constants from P.F. Bernath and R. Colin, "Revised molecular constants and term values for the  $X^2\Pi_i$  and  $B^2\Sigma^+$  states of OH," *J.Mol.Spectrosc.* **257**, 20-23 (2009).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. A. Goldman, W.G. Schoenfeld, D. Goorvitch, C. Chackerian, Jr, H. Dothe, F. Mélen, M.C. Abrams, and J.E.A. Selby, "Updated Line Parameters for OH  $X^2\Pi - X^2\Pi$  ( $v'', v'$ ) Transitions," *JQSRT* **59**, 453-469 (1998).
3. J.R. Gillis, A. Goldman, G. Stark, and C.P. Rinsland, "Line Parameters for the  $A^2\Sigma^+ - X^2\Pi$  Bands of OH," *JQSRT* **68**, 225-230 (2000).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A. Schiffman and D.J. Nesbitt, "Pressure Broadening and Collisional Narrowing in OH ( $v=1-0$ ) rovibrational transitions with Ar, He, O<sub>2</sub>, and N<sub>2</sub>," *J.Chem.Phys.* **100**, 2677-2689 (1994); values are reduced by 10% to make consistent with measured values at Smithsonian Astrophysical Observatory at 118 and 61 cm<sup>-1</sup>.
2. K.V. Chance, D.A. Jennings, K.M. Evenson, M.D. Vanek, I.G. Nolt, J.V. Radostitz, and K. Park, "Pressure Broadening of the 118.455 cm<sup>-1</sup> Rotational Lines of OH by H<sub>2</sub>, He, N<sub>2</sub>, and O<sub>2</sub>," *J.Mol.Spectrosc.* **146**, 375-380 (1991); K. Park, L.R. Zinc, K.M. Evenson, K.V. Chance, and I.G. Nolt, "Pressure Broadening of the 83.869 cm<sup>-1</sup> Rotational Lines of OH by N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, and He," *JQSRT* **55**, 285-287 (1996); A. Schiffman and D.J. Nesbitt, "Pressure Broadening and



Collisional Narrowing in OH ( $v=1-0$ ) rovibrational transitions with Ar, He, O<sub>2</sub>, and N<sub>2</sub>,” *J.Chem.Phys.* **100**, 2677-2689 (1994) - values reduced by 10% to make consistent with measured values at Smithsonian Astrophysical Observatory at 118 and 61 cm<sup>-1</sup>.

**3.** J.R. Gillis, A. Goldman, G. Stark, and C.P. Rinsland, “Line Parameters for the  $A^2\Sigma^+ - X^2\Pi$  Bands of OH,” *JQSRT* **68**, 225-230 (2000).

Temperature dependence of air-broadened half-width

**1.** A. Goldman, W.G. Schoenfeld, D. Goorvitch, C. Chackerian, Jr, H. Dothe, F. Mélen, M.C. Abrams, and J.E.A. Selby, “Updated Line Parameters for OH  $X^2\Pi - X^2\Pi$  ( $v'',v'$ ) Transitions,” *JQSRT* **59**, 453-469 (1998).

## HF [14] 19

### Positions

1. D.A. Jennings, K.M. Evenson, L.R. Zink, C. Demuynck, J.L. Destombes, B. Lemoine, and J.W.C. Johns, "High-Resolution Spectroscopy of HF from 40 to 1100  $\text{cm}^{-1}$ : Highly Accurate Rotational Constants," *J.Mol.Spectrosc.* **122**, 477-480 (1987); ( $\Delta v = 0$ ).
2. G. Guelachvili, "Absolute Wavenumber Measurements of 1-0, 2-0, HF and 2-0,  $\text{H}^{35}\text{Cl}$ ,  $\text{H}^{37}\text{Cl}$  Absorption Bands," *Opt.Comm.* **19**, 150 (1976); ( $\Delta v = 1, 2, \dots$ ).
3. Difference
4. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

### Intensities

1. R.H. Tipping, "Calculation of Spectroscopic Parameters for Diatomic Molecules of Atmospheric Interest," Final Report GL-TR-90-0127, Geophysics Laboratory (1990).
2. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

### Half-widths (air)

1. G. Bachet, *C. R. Acad. Sci. Paris* **274**, 1319 (1972); G. Bachet, "Etude sur les Elargissements par des Gaz Etrangers Comprimés des Raies du Spectre de Rotation Pure de la Molécule HF-II. Perturbation par les Molécules Linéaires Homopolaires," *JQSRT* **14**, 1285 (1974); ( $\Delta v = 0$ ).
2. A.S. Pine and J.P. Looney, " $\text{N}_2$  and Air Broadening in the Fundamental Bands of HF and HCl," *J.Mol.Spectrosc.* **122**, 41-55 (1987); ( $\Delta v = 1$ ).
3. R.E. Meredith and F.G. Smith, "Broadening of hydrogen fluoride lines by  $\text{H}_2$ ,  $\text{D}_2$ , and  $\text{N}_2$ ," *J.Chem.Phys.* **60**, 3388 (1974); overtone bands, measured at  $T=373$  K for  $\text{N}_2$ ; scaled to  $T=296$  K using  $n = 0.5$  and to air by  $\gamma_{\text{air}} = 0.9 \gamma_{\text{N}_2}$ .
4. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

## HCl [15] 15, 17

### Positions

1. J.A. Coxon and J.F. Ogilvie, "Precise potential-energy function for the  $X^1\Sigma^+$  state of hydrogen chloride," *J.Chem.Soc.Faraday Trans. II* **78**, 1345-1362 (1982).
2. G. Guelachvili, "Absolute Wavenumber Measurements of 1-0, 2-0, HF and 2-0,  $H^{35}Cl$ ,  $H^{37}Cl$  Absorption Bands," *Opt.Comm.* **19**, 150 (1976); ( $\Delta v = 1, 2, \dots$ ).
3. Clayton, thesis (1977).
4. Difference
5. D.U. Webb and K.Narahari Rao, "A Heated Absorption Cell for Studying Infrared Absorption Bands," *Appl.Opt.* **5**, 1461-1463 (1966).
6. I.G. Nolt, J.V. Radostitz, G. DiLonardo, K.M. Evenson, D.A. Jennings, K.R. Leopold, M.D. Vanek, L.R. Zink, A. Hinz, and K.V. Chance, "Accurate rotational constants of CO, HCl, and HF: Spectral standards for the 0.3 to 6 THz (10 to 200  $cm^{-1}$ ) region," *J.Mol.Spectrosc.* **125**, 274-287 (1987).
7. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
8. I.E. Gordon predictions using constants from J.A. Coxon and P.G. Hajigeorgiou, "The Radial Hamiltonians for the  $X^1\Sigma^+$  and  $B^1\Sigma^+$  States of HCl," *J.Mol.Spectrosc.* **203**, 49-64 (2000).

### Intensities

1. R.H. Tipping, "Calculation of Spectroscopic Parameters for Diatomic Molecules of Atmospheric Interest," Final Report GL-TR-90-0127, Geophysics Laboratory (1990).
2. E.W. Kaiser, "Dipole Moment and Hyperfine Parameters of  $H^{35}Cl$  and  $D^{35}Cl$ ," *J.Chem.Phys.* **53**, 1686-1703 (1970); data include a correction factor for partition sums.
3. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

### Half-widths (air)

1. A.S. Pine and J.P. Looney, " $N_2$  and Air Broadening in the Fundamental Bands of HF and HCl," *J.Mol.Spectrosc.* **122**, 41-55 (1987).

### Half-widths (self)

1. A.S. Pine and A. Fried, "Self-broadening in the Fundamental Bands of HF and HCl," *J.Mol.Spectrosc.* **114**, 148-162 (1985).

### Temperature dependence of air-broadened half-width

1. A.S. Pine and J.P. Looney, " $N_2$  and Air Broadening in the Fundamental Bands of HF and HCl," *J.Mol.Spectrosc.* **122**, 41-55 (1987).

### Pressure shift (air)

1. A.S. Pine and J.P. Looney, " $N_2$  and Air Broadening in the Fundamental Bands of HF and HCl," *J.Mol.Spectrosc.* **122**, 41-55 (1987).

## HBr [16] 19, 11

### Positions

1. P. Bernage and P. Niay, "High-Resolution Measurements on the Infrared Absorption 5-0 Band of Deuterium Bromide," *J.Mol.Spectrosc.* **63**, 317-321 (1976); P. Bernage, thesis, University of Lille (1976).
2. P. Niay, P. Bernage, C. Coquant, and A. Fayt, "Détermination directe des coefficients du potentiel de Dunham par une méthode de moindres carrés non linéaire appliquée aux nombres d'ondes des raies. Application au cas de la molécule HBr," *Can.J.Phys.* **55**, 1829-1834 (1977).
3. Difference
4. G. DiLonardo, L. Fusina, P. DeNatale, M. Inguscio, and M. Prevedelli, "The Pure Rotation Spectrum of HBr in the Submillimeter-Wave Region," *J.Mol.Spectrosc.* **148**, 86-92 (1991).
5. M.T. Coffey, A. Goldman, J.W. Hannigan, W.G. Mankin, W.G. Schoenfeld, C.P. Rinsland, C. Bernardo, and D.W.T. Griffith, "Improved vibration-rotation (0-1) HBr line parameters for validating high resolution infrared atmospheric spectra measurements," *JQSRT* **60**, 863-867 (1998); A. Goldman, M.T. Coffey, J.W. Hannigan, W.G. Mankin, K. Chance, and C.P. Rinsland, "HBr and HI line parameters update for atmospheric spectroscopy databases," *JQSRT* **82**, 313-318 (2003).

### Intensities

1. C.B. Carlisle, H. Riris, L.G. Wang, G.R. Janik, T.F. Gallagher, A. Lopez Pineiro, and R.H. Tipping, "Measurement of High Overtone Intensities of HBr by Two-Tone Frequency-Modulation Spectroscopy," *J.Mol.Spectrosc.* **130**, 395-406 (1988).
2. M.T. Coffey, A. Goldman, J.W. Hannigan, W.G. Mankin, W.G. Schoenfeld, C.P. Rinsland, C. Bernardo, and D.W.T. Griffith, "Improved vibration-rotation (0-1) HBr line parameters for validating high resolution infrared atmospheric spectra measurements," *JQSRT* **60**, 863-867 (1998); A. Goldman, M.T. Coffey, J.W. Hannigan, W.G. Mankin, K. Chance, and C.P. Rinsland, "HBr and HI line parameters update for atmospheric spectroscopy databases," *JQSRT* **82**, 313-318 (2003).

### Half-widths (air)

1. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).

## HI [17] 17

### Positions

1. G. Guelachvili, P. Niay, and P. Bernage, "Fourier Transform High-Resolution Measurements on the  $2\leftarrow 0$ ,  $3\leftarrow 0$ ,  $4\leftarrow 0$ ,  $5\leftarrow 0$  Infrared Absorption Bands of HI and DI," *J.Mol.Spectrosc.* **85**, 253-270 (1981).
2. Difference
3. A. Goldman, K. Chance, M.T. Coffey, J.W. Hannigan, W.G. Mankin, C.P. Rinsland, "Improved line parameters for the  $X^1\Sigma^+$  (0-0) and (0-1) bands of HI," *JQSRT* **60**, 869-874 (1998); A. Goldman, M.T. Coffey, J.W. Hannigan, W.G. Mankin, K. Chance, and C.P. Rinsland, "HBr and HI line parameters update for atmospheric spectroscopy databases," *JQSRT* **82**, 313-317 (2003).

### Intensities

1. H. Riris, C.B. Carlisle, D.E. Cooper, L-G. Wang, T.F. Gallagher, and R.H. Tipping, "Measurement of the Strengths of  $1\leftarrow 0$  and  $3\leftarrow 0$  Transitions of HI Using Frequency Modulation Spectroscopy," *J.Mol.Spectrosc.* **146**, 381-388 (1991).
2. A. Goldman, K. Chance, M.T. Coffey, J.W. Hannigan, W.G. Mankin, C.P. Rinsland, "Improved line parameters for the  $X^1\Sigma^+$  (0-0) and (0-1) bands of HI," *JQSRT* **60**, 869-874 (1998); A. Goldman, M.T. Coffey, J.W. Hannigan, W.G. Mankin, K. Chance, and C.P. Rinsland, "HBr and HI line parameters update for atmospheric spectroscopy databases," *JQSRT* **82**, 313-317 (2003).

### Half-widths (air)

1. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).



### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.B. Burkholder, P.D. Hammer, C.J. Howard, A.G. Maki, G. Thompson and C. Chackerian Jr., "Infrared Measurements of the ClO Radical," *J.Mol.Spectrosc.* **124**, 139-161 (1987); A.Goldman, J.R. Gillis, C.P. Rinsland, and J.B. Burkholder, "Improved Line Parameters for the  $X^2\Pi$ - $X^2\Pi$  (1-0) Bands of  $^{35}\text{ClO}$  and  $^{37}\text{ClO}$ ," *JQSRT* **52**, 357-359 (1994).
2. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.B. Burkholder, P.D. Hammer, C.J. Howard, and A. Goldman, "Infrared Line Intensity Measurements in the  $\nu = 0-1$  Band of the ClO Radical," *J.Geophys.Res.* **94**, 2225-2234 (1989); A. Goldman, J.R. Gillis, C.P. Rinsland, and J.B. Burkholder, "Improved Line Parameters for the  $X^2\Pi$ - $^2\Pi$ (1-0) Bands of  $^{35}\text{ClO}$  and  $^{37}\text{ClO}$ ," *JQSRT* **52**, 357-359 (1994).
2. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.B. Burkholder, P.D. Hammer, C.J. Howard, and A. Goldman, "Infrared Line Intensity Measurements in the  $\nu = 0-1$  Band of the ClO Radical," *J.Geophys.Res.* **94**, 2225-2234 (1989); A. Goldman, J.R. Gillis, C.P. Rinsland, and J.B. Burkholder, "Improved Line Parameters for the  $X^2\Pi$ - $^2\Pi$ (1-0) Bands of  $^{35}\text{ClO}$  and  $^{37}\text{ClO}$ ," *JQSRT* **52**, 357-359 (1994).
2. A coarse approximation for transitions with  $J'' < 20.5$  based on the linear fit to three measurements from J.J. Oh and E.A. Cohen, "Pressure broadening of ClO by  $\text{N}_2$  and  $\text{O}_2$  near 204 and 649 GHz and new frequency measurements between 632 and 725 GHz," *JQSRT* **52**, 151-156 (1994), and A. Bauer, M. Birk, G. Wagner, J.-M. Colmont, D. Priem, G. Wlodarczak, S. Buehler, A. Von Engeln, K. Kunzi, and A. Perrin, "Study on a spectroscopic database for millimeter and submillimeter wavelength," *Final report of ESA No 11581/95/NL/CN* (1998).

### Temperature dependence of air-broadened halfwidth

1. A coarse approximation for transitions with  $J'' < 20.5$  based on the linear fit to three measurements from J.J. Oh and E.A. Cohen, "Pressure broadening of ClO by  $\text{N}_2$  and  $\text{O}_2$  near 204 and 649 GHz and new frequency measurements between 632 and 725 GHz," *JQSRT* **52**, 151-156 (1994), and A. Bauer, M. Birk, G. Wagner, J.-M. Colmont, D. Priem, G. Wlodarczak, S. Buehler, A. Von Engeln, K. Kunzi, and A. Perrin, "Study on a spectroscopic database for millimeter and submillimeter wavelength," *Final report of ESA No 11581/95/NL/CN* (1998).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.S. Wells, F.R. Petersen, A.G. Maki, and D.J. Sukle, "Heterodyne frequency measurements on the 11.6- $\mu\text{m}$  band of OCS: new frequency/wavelength calibration tables for 11.6- and 5.8- $\mu\text{m}$  OCS bands," *Appl. Opt.* **20**, 1676-1684 (1981).
2. G. Guelachvili, "Nombres d'ondes absolus de la bande  $\nu_3$  de  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  par spectroscopie de Fourier," *Opt. Comm.* **30**, 361-363 (1979).
3. A.G. Maki and J.S. Wells, "Wavenumber Calibration Tables from Heterodyne Frequency Measurements" NIST Special Publication 821 (1991).
4. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).
5. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).
6. T.L. Tan, E.C. Looi, and K.K. Lee, "Hot-Band Spectrum of  $\text{CO}_2$  near  $700\text{ cm}^{-1}$  and the  $\nu_1$  Band of  $\text{OC}^{34}\text{S}$ ," *J.Mol.Spectrosc.* **157**, 261-267 (1993).
7. M. Mürztz, P. Palm, W. Urban, and A.G. Maki, "More Sub-Doppler Heterodyne Frequency Measurements on OCS between 56 and 63 THz," *J.Mol.Spectrosc.* **204**, 281-285 (2000).
8. Line positions calculated by L.R. Brown (2008) based on spectroscopic constants reported in S. Naïm, A. Fayt, H. Bredohl, J.F. Blavier, and I. Dubois, "Fourier Transform Spectroscopy of Carbonyl Sulfide from 3700 to  $4800\text{ cm}^{-1}$  and Selection of a Line-Pointing Program," *J.Mol.Spectrosc.* **192**, 91-101 (1998) and references therein.
9. H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists," *J.Mol.Struct.* **742**, 215-227 (2005).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. G. Blanquet, J. Walrand, I. Hilgers, and D. Lambot, "Spectral Intensities in the  $\nu_1$  Band of Carbonyl Sulfide and its Isotopic Species," *J.Mol.Spectrosc.* **140**, 295-300 (1990).
2. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana,

V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).

3. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).

4. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).

5. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).

6. L.R. Brown/A. Fayt, private communication (1997), for details see L.S. Rothman, A. Barbe, D.Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, and K. Yoshino, "The HITRAN Molecular Spectroscopic Database: Edition of 2000 Including Updates through 2001," *JQSRT* **82**, 5-44 (2003).

7. D. Bermejo, J.L. Domenech, J. Santos, J.-P. Bouanich, and G. Blanquet, "Absolute Line Intensities in the  $2\nu_3$  Band of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ ," *J.Mol.Spectrosc.* **185**, 26-30 (1997).

8. Based on an average value between L. Régalia-Jarlot, A. Hamdouni, X. Thomas, P. Von der Heyden, and A. Barbe, "Line Intensities of the:  $\nu_3$ ,  $4\nu_2$ ,  $\nu_1 + \nu_3$ ,  $3\nu_1$  and  $2\nu_1 + 2\nu_2$  bands of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  molecule," *JQSRT* **74**, 455-470 (2002) and J. Vander Auwera, R. El Hachtouki, K. Amara, and A. Fayt, "Absolute Line Intensities for Carbonyl Sulfide near  $4.85\ \mu\text{m}$ ," Poster D23, Proceedings of the Eighteenth Colloquium on High Resolution Molecular Spectroscopy, Dijon, France, 8-12 Sept. 2003.

9. L. Régalia-Jarlot, A. Hamdouni, X. Thomas, P. Von der Heyden, and A. Barbe, "Line Intensities of the:  $\nu_3$ ,  $4\nu_2$ ,  $\nu_1 + \nu_3$ ,  $3\nu_1$  and  $2\nu_1 + 2\nu_2$  bands of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  molecule," *JQSRT* **74**, 455-470 (2002).

10. J. Vander Auwera and A. Fayt, "Absolute line intensities for carbonyl sulfide from 827 to  $2939\ \text{cm}^{-1}$ ," *J.Mol.Struct.* **780-781**, 134-141 (2006).

11. K. Sung, R.A. Toth, L.R. Brown, and T. Crawford, "Line strength measurements of carbonyl

sulfide ( $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ ) in the  $2\nu_3$ ,  $\nu_1+2\nu_2+\nu_3$ , and  $4\nu_2+\nu_3$  bands,” *JQSRT* **110**, 2082-2101 (2009).

**12.** R.A. Toth, K. Sung, L.R. Brown, and T. Crawford, “Line positions and strengths of 41 bands including 10 OCS isotopologues in the 3850-4200  $\text{cm}^{-1}$  region,” *JQSRT* **111**, 1193–1208 (2010).

**13.** H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, “The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists,” *J.Mol.Struct.* **742**, 215-227 (2005).

#### Half-widths (air)

- 0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, “The HITRAN database: 1986 Edition,” *Appl.Opt.* **26**, 4058-4097 (1987).
- 1.** Polynomial fit by C.P. Rinsland to the data of: J.-P. Bouanich, J. Walrand, S. Albery, and G. Blanquet, “Diode-Laser Measurements of Oxygen-Broadened Linewidths in the  $\nu_1$  Band of OCS,” *J.Mol.Spectrosc.* **123**, 37-47 (1987).
- 2.** A. Mouchet, G. Blanquet, P. Herbin, J. Walrand, C.P. Courtoy, and J.P. Bouanich “Diode Laser Measurements of  $\text{N}_2$ -Broadened line widths in the  $\nu_1$  Band of OCS,” *Can.J.Phys.* **63**, 527-531 (1985); J.P. Bouanich, G. Blanquet, J. Walrand, and C.P. Courtoy, “Diode Laser Measurements of Line Strengths and Collisional halfwidths in the  $\nu_1$  Band of OCS at 298K and 200K,” *JQSRT* **36**, 295-306 (1986); J.P. Bouanich, J. Walrand, S. Albery, and G. Blanquet, “Diode Laser Measurements of Oxygen-Broadened line widths in the  $\nu_1$  Band of OCS,” *J.Mol.Spectrosc.* **123**, 37-47 (1987); J.C. Depannemaecker and J. Lemaire, “Measurement with a Double-Beam Spectrometer of Strengths and Half-widths of  $2\nu_2$  and  $3\nu_2-\nu_2$  OCS Lines,” *J.Mol.Spectrosc.* **128**, 350-359 (1988).
- 3.** L.R. Brown/A. Fayt, private communication (1997), based on Ref. 2 above.
- 4.** M.A. Koshelev and M.Y. Tretyakov, “Collisional broadening and shifting of OCS rotational spectrum lines,” *JQSRT* **110**, 118-128 (2009).

#### Half-widths (self)

- 1.** J.P. Bouanich, G. Blanquet, J. Walrand, and C.P. Courtoy, “Diode Laser Measurements of Line Strengths and Collisional halfwidths in the  $\nu_1$  Band of OCS at 298K and 200K,” *JQSRT* **36**, 295-306 (1986).
- 2.** S. Matton, F. Rohart, R. Bocquet, G. Mouret, D. Bigourd, A. Cuisset, and F. Hindle, “Terahertz spectroscopy applied to the measurement of strengths and self-broadening coefficients for high-J lines of OCS,” *J.Mol.Spectrosc.* **239**, 182-189 (2006).
- 3.** M.A. Koshelev and M.Y. Tretyakov, “Collisional broadening and shifting of OCS rotational spectrum lines,” *JQSRT* **110**, 118-128 (2009).

#### Temperature dependence of air-broadened half-width

- 1.** J.P. Bouanich, G. Blanquet, J. Walrand, and C.P. Courtoy, “Diode Laser Measurements of Line Strengths and Collisional halfwidths in the  $\nu_1$  Band of OCS at 298K and 200K,” *JQSRT* **36**, 295-306 (1986).

## **H<sub>2</sub>CO [20] 126, 136, 128**

### Positions

- 0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
- 1. L.R. Brown, R.H. Hunt, and A.S. Pine, "Wavenumbers, Line Strengths, and Assignments in the Doppler-Limited Spectrum of Formaldehyde from 2700 to 3000 cm<sup>-1</sup>," *J.Mol.Spectrosc.* **75**, 406-428 (1979).
- 2. L.R. Brown, Jet Propulsion Laboratory, private communication.
- 3. A. Perrin, D. Jacquemart, F. Kwabia Tchana, and N. Lacome, "Absolute line intensities measurements and calculations for the 5.7 and 3.6  $\mu$ m bands of formaldehyde," *JQSRT* **110**, 700-716 (2009).

### Intensities

- 0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
- 1. A. Perrin, D. Jacquemart, F. Kwabia Tchana, and N. Lacome, "Absolute line intensities measurements and calculations for the 5.7 and 3.6  $\mu$ m bands of formaldehyde," *JQSRT* **110**, 700-716 (2009).

### Half-widths (air)

- 0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
- 1. A. Perrin, D. Jacquemart, F. Kwabia Tchana, and N. Lacome, "Absolute line intensities measurements and calculations for the 5.7 and 3.6  $\mu$ m bands of formaldehyde," *JQSRT* **110**, 700-716 (2009).

### Temperature dependence of air-broadened half-width

- 1. A. Perrin, D. Jacquemart, F. Kwabia Tchana, and N. Lacome, "Absolute line intensities measurements and calculations for the 5.7 and 3.6  $\mu$ m bands of formaldehyde," *JQSRT* **110**, 700-716 (2009).



## HOCl [21] 165, 167

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.S. Wells, R.L. Sams, and W.J. Lafferty, "The High Resolution Infrared Spectrum of the  $\nu_1$  Band of HOCl," *J.Mol.Spectrosc.* **77**, 349-364 (1979).
2. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
3. J.-M. Flaud, M. Birk, G. Wagner, J. Orphal, S. Klee, and W.J. Lafferty, "The Far-Infrared Spectrum of HOCl: Line Positions and Intensities," *J.Mol.Spectrosc.* **191**, 362-367 (1998).
4. W.J. Lafferty and W.B. Olson, "The High-resolution Infrared Spectra of the  $\nu_2$  and  $\nu_3$  Bands of HOCl," *J.Mol.Spectrosc.* **120**, 359-373 (1986).
5. J. Vander Auwera, J. Kleffmann, J.-M. Flaud, G. Pawelke, H. Buerger, D. Hurtmans, and R. Petrisse, "Absolute  $\nu_2$  Line Intensities of HOCl by Simultaneous Measurements in the Infrared with a Tunable Diode Laser and Far-Infrared Region Using a Fourier Transform Spectrometer," *J.Mol.Spectrosc.* **204**, 36-47 (2000).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. J.-M. Flaud, M. Birk, G. Wagner, J. Orphal, S. Klee, and W.J. Lafferty, "The Far-Infrared Spectrum of HOCl: Line Positions and Intensities," *J.Mol.Spectrosc.* **191**, 362-367 (1998).
3. J. Vander Auwera, J. Kleffmann, J.-M. Flaud, G. Pawelke, H. Buerger, D. Hurtmans, and R. Petrisse, "Absolute  $\nu_2$  Line Intensities of HOCl by Simultaneous Measurements in the Infrared with a Tunable Diode Laser and Far-Infrared Region Using a Fourier Transform Spectrometer," *J.Mol.Spectrosc.* **204**, 36-47 (2000).

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).
2. J. H. Shorter, D. D. Nelson, and M. S. Zahniser, "Air-broadened linewidth measurements in the  $\nu_2$  vibrational band of HOCl," *J.Chem.Soc., Faraday Trans.* **93**, 2933-2935 (1997) measured the air-broadening for two lines in the  $\nu_2$  band. The average of about  $0.1 \text{ cm}^{-1}/\text{atm}$  was used as a default for this band.

### Temperature dependence of air-broadened half-width

1. K. Chance and L.S. Rothman, private communication (2000).

### Positions

1. C.P. Rinsland, R. Zander, A. Goldman, F.J. Murcray, D.G. Murcray, M.R. Gunson, and C.B. Farmer, "The Fundamental Quadrupole Band of <sup>14</sup>N<sub>2</sub>: Line Positions from High-Resolution Stratospheric Solar Absorption Spectra," *J.Mol.Spectrosc.* **148**, 274-279 (1991).
2. C.P. Rinsland, A. Goldman, and J.-M. Flaud, "Infrared Spectroscopic Parameters of COF<sub>2</sub>, SF<sub>6</sub>, ClO, N<sub>2</sub>, and O<sub>2</sub>," *JQSRT* **48**, 693-699 (1992).
3. A. Goldman, University of Denver, private communication (2008) based on A. Goldman, R.H. Tipping, Q. Ma, C.D. Boone, P.F. Bernath, Ph. Demoulin, F. Hase, M. Schneider, J.W. Hannigan, M.T. Coffey, and C.P. Rinsland, "On the line parameters for the  $X^1\Sigma_g^+$  (1-0) infrared quadrupolar transitions of <sup>14</sup>N<sub>2</sub>," *JQSRT* **103**, 168-174 (2007).

### Intensities

1. Ph. Demoulin, C.B. Farmer, C.P. Rinsland, and R. Zander, "Determination of Absolute Strengths of N<sub>2</sub> Quadrupole Lines from High-Resolution Ground-Based IR Solar Observations," *J.Geophys.Res.* **96**, 13003-13008 (1990); HITRAN'86 values scaled by 1.049.
2. H. Li, and R.J. LeRoy, "Quadrupole moment function and absolute infrared quadrupolar intensities for N<sub>2</sub>," *J.Chem.Phys.* **126**, 224301 (2007).

### Half-widths (air)

1. C.P. Rinsland, NASA Langley Research Center, unpublished data.
2. A. Goldman, University of Denver, private communication (2008) based on A. Goldman, R.H. Tipping, Q. Ma, C.D. Boone, P.F. Bernath, Ph. Demoulin, F. Hase, M. Schneider, J.W. Hannigan, M.T. Coffey, and C.P. Rinsland, "On the line parameters for the  $X^1\Sigma_g^+$  (1-0) infrared quadrupolar transitions of <sup>14</sup>N<sub>2</sub>," *JQSRT* **103**, 168-174 (2007).

### Halfwidths (self)

1. A. Goldman, University of Denver, private communication (2008) based on A. Goldman, R.H. Tipping, Q. Ma, C.D. Boone, P.F. Bernath, Ph. Demoulin, F. Hase, M. Schneider, J.W. Hannigan, M.T. Coffey, and C.P. Rinsland, "On the line parameters for the  $X^1\Sigma_g^+$  (1-0) infrared quadrupolar transitions of <sup>14</sup>N<sub>2</sub>," *JQSRT* **103**, 168-174 (2007).

### Temperature dependence of air-broadened half-width

1. A. Goldman, University of Denver, private communication (2008) based on A. Goldman, R.H. Tipping, Q. Ma, C.D. Boone, P.F. Bernath, Ph. Demoulin, F. Hase, M. Schneider, J.W. Hannigan, M.T. Coffey, and C.P. Rinsland, "On the line parameters for the  $X^1\Sigma_g^+$  (1-0) infrared quadrupolar transitions of <sup>14</sup>N<sub>2</sub>," *JQSRT* **103**, 168-174 (2007).

## HCN [23] 124, 134, 125

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. P.K.L. Yin and K.Narahari Rao, "Bands of HCN at  $14\mu$ ," *J.Mol.Spectrosc.* **42**, 385-392 (1972).
2. D.H. Rank, D.P. Eastman, B.S. Rao, and T.A. Wiggins, "Highly Precise Wavelengths in the Infrared. II. HCN,  $N_2O$ , and CO," *JOSA* **51**, 929-936 (1961).
3. A.G. Maki, G.Ch. Mellau, S. Klee, M. Winnewisser, and W. Quapp, "High-Temperature Infrared Measurements in the Region of the Bending Fundamental of  $H^{12}C^{14}N$ ,  $H^{12}C^{15}N$ , and  $H^{13}C^{14}N$ ," *J.Mol.Spectrosc.* **202**, 67-82 (2000).
4. A. Maki, W. Quapp, S. Klee, G.Ch. Mellau, and S. Albert, "Infrared Transitions of  $H^{12}C^{14}N$  and  $H^{12}C^{15}N$  between 500 and  $10000\text{ cm}^{-1}$ ," *J.Mol.Spectrosc.* **180**, 323-336 (1996).
5. F. Maiwald, F. Lewen, V. Ahrens, M. Beaky, R. Gendriesch, A.N. Koroliev, A.A. Negirev, D.G. Paveljev, B. Vowinkel, and G. Winnewisser, "Pure Rotational Spectrum of HCN in the Terahertz Region: Use of a New Planar Schottky Diode Multiplier," *J.Mol.Spectrosc.* **202**, 166-168 (2000).
6. V. Ahrens, F. Lewen, S. Takano, G. Winnewisser, S. Urban, A.A. Negirev, and A.N. Koroliev, *Z. Naturforsch.* **57 a**, 669-681 (2002).
7. S. Thorwirth, H.S.P. Müller, F. Lewen, S. Brünken, V. Ahrens, and G. Winnewisser, *Ap.J.* **585**, L163-L165 (2003).
8. Z. Zelinger, T. Amano, V. Ahrens, S. Brünken, F. Lewen, H.S.P. Müller, and G. Winnewisser, "Submillimeter-wave spectroscopy of HCN in excited vibrational states," *J.Mol.Spectrosc.* **220**, 223-233 (2003).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A. Maki, W. Quapp, S. Klee, G.Ch. Mellau, and S. Albert, "The CN Mode of HCN: A Comparative Study of the Variation of the Transition Dipole and Herman-Wallis Constants for Seven Isotopomers and the Influence of Vibration-Rotation Interaction," *J.Mol.Spectrosc.* **174**, 365-378 (1995).
2. A. Maki, W. Quapp, and S. Klee, "Intensities of Hot-Band Transitions: HCN Hot Bands," *J.Mol.Spectrosc.* **171**, 420-434 (1995).
3. A.G. Maki, "Microwave Spectra of Molecules of Astrophysical Interest VI. Carbonyl Sulfide and Hydrogen Cyanide," *J.Phys.Chem.Ref.Data* **3**, 221-244 (1974).

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. Polynomial fit by M.A.H. Smith, NASA Langley Research Center, using: C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, D.C. Benner, S.W. Sharpe, and R.L. Sams, "A multispectrum analysis of the  $\nu_1$  band of  $H^{12}C^{14}N$ : Part II. Air- and  $N_2$ -broadening, shifts and their temperature dependences," *JQSRT* **82**, 343-362 (2003); V. Malathy Devi, D.C. Benner, M.A.H. Smith, C.P.

- Rinsland, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $2\nu_2$  spectral region of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Intensities, broadening and pressure-shift coefficients,” *JQSRT* **87**, 339-366 (2004).
2. C. Yang, J. Buldyreva, I.E. Gordon, F. Rohart, A. Cuisset, G. Mouret, R. Bocquet, and F. Hindle, “Oxygen, nitrogen and air broadening of HCN spectral lines at terahertz frequencies,” *JQSRT* **109**, 2857-2868 (2008).

#### Half-widths (self)

1. Polynomial fit by M.A.H. Smith, NASA Langley Research Center, using: V. Malathy Devi, D.C. Benner, M.A.H. Smith, C.P. Rinsland, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $\nu_1$  band of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Part I. Intensities, self-broadening and self-shift coefficients” *JQSRT* **82**, 319-342 (2003); C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, D.C. Benner, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $\nu_1$  band of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Part II. Air- and  $\text{N}_2$ -broadening, shifts and their temperature dependences,” *JQSRT* **82**, 343-362 (2003).

#### Temperature dependence of air-broadened half-width

1. Polynomial fit by M.A.H. Smith, NASA Langley Research Center, using: V. Malathy Devi, D.C. Benner, M.A.H. Smith, C.P. Rinsland, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $2\nu_2$  spectral region of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Intensities, broadening and pressure-shift coefficients,” *JQSRT* **87**, 339-366 (2004).

#### Pressure shift (air)

1. Polynomial fit by M.A.H. Smith, NASA Langley Research Center, using: C.P. Rinsland, V. Malathy Devi, M.A.H. Smith, D.C. Benner, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $\nu_1$  band of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Part II. Air- and  $\text{N}_2$ -broadening, shifts and their temperature dependences,” *JQSRT* **82**, 343-362 (2003); V. Malathy Devi, D.C. Benner, M.A.H. Smith, C.P. Rinsland, S.W. Sharpe, and R.L. Sams, “A multispectrum analysis of the  $2\nu_2$  spectral region of  $\text{H}^{12}\text{C}^{14}\text{N}$ : Intensities, broadening and pressure-shift coefficients,” *JQSRT* **87**, 339-366 (2004).

## CH<sub>3</sub>Cl [24] 215, 217

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. P. Jensen, S. Brodersen, and G. Guelachvili, "Determination of  $A_0$  for CH<sub>3</sub><sup>35</sup>Cl and CH<sub>3</sub><sup>37</sup>Cl from the  $\nu_4$  Infrared and Raman Bands," *J.Mol.Spectrosc.* **88**, 378-393 (1981).
2. M. Betrencourt, M. Morillon-Chapey, G. Blanquet, and J. Walrand, "Diode-Laser Spectroscopy of Methyl Chloride Near 14  $\mu\text{m}$  toward Its Detection in the Stratosphere," *J.Mol.Spectrosc.* **128**, 433-443 (1988).
3. C. Chackerian, Jr., L.R. Brown, N. Lacome, and G. Tarrago, "Methyl Chloride  $\nu_5$  Region Line Shape Parameters and Rotational Constants for the  $\nu_2$ ,  $\nu_5$  and  $2\nu_3$  Vibrational Bands," *J.Mol.Spectrosc.* **191**, 148-157 (1998).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
5. A. Nikitin, J.-P. Champion, and H. Burger, "Global analysis of <sup>12</sup>CH<sub>3</sub><sup>35</sup>Cl and <sup>12</sup>CH<sub>3</sub><sup>37</sup>Cl: simultaneous fit of the lower five polyads (0-2600 cm<sup>-1</sup>)," *J.Mol.Spectrosc.* **230**, 174-184 (2005).
6. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Muller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998). Line parameters were taken in August 2010.

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. M. Dang-Nhu, G. Blanquet, J. Walrand, and F. Derie, "Spectral intensities in the  $\nu_3$ -band of <sup>13</sup>CH<sub>3</sub><sup>35</sup>Cl at 13 $\mu\text{m}$ ," *Mol.Phys.* **65**, 77-83 (1988).
2. G. Blanquet, J. Walrand, and M. Dang-Nhu, "Spectral Intensities in the  $\nu_3$  Band of <sup>13</sup>CH<sub>3</sub><sup>37</sup>Cl at 13 $\mu\text{m}$ ," *J.Mol.Spectrosc.* **133**, 471-474 (1989).
3. C. Chackerian, Jr., L.R. Brown, N. Lacome, and G. Tarrago, "Methyl Chloride  $\nu_5$  Region Line Shape Parameters and Rotational Constants for the  $\nu_2$ ,  $\nu_5$  and  $2\nu_3$  Vibrational Bands," *J.Mol.Spectrosc.* **191**, 148-157 (1998).
4. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998).
5. A. Nikitin, J.-P. Champion, and H. Burger, "Global analysis of <sup>12</sup>CH<sub>3</sub><sup>35</sup>Cl and <sup>12</sup>CH<sub>3</sub><sup>37</sup>Cl: simultaneous fit of the lower five polyads (0-2600 cm<sup>-1</sup>)," *J.Mol.Spectrosc.* **230**, 174-184 (2005).
6. Intensities from Ref. 5 were scaled, so that the band strengths would match those from various experiments when available. In case no experimental information was available, bands were scaled to closely resemble the appearance of the PNNL spectrum (I. Gordon and D. Plutov) (2010).
7. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Muller, "Submillimeter, Millimeter, and Microwave Spectral Line Catalog," *JQSRT* **60**, 883-890 (1998). Line parameters were taken in August 2010.

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L.



Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).

1. G. Blanquet, J. Walrand, and J.P. Bouanich, "Diode-Laser Measurements of O<sub>2</sub>-Broadening Coefficients in the  $\nu_3$  Band of CH<sub>3</sub><sup>35</sup>Cl," *J.Mol.Spectrosc.* **159**, 137-141 (1993); G. Blanquet, J. Walrand, and J.P. Bouanich, "Diode-Laser Measurements of N<sub>2</sub>-Broadening Coefficients in the  $\nu_3$  Band of CH<sub>3</sub><sup>35</sup>Cl," *J.Mol.Spectrosc.* **160**, 253-257 (1993); J.P. Bouanich, G. Blanquet, and J. Walrand, "Theoretical O<sub>2</sub> and N<sub>2</sub> Broadening Coefficients of CH<sub>3</sub>Cl Spectral Lines," *J.Mol.Spectrosc.* **161**, 416-426 (1993).
2. J.-P. Bouanich, private communication (2003), based on the work of J.-P. Bouanich, G. Blanquet, J.-C. Populaire, and J. Walrand, "N<sub>2</sub>-Broadening for Methyl Chloride at Low Temperature by Diode-Laser Spectroscopy," *J.Mol.Spectrosc.* **208**, 72-78 (2001).

#### Half-widths (self)

1. C. Chackerian, Jr., L.R Brown, N. Lacome, and G. Tarrago, "Methyl Chloride  $\nu_5$  Region Line Shape Parameters and Rotational Constants for the  $\nu_2$ ,  $\nu_5$  and  $2\nu_3$  Vibrational Bands," *J.Mol.Spectrosc.* **191**, 148-157 (1998).

#### Temperature dependence of air-broadened half-width

1. J.-P. Bouanich, G. Blanquet, J.-C. Populaire, and J. Walrand, "N<sub>2</sub>-Broadening for Methyl Chloride at Low Temperature by Diode-Laser Spectroscopy," *J.Mol.Spectrosc.* **208**, 72-78 (2001).

#### Shift

1. Crude estimate of the shift based on comparison with the PNNL spectrum.

Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.J. Hillman, D.E. Jennings, W.B. Olson, and A. Goldman, "High-Resolution Infrared Spectrum of Hydrogen Peroxide: The  $\nu_6$  Fundamental Band," *J.Mol.Spectrosc.* **117**, 46-59 (1986).
2. J. Hillman, NASA Goddard Space Flight Center, private communication.
3. A. Perrin, Univ. Paris, private communication (1997).
4. A. Perrin, J.-M. Flaud, C. Camy-Peyret, R. Schermaul, M. Winnewisser, J.-Y. Mandin, V. Dana, M Badaoui, and J. Koput, "Line Intensities in the Far-Infrared Spectrum of H<sub>2</sub>O<sub>2</sub>," *J.Mol.Spectrosc.* **176**, 287-296 (1996).
5. A. Perrin, A. Valentin, J.-M. Flaud, C. Camy-Peyret, L. Schriver, A. Schriver, and Ph. Arcas, "The 7.9 $\mu$ m band of hydrogen peroxide: line positions and intensities," *J.Mol.Spectrosc.* **171**, 358-373 (1995).

Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. J.D. Rogers and J.J. Hillman, "Prediction of absolute infrared intensities for the fundamental vibrations of H<sub>2</sub>O<sub>2</sub>," *J.Chem.Phys.* **75**, 1085 (1981); *ibid* **76**, 4046 (1982); F.P.J. Valero, D. Goorvitch, F.S. Bonomo, and R.W. Boese, "Intensity of the hydrogen peroxide  $\nu_6(b)$  band around 1266 cm<sup>-1</sup>," *Appl. Opt.* **20**, 4097-4101 (1981); H. Niki, P.D. Maker, C.M. Savage, and L.P. Breitenbach, "An FTIR Study of the Mechanism for the Gas Phase Reaction between HO<sub>2</sub> Radicals," *Chem.Phys.Lett.* **73**, 43 (1980); J.J. Hillman, "On the Submillimeter Spectrum of Hydrogen Peroxide," *J.Mol.Spectrosc.* **95**, 236-238 (1982).
2. A. Perrin, Univ. Paris, private communication (1997).
3. A. Perrin, J.-M. Flaud, C. Camy-Peyret, R. Schermaul, M. Winnewisser, J.-Y. Mandin, V. Dana, M Badaoui, and J. Koput, "Line Intensities in the Far-Infrared Spectrum of H<sub>2</sub>O<sub>2</sub>," *J.Mol.Spectrosc.* **176**, 287-296 (1996).
4. S. Klee, M. Winnewisser, A. Perrin, and J.-M. Flaud, "Absolute line intensities for the  $\nu_6$  band of H<sub>2</sub>O<sub>2</sub>," *J.Mol.Spectrosc.* **195**, 154-161 (1999).

Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. V. Malathy Devi, C.P. Rinsland, M.A.H. Smith, D.C. Benner, and B. Fridovitch, "Tunable diode laser measurements of air-broadened linewidths in the  $\nu_6$  band of H<sub>2</sub>O<sub>2</sub>," *Appl. Opt.* **25**, 1844-1847 (1986).

Temperature dependence of air-broadened half-width

1. J.-M. Flaud, C. Piccolo, B. Carli, A. Perrin, L.H. Coudert, J.L. Teffo, and L.R. Brown, "Molecular line parameters for the MIPAS (Michelson Interferometer for Passive Atmospheric

Sounding) experiment,” *Atmos.Oceanic Opt.* **16**, 172-182 (2003).

Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. K.F. Palmer, M.E. Mickelson, and K.Narahari Rao, "Investigations of Several Infrared Bands of <sup>12</sup>C<sub>2</sub>H<sub>2</sub> and studies of the Effects of Vibrational Rotational Interactions," *J.Mol.Spectrosc.* **44**, 131-144 (1972).
2. J. Vander Auwera, D. Hurtmans, M. Carleer, and M. Herman, "The  $\nu_3$  Fundamental in C<sub>2</sub>H<sub>2</sub>," *J.Mol.Spectrosc.* **157**, 337-357 (1993).
3. J.J. Hillman, D.E. Jennings, G.W. Halsey, S. Nadler, and W.E. Blass, "An Infrared Study of the Bending Region of Acetylene," *J.Mol.Spectrosc.* **146**, 389-401 (1991).
4. M. Weber, W.E. Blass, G.W. Halsey, J.J. Hillman, and W.C. Maguire, "l-Resonance effects in the  $\nu_5$ ,  $2\nu_5$ - $\nu_5$ , and  $\nu_4$ + $\nu_5$ - $\nu_4$  bands of C<sub>2</sub>H<sub>2</sub> and <sup>13</sup>C<sup>12</sup>CH<sub>2</sub> near 13.7  $\mu$ m," *Spectrochim.Acta* **48A**, 1203-1226 (1992).
5. Y. Kabbadj, M. Herman, G. Di Lonardo, L. Fusina, and J.W.C. Johns, "The bending energy levels of C<sub>2</sub>H<sub>2</sub>," *J.Mol.Spectrosc.* **150**, 535-565 (1991).
6. J. Plíva, "Spectrum of acetylene in the 5-micron region," *J.Mol.Spectrosc.* **44**, 145-164 (1972); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, X. Thomas, P. Von der Heyden, "Multispectrum fitting measurements of line parameters for 5 $\mu$ m cold bands of acetylene," *JQSRT* **75**, 397-422 (2002); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, "The spectrum of acetylene in the 5- $\mu$ m region from new line parameter measurements," *JQSRT* **76**, 237-267 (2003).
7. C.P. Rinsland, A. Baldacci, and K.N. Rao, "Acetylene bands observed in carbon stars: a laboratory study and an illustrative example of its applications to IRC+10216," *Astrophys.J.Suppl.Ser.* **49**, 487-513 (1982).
8. G. Di Lonardo, A. Baldan, G. Bramati, and L. Fusina, "The intrared spectrum of <sup>12</sup>C<sup>13</sup>CH<sub>2</sub>: the bending states up to  $\nu_4$ + $\nu_5$  = 4," *J.Mol.Spectrosc.* **213**, 57-63 (2002).
9. Q. Kou, G. Guelachvili, M. Abbouti Temsamani, and M. Herman, "The absorption spectrum of C<sub>2</sub>H<sub>2</sub> around  $\nu_1$ + $\nu_3$ : energy standards in the 1.5  $\mu$ m region and vibrational clustering," *Can.J.Phys.* **72**, 1241-1250 (1994).
10. O.M. Lyulin, V.I. Perevalov, J.-Y. Mandin, V. Dana, F. Gueye, P. Von Der Heyden, X. Thomas, D. Décatoire, L. Regalia-Jarlot, D. Jacquemart, and N. Lacome, "Line intensities of acetylene: measurements in the 2.5- $\mu$ m region and approach in the  $\Delta P$  = 4 and 6 series," *JQSRT* **103**, 496-523 (2007).
11. D. Jacquemart, N. Lacome, J.-Y. Mandin, V. Dana, O.M. Lyulin, and V.I. Perevalov, "Multispectrum fitting of line parameters for <sup>12</sup>C<sub>2</sub>H<sub>2</sub> in the 3.8- $\mu$ m spectral region," *JQSRT* **103**, 478-495 (2007).
12. D. Jacquemart, N. Lacome, J.-Y. Mandin, V. Dana, H. Tran, F.K. Gueye, O.M. Lyulin, V.I. Perevalov, and L. Régalia-Jarlot, "The IR spectrum of <sup>12</sup>C<sub>2</sub>H<sub>2</sub>: line intensity measurements in the 1.4  $\mu$ m region and update of the databases," *JQSRT* **110**, 717-732 (2009).
13. D. Jacquemart, N. Lacome, and J.-Y. Mandin, "Line intensities of <sup>12</sup>C<sub>2</sub>H<sub>2</sub> in the 1.3, 1.2, and 1  $\mu$ m spectral regions," *JQSRT* **110**, 733-742 (2009).
14. L. Gomez, D. Jacquemart, N. Lacome, and J.-Y. Mandin, "Line intensities of <sup>12</sup>C<sub>2</sub>H<sub>2</sub> in the 7.7  $\mu$ m spectral region," *JQSRT* **110**, 2102-2114 (2009).
15. L. Gomez, D. Jacquemart, N. Lacome, and J.-Y. Mandin, "New line intensity measurements

for  $^{12}\text{C}_2\text{H}_2$  and HITRAN format line list for applications,” *JQSRT* **111**, 2256-2264 (2010).

**16.** MEP 2005, CIPM recommended values for absorbing molecule  $^{13}\text{C}_2\text{H}_2$ ,

[http://www.bipm.org/utis/common/pdf/mep/M-e-P\\_C2H2\\_1.54.pdf](http://www.bipm.org/utis/common/pdf/mep/M-e-P_C2H2_1.54.pdf).

**17.** K. Nakagawa, M. de Labachellerie, Y. Awaji, and M. Kourogi, “Accurate optical frequency atlas of the 1.5- $\mu\text{m}$  bands of acetylene,” *J.Opt.Soc.Am.* **13**, 2708-2714 (1996).

**18.** A. Jolly, Y. Benilan, E. Cané, L. Fusina, F. Tamassia, A. Fayt, S. Robert, M. Herman, “Measured integrated band intensities and simulated line-by-line spectra for  $\text{C}_2\text{HD}$  between 25 and 2.5  $\mu\text{m}$ , and new global vibration rotation parameters for the bending vibrations,” *JQSRT* **111**, 2256-2264 (2010).

**19.** H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, “The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists,” *J.Mol.Struct.* **742**, 215-227 (2005). Data taken in March 2011.

### Intensities

**0.** L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, “The HITRAN database: 1986 Edition,” *Appl.Opt.* **26**, 4058-4097 (1987).

**1.** J.R. Podolske, M. Loewenstein, and P. Varanasi, “Diode Laser Line Strength Measurements of the  $(\nu_4 + \nu_5)^0$  Band of  $^{12}\text{C}_2\text{H}_2$ ,” *J.Mol.Spectrosc.* **107**, 241-249 (1984).

**2.** J. Vander Auwera, D. Hurtmans, M. Carleer, and M. Herman, “The  $\nu_3$  Fundamental in  $\text{C}_2\text{H}_2$ ,” *J.Mol.Spectrosc.* **157**, 337-357 (1993).

**3.** M. Weber, Ph.D. thesis, University of Tennessee (1992).

**4.** J.-Y. Mandin, V. Dana, and C. Claveau, “Line intensities in the  $\nu_5$  band of acetylene  $^{12}\text{C}_2\text{H}_2$ ,” *JQSRT* **67**, 429-446 (2000).

**5.** D. Jacquemart, C. Claveau, J.-Y. Mandin, and V. Dana, “Line intensities of hot bands in the 13.6  $\mu\text{m}$  spectral region of acetylene  $^{12}\text{C}_2\text{H}_2$ ,” *JQSRT* **69**, 81-101 (2001).

**6.** J. Vander Auwera, “Absolute Intensities Measurements in the  $\nu_4+\nu_5$  Band of  $^{12}\text{C}_2\text{H}_2$ : Analysis of Herman-Wallis Effects and Forbidden Transitions,” *J.Mol.Spectrosc.* **201**, 143-150 (2000).

**7.** D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, X. Thomas, P. Von der Heyden, “Multispectrum fitting measurements of line parameters for 5 $\mu\text{m}$  cold bands of acetylene,” *JQSRT* **75**, 397-422 (2002); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, “The spectrum of acetylene in the 5- $\mu\text{m}$  region from new line parameter measurements,” *JQSRT* **76**, 237-267 (2003).

**8.** D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, “The spectrum of acetylene in the 5- $\mu\text{m}$  region from new line parameter measurements,” *JQSRT* **76**, 237-267 (2003); D. Jacquemart, J.-Y. Mandin, V. Dana, C. Claveau, J. Vander Auwera, M. Herman, L.S. Rothman, L. Régalia-Jarlot, and A. Barbe, “The IR acetylene spectrum in HITRAN: update and new results,” *JQSRT* **82**, 363-382 (2003).

**9.** R. El Hachtouki and J. Vander Auwera, “Absolute Line Intensities in Acetylene: The 1.5- $\mu\text{m}$  Region,” *J.Mol.Spectrosc.* **216**, 355-362 (2002).

**10.** O.M. Lyulin, V.I. Perevalov, J.-Y. Mandin, V. Dana, F. Gueye, P. Von Der Heyden, X. Thomas, D. Décatoire, L. Regalia-Jarlot, D. Jacquemart, and N. Lacome, “Line intensities of acetylene: measurements in the 2.5- $\mu\text{m}$  region and approach in the  $\Delta P = 4$  and 6 series,” *JQSRT* **103**, 496-523 (2007).

**11.** D. Jacquemart, N. Lacome, J.-Y. Mandin, V. Dana, O.M. Lyulin, and V.I. Perevalov, “Multispectrum fitting of line parameters for  $^{12}\text{C}_2\text{H}_2$  in the 3.8- $\mu\text{m}$  spectral region,” *JQSRT* **103**, 478-495 (2007).



12. D. Jacquemart, N. Lacome, J.-Y. Mandin, V. Dana, H. Tran, F.K. Gueye, O.M. Lyulin, V.I. Perevalov, and L. Régalia-Jarlot, "The IR spectrum of  $^{12}\text{C}_2\text{H}_2$ : line intensity measurements in the 1.4  $\mu\text{m}$  region and update of the databases," *JQSRT* **110**, 717-732 (2009).
13. D. Jacquemart, N. Lacome, and J.-Y. Mandin, "Line intensities of  $^{12}\text{C}_2\text{H}_2$  in the 1.3, 1.2, and 1  $\mu\text{m}$  spectral regions," *JQSRT* **110**, 733-742 (2009).
14. L. Gomez, D. Jacquemart, N. Lacome, and J.-Y. Mandin, "Line intensities of  $^{12}\text{C}_2\text{H}_2$  in the 7.7  $\mu\text{m}$  spectral region," *JQSRT* **110**, 2102-2114 (2009).
15. L. Gomez, D. Jacquemart, N. Lacome, and J.-Y. Mandin, "New line intensity measurements for  $^{12}\text{C}_2\text{H}_2$  and HITRAN format line list for applications," *JQSRT* **111**, 2256-2264 (2010).
16. A. Jolly, Y. Benilan, E. Cané, L. Fusina, F. Tamassia, A. Fayt, S. Robert, M. Herman, "Measured integrated band intensities and simulated line-by-line spectra for  $\text{C}_2\text{HD}$  between 25 and 2.5  $\mu\text{m}$ , and new global vibration rotation parameters for the bending vibrations," *JQSRT* **111**, 2256-2264 (2010).
17. H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists," *J.Mol.Struct.* **742**, 215-227 (2005). Data taken in March 2011.

#### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl.Opt.* **26**, 4058-4097 (1987).
1. V.Malathy Devi, D.C. Benner, C.P. Rinsland, M.A.H. Smith, and B.D. Sidney, "Tunable Diode Laser Measurements of  $\text{N}_2$ - and Air-Broadened Halfwidths: Lines in the  $(\nu_4 + \nu_5)^0$  Band of  $^{12}\text{C}_2\text{H}_2$  Near 7.4  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **114**, 49-53 (1985).
2. D. Lambot, G. Blanquet, and J.-P. Bouanich, "Diode laser measurements of collisional broadening in the  $\nu_5$  band of  $\text{C}_2\text{H}_2$  perturbed by  $\text{O}_2$  and  $\text{N}_2$ ," *J.Mol.Spectrosc.* **136**, 86-92 (1989); J.-P. Bouanich, D. Lambot, G. Blanquet, and J. Walrand, " $\text{N}_2$ - and  $\text{O}_2$ -broadening coefficients of  $\text{C}_2\text{H}_2$  IR lines," *J.Mol.Spectrosc.* **140**, 195-213. (1990); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, "The spectrum of acetylene in the 5- $\mu\text{m}$  region from new line parameter measurements," *JQSRT* **76**, 237-267 (2003).

#### Half-widths (self)

1. D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, X. Thomas, P. Von der Heyden, "Multispectrum fitting measurements of line parameters for 5 $\mu\text{m}$  cold bands of acetylene," *JQSRT* **75**, 397-422 (2002); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, "The spectrum of acetylene in the 5- $\mu\text{m}$  region from new line parameter measurements," *JQSRT* **76**, 237-267 (2003).

#### Temperature dependence of air-broadened half-width

1. J.-P. Bouanich, D. Lambot, G. Blanquet, and J. Walrand, " $\text{N}_2$ - and  $\text{O}_2$ -broadening coefficients of  $\text{C}_2\text{H}_2$  IR lines" *J.Mol.Spectrosc.* **140**, 195-213 (1990); J.-P. Bouanich, G. Blanquet, J.-C. Populaire, and J. Walrand, "Nitrogen broadening of acetylene lines in the  $\nu_5$  band at low temperature," *J.Mol.Spectrosc.* **190**, 7-14. (1998); J.-P. Bouanich, G. Blanquet, and J. Walrand, "Oxygen broadening of acetylene lines in the  $\nu_5$  band at low temperature," *J.Mol.Spectrosc.* **194**, 269-277 (1999); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, "The spectrum of acetylene in the 5- $\mu\text{m}$  region from new line parameter measurements," *JQSRT* **76**, 237-267 (2003).

Pressure shift (air)

1. A. Babay, M. Ibrahimi, V. Lemaire, B. Lemoine, F. Rohart, and J.-P. Bouanich, “Line frequency shifting in the  $\nu_5$  band of  $C_2H_2$ ,” *JQSRT* **59**, 195-202 (1998); D. Jacquemart, J.-Y. Mandin, V. Dana, L. Régalia-Jarlot, J.J. Plateaux, D. Décatoire, and L.S. Rothman, “The spectrum of acetylene in the 5- $\mu m$  region from new line parameter measurements,” *JQSRT* **76**, 237-267 (2003).

Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A. Goldman, M. Dang-Nhu, and J.P. Bouanich, "Ethane 3 $\mu$ m Spectral Clusters of Atmospheric Interest," *JQSRT* **41**, 17-21 (1989).
2. S.J. Daunt, W.E. Blass, G.W. Halsey, K. Fox, and R.J. Lovell, "High-Resolution Infrared Spectrum and Analysis of the  $\nu_9$  Band of Ethane at 12.17  $\mu$ m," *J.Mol.Spectrosc.* **86**, 327-343 (1981).
3. A.S. Pine and W.J. Lafferty, "Torsional Splittings and Assignments of the Doppler-Limited Spectrum of Ethane in the C-H Stretching Region," *J.Res.NBS* **87**, 237-256 (1982).
4. C.P. Rinsland, N.B. Jones, B.J. Connor, J.A. Logan, N.S. Pougatchev, A. Goldman, F.J. Murcray, T.M. Stephen, A.S. Pine, R. Zander, E. Mahieu, and P. Demoulin, "Northern and southern hemisphere ground-based infrared spectroscopic measurements of tropospheric carbon monoxide and ethane," *J.Geophys.Res.* **103**, 28,197-28,217 (1998).
5. A.S. Pine and C.P. Rinsland, "The role of torsional hot bands in modeling atmospheric ethane," *JQSRT* **62**, 445-458 (1999).
6. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, "Toward an accurate database for the 12  $\mu$ m region of the ethane spectrum," *Ap.J.* **662**, 750-757 (2007).
7. M. Weber, D.C. Reuter, D.E. Jennings, W.E. Blass, and J.J. Hillman, "A spectral atlas of the  $\nu_{12}$  fundamental of  $^{13}\text{C}^{12}\text{CH}_6$  in the 12  $\mu$ m region," NASA Technical Memorandum 104601, Greenbelt; 1994.

Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A. Goldman, M. Dang-Nhu, and J.P. Bouanich, "Ethane 3 $\mu$ m Spectral Clusters of Atmospheric Interest," *JQSRT* **41**, 17-21 (1989).
2. C.P. Rinsland, N.B. Jones, B.J. Connor, J.A. Logan, N.S. Pougatchev, A. Goldman, F.J. Murcray, T.M. Stephen, A.S. Pine, R. Zander, E. Mahieu, and P. Demoulin, "Northern and southern hemisphere ground-based infrared spectroscopic measurements of tropospheric carbon monoxide and ethane," *J.Geophys.Res.* **103**, 28,197-28,217 (1998).
3. A.S. Pine and C.P. Rinsland, "The role of torsional hot bands in modeling atmospheric ethane," *JQSRT* **62**, 445-458 (1999).
4. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, "Toward an accurate database for the 12  $\mu$ m region of the ethane spectrum," *Ap.J.* **662**, 750-757 (2007).
5. M. Weber, D.C. Reuter, D.E. Jennings, W.E. Blass, and J.J. Hillman, "A spectral atlas of the  $\nu_{12}$  fundamental of  $^{13}\text{C}^{12}\text{CH}_6$  in the 12  $\mu$ m region," NASA Technical Memorandum 104601, Greenbelt; 1994.

Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. A.S. Pine and S.C. Stone, "Torsional tunneling and A1-A2 splittings and air-broadening of

the  $^1Q0$  and  $^1Q3$  subbranches of the  $\nu_7$  band of ethane,” *J.Mol.Spectrosc.* **175**, 21-30 (1996); C.P. Rinsland, N.B. Jones, B.J. Connor, J.A. Logan, N.S. Pougatchev, A. Goldman, F.J. Murcray, T.M. Stephen, A.S. Pine, R. Zander, E. Mahieu, and P. Demoulin, “Northern and southern hemisphere ground-based infrared spectroscopic measurements of tropospheric carbon monoxide and ethane,” *J.Geophys.Res.* **103**, 28,197-28,217 (1998).

3. A.S. Pine and C.P. Rinsland, “The role of torsional hot bands in modeling atmospheric ethane,” *JQSRT* **62**, 445-458 (1999).

4. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, “Toward an accurate database for the 12  $\mu\text{m}$  region of the ethane spectrum,” *Ap.J.* **662**, 750-757 (2007).

#### Half-widths (self)

1. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, “Toward an accurate database for the 12  $\mu\text{m}$  region of the ethane spectrum,” *Ap.J.* **662**, 750-757 (2007).

#### Temperature dependence of air-broadened half-width

1. A.S. Pine and C.P. Rinsland, “The role of torsional hot bands in modeling atmospheric ethane,” *JQSRT* **62**, 445-458 (1999).

2. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, “Toward an accurate database for the 12  $\mu\text{m}$  region of the ethane spectrum,” *Ap.J.* **662**, 750-757 (2007).

#### Pressure shift (air)

1. A.S. Pine and C.P. Rinsland, “The role of torsional hot bands in modeling atmospheric ethane,” *JQSRT* **62**, 445-458 (1999).

### Positions

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. G. Tarrago, M. Dang-Nhu, and A. Goldman, "Analysis of Phosphine Absorption in the Region 9-10  $\mu\text{m}$  and High Resolution Line-by-Line Simulation of the  $\nu_2$  and  $\nu_4$  Bands," *J.Mol.Spectrosc.* **88**, 311-322 (1981).
2. L.R. Brown, R.L. Sams, I. Kleiner, C. Cottaz, and L. Sagui, "Line Intensities of the Phosphine Dyad at 10  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **215**, 178-203 (2002).
3. G. Tarrago, N. Lacome, A. Levy, G. Guelachvili, B. Benzard, and P. Drossart, "Phosphine Spectrum at 4-5  $\mu\text{m}$ : Analysis and Line-by-Line Simulation of  $2\nu_2$ ,  $\nu_2 + \nu_4$ ,  $2\nu_4$ ,  $\nu_1$ , and  $\nu_3$  Bands," *J.Mol.Spectrosc.* **154**, 30-42 (1992).
4. R.A.H. Butler, L. Sagui, I. Kleiner, and L.R. Brown, "The absorption spectrum of phosphine (PH<sub>3</sub>) between 2.8 and 3.7  $\mu\text{m}$ : Line positions, intensities, and assignments," *J.Mol.Spectrosc.* **238**, 178-192 (2006).

### Intensities

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. L.R. Brown, R.L. Sams, I. Kleiner, C. Cottaz, and L. Sagui, "Line Intensities of the Phosphine Dyad at 10  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **215**, 178-203 (2002).
2. G. Tarrago, N. Lacome, A. Levy, G. Guelachvili, B. Benzard, and P. Drossart, "Phosphine Spectrum at 4-5  $\mu\text{m}$ : Analysis and Line-by-Line Simulation of  $2\nu_2$ ,  $\nu_2 + \nu_4$ ,  $2\nu_4$ ,  $\nu_1$ , and  $\nu_3$  Bands," *J.Mol.Spectrosc.* **154**, 30-42 (1992).
3. R.A.H. Butler, L. Sagui, I. Kleiner, and L.R. Brown, "The absorption spectrum of phosphine (PH<sub>3</sub>) between 2.8 and 3.7  $\mu\text{m}$ : Line positions, intensities, and assignments," *J.Mol.Spectrosc.* **238**, 178-192 (2006).

### Half-widths (air)

0. L.S. Rothman, R.R. Gamache, A. Goldman, L.R. Brown, R.A. Toth, H.M. Pickett, R.L. Poynter, J.-M. Flaud, C. Camy-Peyret, A. Barbe, N. Husson, C.P. Rinsland, and M.A.H. Smith, "The HITRAN database: 1986 Edition," *Appl. Opt.* **26**, 4058-4097 (1987).
1. L.R. Brown, R.L. Sams, I. Kleiner, C. Cottaz, and L. Sagui, "Line Intensities of the Phosphine Dyad at 10  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **215**, 178-203 (2002).
2. Scaled by 0.9 from the nitrogen-broadened widths in R.A.H. Butler, L. Sagui, I. Kleiner, and L.R. Brown, "The absorption spectrum of phosphine (PH<sub>3</sub>) between 2.8 and 3.7  $\mu\text{m}$ : Line positions, intensities, and assignments," *J.Mol.Spectrosc.* **238**, 178-192 (2006).

### Half-widths (self)

1. L.R. Brown, R.L. Sams, I. Kleiner, C. Cottaz, and L. Sagui, "Line Intensities of the Phosphine Dyad at 10  $\mu\text{m}$ ," *J.Mol.Spectrosc.* **215**, 178-203 (2002).
2. R.A.H. Butler, L. Sagui, I. Kleiner, and L.R. Brown, "The absorption spectrum of phosphine (PH<sub>3</sub>) between 2.8 and 3.7  $\mu\text{m}$ : Line positions, intensities, and assignments," *J.Mol.Spectrosc.* **238**, 178-192 (2006).



Temperature dependence of air-broadened half-width

**1.** R.A.H. Butler, L. Sagui, I. Kleiner, and L.R. Brown, “The absorption spectrum of phosphine (PH<sub>3</sub>) between 2.8 and 3.7  $\mu\text{m}$ : Line positions, intensities, and assignments,” *J.Mol.Spectrosc.* **238**, 178-192 (2006).

Positions

1. L.R. Brown and E.A. Cohen, "The C-O Stretch Regions of COF<sub>2</sub>: the Interaction of the  $\nu_1$ ,  $2\nu_2$ , and  $2\nu_3 + \nu_6$  Bands," private communication (1991).
2. E.A. Cohen and W. Lewis-Bevan, "Further Measurements of the Rotational Spectrum of COF<sub>2</sub>: Improved Molecular Constants for the Ground and  $\nu_2$  States," *J.Mol.Spectrosc.* **148**, 378-384 (1991).
3. C. Camy-Peyret, J.-M. Flaud, A. Goldman, F.J. Murcray, R.D. Blatherwick, F.S. Bonomo, D.G. Murcray, and C.P. Rinsland, "The  $\nu_4$  Band of Carbonyl Fluoride," *J.Mol.Spectrosc.* **149**, 481-490 (1991).
4. A. Goldman, C.P. Rinsland, R.D. Blatherwick, and F.S. Bonomo, "Spectroscopic line parameters for the  $\nu_6$  band of carbonyl fluoride," *Appl.Opt.* **29**, 1860-1863 (1990).
5. C.P. Rinsland, NASA Langley Research Center, private communication (1992).
6. L.R. Brown, Jet Propulsion Laboratory, private communication (1992).
7. L.R. Brown, Jet Propulsion Laboratory, private communication (2001).

Intensities

1. L.R. Brown and E.A. Cohen, "The C-O Stretch Regions of COF<sub>2</sub>: the Interaction of the  $\nu_1$ ,  $2\nu_2$ , and  $2\nu_3 + \nu_6$  Bands," private communication (1991).
2. E.A. Cohen and W. Lewis-Bevan, "Further Measurements of the Rotational Spectrum of COF<sub>2</sub>: Improved Molecular Constants for the Ground and  $\nu_2$  States," *J.Mol.Spectrosc.* **148**, 378-384 (1991).
3. C. Camy-Peyret, J.-M. Flaud, A. Goldman, F.J. Murcray, R.D. Blatherwick, F.S. Bonomo, D.G. Murcray, and C.P. Rinsland, "The  $\nu_4$  Band of Carbonyl Fluoride," *J.Mol.Spectrosc.* **149**, 481-490 (1991).
4. A. Goldman, C.P. Rinsland, R.D. Blatherwick, and F.S. Bonomo, "Spectroscopic line parameters for the  $\nu_6$  band of carbonyl fluoride," *Appl.Opt.* **29**, 1860-1863 (1990).
7. L.R. Brown, Jet Propulsion Laboratory, private communication (2001).

Half-widths (air)

1. R.D. May, "Line Intensities and Collisional-broadening Parameters for the  $\nu_4$  and  $\nu_6$  Bands of Carbonyl Fluoride," *JQSRT* **48**, 701-712 (1992).

Positions

1. C.P. Rinsland, L.R. Brown, and C.B. Farmer, "Infrared Spectroscopic Detection of Sulfur Hexafluoride (SF<sub>6</sub>) in the Lower Stratosphere and Upper Troposphere," *J.Geophys.Res.* **95**, 5577-5585 (1990); B. Bobin, C.J. Borde, J. Borde, and C. Breant, "Vibration-Rotation Molecular Constants for the Ground and ( $\nu_3=1$ ) States of <sup>32</sup>SF<sub>6</sub> from Saturated Absorption Spectroscopy," *J.Mol.Spectrosc.* **121**, 91-127 (1987); B. Bobin, private communication (1990).
2. C.P. Rinsland, NASA Langley Research Center, private communication (1992).
3. O. Acef, C.J. Bordé, A. Clairon, G. Pierre, and B. Sartakov, "New Accurate Fit of an Extended Set of Saturation Data for the  $\nu_3$  Band of SF<sub>6</sub>: Comparison of Hamiltonians in the Spherical and Cubic Tensor Formalisms," *J.Mol.Spectrosc.* **199**, 188-204 (2000); V. Boudon, G. Pierre, "Rovibrational spectroscopy of sulphur hexafluoride: A review" *Recent Research Developments in Molecular Spectroscopy*, S.G. Pandalai, Editor, *Transworld Research Network*, Trivandrum, India **1**, 25-55 (2002).
4. The calculations were performed by V. Boudon (2008) with the HTDS software (<http://icb.u-bourgogne.fr/OMR/SMA/SHTDS>) using data reviewed in V. Boudon, G. Pierre, "Rovibrational spectroscopy of sulphur hexafluoride: A Review," in *Recent Research Developments in Molecular Spectroscopy*, S.G. Pandalai, Editor, *Transworld Research Network*, Trivandrum, India **1**, 25-55 (2002).
5. The calculations were performed by V. Boudon (2008) with the HTDS software (<http://icb.u-bourgogne.fr/OMR/SMA/SHTDS>) using data from V. Boudon, G. Pierre, H. Burger, "High Resolution Spectroscopy and Analysis of the  $\nu_4$  Bending Region of SF<sub>6</sub> Near 615 cm<sup>-1</sup>" *J.Mol.Spectrosc.* **205**, 304-311 (2001).

Intensities

1. C.P. Rinsland, L.R. Brown, and C.B. Farmer, "Infrared Spectroscopic Detection of Sulfur Hexafluoride (SF<sub>6</sub>) in the Lower Stratosphere and Upper Troposphere," *J.Geophys.Res.* **95**, 5577-5585 (1990); K. Fox, *Opt.Comm.* **19**, 397-400 (1976); B. Bobin, private communication (1990).
2. O. Acef, C.J. Bordé, A. Clairon, G. Pierre, B. Sartakov, "New Accurate Fit of an Extended Set of Saturation Data for the  $\nu_3$  Band of SF<sub>6</sub>: Comparison of Hamiltonians in the Spherical and Cubic Tensor Formalisms," *J.Mol.Spectrosc.* **199**, 188-204 (2000); V. Boudon, G. Pierre, "Rovibrational spectroscopy of sulphur hexafluoride: A review in recent research developments in molecular spectroscopy," S. G. Pandalai Editor, *Transworld Research Network*, Trivandrum, India **1**, 25-55 (2002).
3. The calculations were performed by V. Boudon (2008) with the HTDS software (<http://icb.u-bourgogne.fr/OMR/SMA/SHTDS>) using data from K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn, "Analysis of the  $\nu_4$  (615 cm<sup>-1</sup>) region of the Fourier transform and diode laser spectra of SF<sub>6</sub>," *J.Mol.Spectrosc.*, **76**, 322-340 (1979) and W.B. Person, and B.J. Krohn, "Coriolis intensity perturbations of the  $\nu_4$  band of SF<sub>6</sub>," *J.Mol.Spectrosc.*, **98**, 229-257 (1983).

Half-widths (air)

1. C.P. Rinsland, L.R. Brown, and C.B. Farmer, "Infrared Spectroscopic Detection of Sulfur Hexafluoride (SF<sub>6</sub>) in the Lower Stratosphere and Upper Troposphere," *J.Geophys.Res.* **95**, 5577-5585 (1990); G.D.T. Tejwani and K. Fox, "Calculated self- and foreign-gas-broadened linewidths for SF<sub>6</sub>," *JQSRT* **37**, 541-546 (1987).

Half-widths (self)

1. G.D.T. Tejawani and K. Fox, “Calculated self- and foreign-gas-broadened linewidths for SF<sub>6</sub>,” *JQSRT* **37**, 541-546 (1987).

Temperature dependence of air-broadened half-width

1. G.D.T. Tejawani and K. Fox, “Calculated self- and foreign-gas-broadened linewidths for SF<sub>6</sub>,” *JQSRT* **37**, 541-546 (1987).

## **H<sub>2</sub>S [31] 121,141,131**

### Positions

1. A. Goldman and J.R. Gillis, "Line Parameters and Line by Line Calculations for Molecules of Stratospheric Interest," University of Denver Progress Report (1984).
2. J.-M. Flaud, C. Camy-Peyret, and J.W.C. Johns, "The far infrared spectrum of hydrogen sulfide. The (000) rotational constants of H<sub>2</sub><sup>32</sup>S, H<sub>2</sub><sup>33</sup>S and H<sub>2</sub><sup>34</sup>S," *Can.J.Phys.* **61**, 1462-1473 (1983).
3. L. Sinitsa, Institute of Atmospheric Optics (Tomsk), private communication (1994).
4. L. Lechuga-Fossat, J.-M. Flaud, C. Camy-Peyret, and J.W.C. Johns, "The spectrum of natural hydrogen sulfide between 2150 and 2950 cm<sup>-1</sup>," *Can.J.Phys.* **62**, 1889-1923 (1984).
5. L.R. Brown, J.A. Crisp, D. Crisp, V. Naumenko, M.A. Smirnov, L.N. Sinitsa, and A. Perrin, "The Absorption Spectrum of H<sub>2</sub>S between 2150 and 4260 cm<sup>-1</sup>: Analysis of the Positions and Intensities in the First [2ν<sub>2</sub>, ν<sub>1</sub> and ν<sub>3</sub>] and Second [3ν<sub>2</sub>, ν<sub>1</sub> + ν<sub>2</sub> and ν<sub>2</sub> + ν<sub>3</sub>] Triad Region," *J.Mol. Spectrosc.* **188**, 148-174 (1998).

### Intensities

1. A. Goldman and J.R. Gillis, "Line Parameters and Line by Line Calculations for Molecules of Stratospheric Interest," University of Denver Progress Report (1984).
2. J.-M. Flaud, C. Camy-Peyret, and J.W.C. Johns, "The far infrared spectrum of hydrogen sulfide. The (000) rotational constants of H<sub>2</sub><sup>32</sup>S, H<sub>2</sub><sup>33</sup>S and H<sub>2</sub><sup>34</sup>S," *Can.J.Phys.* **61**, 1462-1473 (1983).
3. L. Sinitsa, Institute of Atmospheric Optics (Tomsk), private communication (1994).
4. L. Lechuga-Fossat, J.-M. Flaud, C. Camy-Peyret, and J.W.C. Johns, "The spectrum of natural hydrogen sulfide between 2150 and 2950 cm<sup>-1</sup>," *Can.J.Phys.* **62**, 1889-1923 (1984).
5. L.R. Brown, J.A. Crisp, D. Crisp, O. V. Naumenko, M.A. Smirnov, L.N. Sinitsa, and A. Perrin, "The Absorption Spectrum of H<sub>2</sub>S between 2150 and 4260 cm<sup>-1</sup>: Analysis of the Positions and Intensities in the First [2ν<sub>2</sub>, ν<sub>1</sub> and ν<sub>3</sub>] and Second [3ν<sub>2</sub>, ν<sub>1</sub> + ν<sub>2</sub> and ν<sub>2</sub> + ν<sub>3</sub>] Triad Region," *J.Mol. Spectrosc.* **188**, 148-174 (1998).

### Half-widths (air)

1. A. Goldman and J.R. Gillis, "Line Parameters and Line by Line Calculations for Molecules of Stratospheric Interest," University of Denver Progress Report (1984).
2. J. Waschull, F. Kuhnemann, and B. Sumpf, "Self-, air- and Helium Broadening of the ν<sub>2</sub> band of H<sub>2</sub>S," *J.Mol.Spectrosc.* **165**, 150-158 (1994).
3. B. Sumpf, I Meusel, and H.-D. Kronfeldt, "Self- and air-Broadening in the ν<sub>1</sub> and ν<sub>3</sub> bands of H<sub>2</sub>S," *J.Mol.Spectrosc.* **177**, 143-145 (1996).
4. A. Kissel, B. Sumpf, H.-D. Kronfeldt, B.A. Tikhomirov, and Yu.N. Ponomarev, "Molecular-Gas-Pressure-Induced Line-Shift and Line-Broadening in the ν<sub>2</sub>-Band of H<sub>2</sub>S," *J.Mol.Spectrosc.* **216**, 345-354 (2002).
5. B. Sumpf, A. Kissel, and H.-D. Kronfeldt, "Line-Broadening and Line-Shift in the ν<sub>1</sub>, ν<sub>3</sub>, and 2ν<sub>2</sub> bands of H<sub>2</sub>S," in preparation.
6. Average values of Refs 2-5.

### Half-widths (self)

1. J. Waschull, F. Kuhnemann, and B. Sumpf, "Self-, air- and Helium Broadening of the ν<sub>2</sub> band of H<sub>2</sub>S," *J.Mol.Spectrosc.* **165**, 150-158 (1994).

2. B. Sumpf, I Meusel, and H.-D. Kronfeldt, "Self- and air-Broadening in the  $\nu_1$  and  $\nu_3$  bands of  $\text{H}_2\text{S}$ ," *J.Mol.Spectrosc.* **177**, 143-145 (1996).
3. B. Sumpf, "Experimental Investigation of the Self-Broadening Coefficients in the  $\nu_1 + \nu_3$  band of  $\text{SO}_2$  and the  $2\nu_2$  band of  $\text{H}_2\text{S}$ ," *J.Mol.Spectrosc.* **181**, 160-167 (1997).
4. Average values of Refs 1-3.

Pressure shift (air)

1. A. Kissel, B. Sumpf, H.-D. Kronfeldt, B.A. Tikhomirov, and Yu.N. Ponomarev, "Molecular-Gas-Pressure-Induced Line-Shift and Line-Broadening in the  $\nu_2$ -Band of  $\text{H}_2\text{S}$ ," *J.Mol.Spectrosc.* **216**, 345-354 (2002).
2. B. Sumpf, A. Kissel, and H.-D. Kronfeldt, "Line-Broadening and Line-Shift in the  $\nu_1$ ,  $\nu_3$ , and  $2\nu_2$  bands of  $\text{H}_2\text{S}$ ," in preparation
3. L.S. Rothman, D. Jacquemart, A. Barbe, D.C. Benner, M. Birk, L.R. Brown, M. Carleer, C. Chackerian Jr, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, and G. Wagner, "The *HITRAN* 2004 Molecular Spectroscopic Database," *JQSRT* **96**, 139-204 (2005).



### Positions

1. A. Goldman, F.H. Murcray, D.G. Murcray, and C.P. Rinsland, "A Search for Formic Acid in the Upper Troposphere: A Tentative Identification of the  $1105\text{ cm}^{-1}$   $\nu_6$  band Q branch in High Resolution Balloon-borne Absorption Spectra," *Geophys.Res.Let.* **11**, 307-310 (1984); A. Goldman and J.R. Gillis, "Line Parameters and Line-by-line Calculations for Molecules of Stratospheric Interest," Progress Report, Dept. of Physics, Univ. Denver (1984).
2. A. Perrin, C.P. Rinsland, and A. Goldman, "Spectral parameters for the  $\nu_6$  region of HCOOH and its measurement in the infrared tropospheric spectrum," *J.Geophys.Res.* **104**, 18,661-18,666 (1999).
3. J. Vander Auwera, private communication (2004), based on J. Vander Auwera, "High-Resolution Investigation of the Far-Infrared Spectrum of Formic Acid," *J.Mol.Spectrosc.* **155**, 136-142 (1992).
4. A. Perrin and J. Vander Auwera, "An improved database for the  $9\text{ }\mu\text{m}$  region of the formic acid spectrum," *JQSRT* **108**, 363-370 (2007).
5. A. Perrin, J. Vander Auwera, and Z. Zelinger, "High-resolution Fourier transform study of the  $\nu_3$  fundamental band of *trans*-formic acid," *JQSRT* **110**, 743-755 (2009).

### Intensities

1. A. Goldman, F.H. Murcray, D.G. Murcray, and C.P. Rinsland, "A Search for Formic Acid in the Upper Troposphere: A Tentative Identification of the  $1105\text{ cm}^{-1}$   $\nu_6$  band Q branch in High Resolution Balloon-borne Absorption Spectra," *Geophys.Res.Let.* **11**, 307-310 (1984); A. Goldman and J.R. Gillis, "Line Parameters and Line-by-line Calculations for Molecules of Stratospheric Interest," Progress Report, Dept. of Physics, Univ. Denver (1984).
2. A. Perrin, C.P. Rinsland, and A. Goldman, "Spectral parameters for the  $\nu_6$  region of HCOOH and its measurement in the infrared tropospheric spectrum," *J.Geophys.Res.* **104**, 18,661-18,666 (1999).
3. J. Vander Auwera, private communication (2004), based on J. Vander Auwera, "High-Resolution Investigation of the Far-Infrared Spectrum of Formic Acid," *J.Mol.Spectrosc.* **155**, 136-142 (1992).
4. A. Perrin and J. Vander Auwera, "An improved database for the  $9\text{ }\mu\text{m}$  region of the formic acid spectrum," *JQSRT* **108**, 363-370 (2007); J. Vander Auwera, K. Didriche, A. Perrin, and F. Keller, "Absolute line intensities for formic acid and dissociation constant of the dimer," *J.Chem.Phys* **126**, 124311 (2007).
5. A. Perrin, J. Vander Auwera, and Z. Zelinger, "High-resolution Fourier transform study of the  $\nu_3$  fundamental band of *trans*-formic acid," *JQSRT* **110**, 743-755 (2009).

### Half-widths (air)

1. A. Goldman and J.R. Gillis, "Line Parameters and Line-by-line Calculations for Molecules of Stratospheric Interest," Progress Report, Dept. of Physics, Univ. Denver (1984).
2. A. Perrin and J. Vander Auwera, "An improved database for the  $9\text{ }\mu\text{m}$  region of the formic acid spectrum," *JQSRT* **108**, 363-370 (2007).

### Half-widths (self)

1. A. Perrin, C.P. Rinsland, and A. Goldman, "Spectral parameters for the  $\nu_6$  region of HCOOH and its measurement in the infrared tropospheric spectrum," *J.Geophys.Res.* **104**, 18,661-18,666

(1999).

2. A. Perrin and J. Vander Auwera, “An improved database for the 9  $\mu\text{m}$  region of the formic acid spectrum,” *JQSRT* **108**, 363-370 (2007). Note that the value takes into account the contribution from the dimer.

Temperature dependence of air-broadened half-width

1. A. Goldman, private communication (1996).

## HO<sub>2</sub> [33] 166

### Positions

1. C. Yamada, Y. Endo, and E. Hirota, "Difference frequency laser spectroscopy of the  $\nu_1$  band of the HO<sub>2</sub> radical," *J.Chem.Phys.* **78**, 4379-4384 (1983).
2. K. Nagai, Y. Endo, and E. Hirota, "Diode Laser Spectroscopy of the HO<sub>2</sub>  $\nu_2$  Band," *J.Mol.Spectrosc.* **89**, 520-527 (1981).
3. D.D. Nelson, Jr., and M.S. Zahniser, "Diode Laser Spectroscopy of the  $\nu_3$  Vibration of the HO<sub>2</sub> Radical," *J.Mol.Spectrosc.* **150**, 527-534 (1991).
4. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

### Intensities

1. M.S. Zahniser, K.E. McCurdy, and A.C. Stanton, "Quantitative Spectroscopic Studies of the HO<sub>2</sub> Radical: Band Strength Measurements for the  $\nu_1$  and  $\nu_2$  Vibrational Bands," *J.Phys.Chem.* **93**, 1065-1070 (1989).
2. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

### Half-widths (air)

1. D.D. Nelson and M.S. Zahniser "Air broadening measurements for the  $\nu_2$  vibrational band of the hydroperoxyl radical," *J.Mol.Spectrosc.* **166**, 273-279 (1994).
2. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52**, 447-457 (1994).

Positions

1. L.R. Zink, K.M. Evenson, F. Matsushima, T. Nelis, and R. L. Robinson, “Atomic oxygen fine-structure splittings with tunable far-infrared spectroscopy,” *Astrophys.J.* **371**, L85-L86 (1991).

Intensities

1. H.M. Pickett, R.L. Poynter, E.A. Cohen, M.L. Delitsky, J.C. Pearson, and H.S.P. Müller, “Submillimeter, Millimeter, and Microwave Spectral Line Catalog,” JPL Publication 800-23, rev. 4 (1996).

Half-widths (air)

1. Does not have the standard HITRAN definition of Lorentz air broadening, but a default value of  $0.05 \text{ cm}^{-1}/\text{atm}$  was appended.

## **ClONO<sub>2</sub> [35] 5646, 7646**

### Positions

**1.** W. Bell, G. Duxbury, and D.D. Stuart, "High-Resolution Spectra of the  $\nu_4$  Band of Chlorine Nitrate," *J.Mol.Spectrosc.* **152**, 283-297 (1992); A. Goldman, C.P. Rinsland, F.J. Murcray, R.D. Blatherwick, and D.G. Murcray, "High Resolution Studies of Heavy NO<sub>y</sub> Molecules in Atmospheric Spectra," *JQSRT* **52**, 367-377 (1994).

### Intensities

**1.** A. Goldman, C.P. Rinsland, F.J. Murcray, R.D. Blatherwick, and D.G. Murcray, "High Resolution Studies of Heavy NO<sub>y</sub> Molecules in Atmospheric Spectra," *JQSRT* **52**, 367-377 (1994).

### Half-widths (air)

**1.** A. Goldman, C.P. Rinsland, F.J. Murcray, R.D. Blatherwick, and D.G. Murcray, "High Resolution Studies of Heavy NO<sub>y</sub> Molecules in Atmospheric Spectra," *JQSRT* **52**, 367-377 (1994).

### Positions

1. Positions based on a fit by D.R. Smith, AF Phillips Lab, using data of F.P. Billingsley, *Chem.Phys.Lett.* **23**, 160-166 (1973), K.P. Huber and G. Herzberg, "Molecular Spectra and Molecular Structure IV. Constants of Diatomic Molecules," Van Nostrand Reinhold Co., NY (1979), and D.R. Smith, E.R. Huppi, and R.M. Nadile, "Improved Rotational Constants for the Ground Electronic State of NO<sup>+</sup> from Atmospheric Emission Spectra," private communication; D.R. Smith, E.R. Huppi, and J.O. Wise, "Observation of highly rotationally excited NO<sup>+</sup> emissions in the themosphere," *J.Atmos.Solar-Terrestrial Phys.* **62**, 1189-1198 (2000).
2. Positions based on a fit by I. Gordon (2006), using data of W.C. Ho, I. Ozier, D.T. Cramb, and M.C.L. Gerry, "Diode Laser Spectroscopy of the Vibrational Fundamental of NO<sup>+</sup>," *J.Mol.Spectrosc.* **149**, 559-561 (1991); G. Hilpert, H. Linnartz, M. Havenith, J.J. ter Meulen, and W.L. Meerts, "Tunable infrared and far-infrared direct absorption spectroscopy of molecular ions in a supersonic jet expansion," *Chem.Phys.Letters.* **219**, 384-388 (1994); M. López-Puertas, J.-M. Flaud, J. Peralta-Calvillo, B. Funke, and S. Gil-López, "NO<sup>+</sup> fundamental and first hot ro-vibrational line frequencies from MIPAS/Envisat atmospheric spectra," *J.Mol.Spectrosc.* **237**, 218-224 (2006); W.C. Bowman, E. Herbst, and F.C. De Lucia, "Millimeter and submillimeter spectrum of NO<sup>+</sup>," *J.Chem.Phys.* **77**, 4261-4262 (1982); E. Miescher, "Rotationsanalyse der NO<sup>+</sup>-banden," *Helv.Phys.Acta* **29**, 135-144 (1956).

### Intensities

1. H.-J. Werner and P. Rosmus, "Ab Initio Calculations of Radiative Transition Probabilities in the X<sup>1</sup>Σ<sup>+</sup> Ground State of the NO<sup>+</sup> Ion," *J.Mol.Spectrosc.* **96**, 362-367 (1982).

### Half-widths (air)

1. Default value of 0.06 cm<sup>-1</sup>/atm chosen, but applications are most likely not required to work in Lorentzian regime.



## **HOBr [37] 169, 161**

### Positions

1. E.A. Cohen, G.A. McRae, T.L. Tan, R.R. Friedl, J.W.C. Johns, and N. Noël, “The  $\nu_1$  Band of HOBr,” *J.Mol.Spectrosc.* **173**, 55-61 (1995).

### Intensities

1. Y. Koga, H. Takeo, S. Kondo, M. Sugie, C. Matsumura, G.A. Rae, and E.A. Cohen, “The Rotational Spectra, Molecular Structure, Dipole Moment, and Hyperfine Constants of HOBr and DOBr,” *J.Mol.Spectrosc.* **138**, 467-481 (1989).

### Half-widths (air)

1. A constant value of  $0.06 \text{ cm}^{-1}/\text{atm}$  has been assumed for the air-broadened halfwidth with a temperature-dependence coefficient  $n = 0.67$ .

## **C<sub>2</sub>H<sub>4</sub> [38] 221, 231**

### Positions

1. I. Cauuet, J. Walrand, G. Blanquet, A. Valentin, L. Henry, Ch. Lambeau, M. DeVleeschouwer, and A. Fayt, "Extension to Third-Order Coriolis Terms of the Analysis of  $\nu_{10}$ ,  $\nu_7$ , and  $\nu_4$  Levels of Ethylene on the Basis of Fourier Transform and Diode Laser Spectra," *J.Mol.Spectrosc.* **139**, 191-214 (1990); J. Legrand, M. Azizi, F. Herlemont, and A. Fayt, "Saturation Spectroscopy of C<sub>2</sub>H<sub>4</sub> Using a CO<sub>2</sub> Laser Sideband Spectrometer," *J.Mol.Spectrosc.* **171**, 13-21 (1995); E. Rusinek, H. Fichoux, M. Khelkhal, F. Herlemont, J. Legrand, and A. Fayt, "Subdoppler study of the  $\nu_7$  band of C<sub>2</sub>H<sub>4</sub> with a CO<sub>2</sub> Laser Sideband Spectrometer," *J.Mol.Spectrosc.* **189**, 64-73 (1998).
2. A.S. Pine, "Tunable laser survey of molecular air pollutants," Final Report NSF/ASRA/DAR 78-24562, MIT, Lexington, MA (1980).
3. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the  $\nu_{12}$  band of ethylene near 1450 cm<sup>-1</sup>: An experimental and theoretical study," *JQSRT* **109**, 952-962 (2008).

### Intensities

1. I. Cauuet, J. Walrand, G. Blanquet, A. Valentin, L. Henry, Ch. Lambeau, M. DeVleeschouwer, and A. Fayt, "Extension to Third-Order Coriolis Terms of the Analysis of  $\nu_{10}$ ,  $\nu_7$ , and  $\nu_4$  Levels of Ethylene on the Basis of Fourier Transform and Diode Laser Spectra," *J.Mol.Spectrosc.* **139**, 191-214 (1990); W.E. Blass, L. Jennings, A.C. Ewing, S.J. Daunt, M.C. Weber, L. Senesac, S. Hager, J.J. Hillman, D.C. Reuter, and J.M. Sirota, "Absolute intensities in the  $\nu_7$  band of ethylene: tunable laser measurements used to calibrate FTS broadband spectra," *JQSRT* **68**, 467-472 (2001).
2. A.S. Pine, "Tunable laser survey of molecular air pollutants," Final Report NSF/ASRA/DAR 78-24562, MIT, Lexington, MA (1980); M. Dang-Nhu, A.S. Pine, A. Fayt, M. DeVleeschouwer, and C. Lambeau, "Les intensités dans la pentade  $\nu_{11}$ ,  $\nu_2 + \nu_{12}$ ,  $2\nu_{10} + \nu_{12}$ ,  $\nu_9$  et  $\nu_3 + \nu_8 + \nu_{10}$  de <sup>12</sup>C<sub>2</sub>H<sub>4</sub>," *Can.J.Phys.* **61**, 514-521 (1983).
3. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the  $\nu_{12}$  band of ethylene near 1450 cm<sup>-1</sup>: An experimental and theoretical study," *JQSRT* **109**, 952-962 (2008).

### Half-widths (air)

1. J.F. Brannon, Jr. and P. Varanasi, "Tunable Diode Laser Measurements on the 951.7393 cm<sup>-1</sup> Line of <sup>12</sup>C<sub>2</sub>H<sub>4</sub> at Planetary Atmospheric Temperatures," *JQSRT* **47**, 237-242 (1992).
2. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the  $\nu_{12}$  band of ethylene near 1450 cm<sup>-1</sup>: An experimental and theoretical study," *JQSRT* **109**, 952-962 (2008).

### Half-widths (self)

1. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the  $\nu_{12}$  band of ethylene near 1450 cm<sup>-1</sup>: An experimental and theoretical study," *JQSRT* **109**, 952-962 (2008).

### Temperature dependence of air-broadened half-width

1. J.F. Brannon, Jr. and P. Varanasi, "Tunable Diode Laser Measurements on the 951.7393 cm<sup>-1</sup> Line of <sup>12</sup>C<sub>2</sub>H<sub>4</sub> at Planetary Atmospheric Temperatures," *JQSRT* **47**, 237-242 (1992).

## CH<sub>3</sub>OH [39] 2161

### Positions

1. L.H. Xu, R.M. Lees, P. Wang, L.R. Brown, I. Kleiner, and J.W.C. Johns, "New assignments, line intensities and HITRAN database for CH<sub>3</sub>OH at 10  $\mu$ m," *J.Mol.Spectrosc.* **228**, 453-470 (2004).
2. H.S.P. Müller, S. Thorwirth, D.A. Roth, and G Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS," *A&A* **370**, L49-L52 (2001).

### Intensities

1. L.H. Xu, R.M. Lees, P. Wang, L.R. Brown, I. Kleiner, and J.W.C. Johns, "New assignments, line intensities and HITRAN database for CH<sub>3</sub>OH at 10  $\mu$ m," *J.Mol.Spectrosc.* **228**, 453-470 (2004).
2. H.S.P. Müller, S. Thorwirth, D.A. Roth, and G Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS," *A&A* **370**, L49-L52 (2001).

### Half-widths (air)

1. L.H. Xu, R.M. Lees, P. Wang, L.R. Brown, I. Kleiner, and J.W.C. Johns, "New assignments, line intensities and HITRAN database for CH<sub>3</sub>OH at 10  $\mu$ m," *J.Mol.Spectrosc.* **228**, 453-470 (2004).

### Half-widths (self)

1. L.H. Xu, R.M. Lees, P. Wang, L.R. Brown, I. Kleiner, and J.W.C. Johns, "New assignments, line intensities and HITRAN database for CH<sub>3</sub>OH at 10  $\mu$ m," *J.Mol.Spectrosc.* **228**, 453-470 (2004).

### Temperature dependence of air-broadened half-width

1. L.H. Xu, R.M. Lees, P. Wang, L.R. Brown, I. Kleiner, and J.W.C. Johns, "New assignments, line intensities and HITRAN database for CH<sub>3</sub>OH at 10  $\mu$ m," *J.Mol.Spectrosc.* **228**, 453-470 (2004).

## CH<sub>3</sub>Br [40] 219, 211

### Positions

1. D. Jacquemart, F. Kwabia Tchana, N. Lacome, and I. Kleiner, "A complete set of line parameters for CH<sub>3</sub>Br in the 10- $\mu$ m spectral region," *JQSRT* **105**, 264-302 (2007).
2. F. Kwabia Tchana, I. Kleiner, J. Orphal, N. Lacome, and O. Bouba, "New analysis of the Coriolis-interacting  $\nu_2$  and  $\nu_5$  bands of CH<sub>3</sub><sup>79</sup>Br and CH<sub>3</sub><sup>81</sup>Br," *J Mol Spectrosc* **228**, 441-452 (2004).

### Intensities

1. D. Jacquemart, F. Kwabia Tchana, N. Lacome, and I. Kleiner, "A complete set of line parameters for CH<sub>3</sub>Br in the 10- $\mu$ m spectral region," *JQSRT* **105**, 264-302 (2007).
2. F. Kwabia Tchana, D. Jacquemart, N. Lacome, I. Kleiner, and J. Orphal, "Absolute line intensities in methyl bromide: The 7- $\mu$ m region," *J Mol Spectrosc* **235**, 132-143 (2006).

### Halfwidths (air)

1. D. Jacquemart, F. Kwabia Tchana, N. Lacome, and I. Kleiner, "A complete set of line parameters for CH<sub>3</sub>Br in the 10- $\mu$ m spectral region," *JQSRT* **105**, 264-302 (2007).

### Halfwidths (self)

1. D. Jacquemart, F. Kwabia Tchana, N. Lacome, and I. Kleiner, "A complete set of line parameters for CH<sub>3</sub>Br in the 10- $\mu$ m spectral region," *JQSRT* **105**, 264-302 (2007).

### Temperature dependence of air-broadened half-width

1. D. Jacquemart and H. Tran, "Temperature dependence of self- and N<sub>2</sub>-broadening coefficients for CH<sub>3</sub>Br in the 10- $\mu$ m spectral region," *JQSRT* **109**, 569-579 (2008).

Positions

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

Intensities

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

Halfwidths (air)

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

Halfwidths (self)

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

Temperature dependence of air-broadened half-width

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

Shifts

1. C.P. Rinsland, V. Malathy Devi, D. Chris Benner, T.A. Blake, R.L. Sams, L.R. Brown, I. Kleiner, A. Dehayem-Kamadjeu, H.S.P. Müller, R.R. Gamache, D.L. Niles, and T. Masiello, "Multispectrum analysis of the  $\nu_4$  band of CH<sub>3</sub>CN: Positions, intensities, self- and N<sub>2</sub>-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

## CF<sub>4</sub> [42] 29

### Positions

1. V. Boudon, Université de Bourgogne, private communication (2008).

### Intensities

1. V. Boudon, Université de Bourgogne, private communication (2008).

### Half-widths (air)

1. S. Höjer and R.D. May, “Air-Broadening Coefficients for the  $\nu_3$  Band of CF<sub>4</sub>,” *J.Mol.Spectrosc.* **178**, 139-142 (1996).

### Half-widths (self)

1. Estimate (0.08 cm<sup>-1</sup>atm<sup>-1</sup>).

### Temperature dependence of air-broadened half-width

1. S. Höjer and R.D. May, “Air-Broadening Coefficients for the  $\nu_3$  Band of CF<sub>4</sub>,” *J.Mol.Spectrosc.* **178**, 139-142 (1996).



## CS [46] 22, 23, 24, 32

### Positions

1. H.S.P. Müller, F. Schlöder, J. Stutzki, and G. Winnewisser, “The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists,” *J.Mol.Struct.* **742**, 215-227 (2005). Data adopted in June 2011.

### Intensities

1. S. Chandra, W.H. Kegel, R.J. Le Roy, and T. Hertenstein, “Einstein A-coefficients for Vib-rotational Transitions in CS,” *Astron.Astrophys.Suppl.Ser.* **114**, 175-177 (1995). (Intensities obtained from conversion of Einstein A-coefficients.)

### Half-widths (air)

1. G. Blanquet, J. Walrand, and J.-P. Bouanich, “N<sub>2</sub> Broadening of Carbon Disulfide <sup>12</sup>C<sup>32</sup>S<sub>2</sub> in the  $\nu_3$  and  $\nu_3-\nu_1$  Bands,” *J.Mol.Spectrosc.* **198**, 408-415 (1999). (Estimate obtained from extrapolating CS nitrogen-broadening parameters from CS<sub>2</sub>-nitrogen broadening parameters by comparing CO to CO<sub>2</sub> air-broadening parameters found in the HITRAN2008 database.)

### Half-widths (self)

1. F. Misago, M. Lepère, J.-P. Bouanich, and G. Blanquet, “Self-broadening Coefficients in the  $\nu_3-\nu_1$  Band of CS<sub>2</sub>,” *J.Mol.Spectrosc.* **254**, 16-19 (2009). (Estimate obtained from extrapolating CS nitrogen-broadening parameters from CS<sub>2</sub>-nitrogen broadening parameters by comparing CO to CO<sub>2</sub> self-broadening parameters found in the HITRAN2008 database.)

### Temperature dependence of air-broadened half-width

1. Default value of 0.75 chosen.

**\*\* Cross-section files \*\***

1. S.T. Massie, A. Goldman, D.G. Murcray, and J.C. Gille, "Approximate absorption cross sections of F12, F11, ClONO<sub>2</sub>, N<sub>2</sub>O<sub>5</sub>, HNO<sub>3</sub>, CCl<sub>4</sub>, CF<sub>4</sub>, F21, F113, F114, and HNO<sub>4</sub>," *Appl. Opt.* **24**, 3426-3427 (1985).
2. A.H. McDaniel, C.A. Cantrell, J.A. Davidson, R.E. Shetter, and J.G. Calvert, "The Temperature Dependent, Infrared Absorption Cross Sections for the Chlorofluorocarbons: CFC-11, CFC-12, CFC-13, CFC-14, CFC-22, CFC-113, CFC-114, and CFC-115," *J. Atmos. Chem.* **12**, 211-227(1991); S.T. Massie, A. Goldman, A.H. McDaniel, C.A. Cantrell, J.A. Davidson, R.E. Shetter, and J.G. Calvert, "Temperature Dependent Infrared Cross Sections for CFC-11, CFC-12, CFC-13, CFC-14, CFC-22, CFC-113, CFC-114, and CFC-115," NCAR Technical Note/TN-358+STR (1991).
3. C.A. Cantrell, J.A. Davidson, A.H. McDaniel, R.E. Shetter, and J.G. Calvert, "Infrared Absorption Cross Sections for N<sub>2</sub>O<sub>5</sub>," *Chem. Phys. Lett.* **148**, 358-363 (1988).
4. J.J. Orlando, G.S. Tyndall, A. Huang, and J.G. Calvert, "Temperature Dependence of the Infrared Absorption Cross Sections of Carbon Tetrachloride," *Geophys. Res. Lett.* **19**, 1005-1008 (1992).
5. J. Ballard, W.B. Johnston, M.R. Gunson, and P.T. Wassell, "Absolute Absorption Coefficients of ClONO<sub>2</sub> Infrared Bands at Stratospheric Temperatures," *J. Geophys. Res.* **93**, 1659-1665 (1988).
6. J. Orphal, M. Morillon-Chapey, and G. Guelachvili, "High-Resolution Absorption Cross Sections of Chlorine Nitrate in the  $\nu_2$  Band Region around 1292 cm<sup>-1</sup> at Stratospheric Temperatures," *J. Geophys. Res. D* **99**, 14549-14555 (1994).
7. K. Yoshino, D.E. Freeman, and W.H. Parkinson, "High Resolution Absorption Cross-Section Measurements of N<sub>2</sub>O at 295-299K in the Wavelength Region 170-222 nm," *Planet. Space Sci.* **32**, 1219-1222 (1984).
8. D.E. Freeman, K. Yoshino, J.R. Esmond, and W.H. Parkinson, "High Resolution Absorption Cross Sections Measurements of SO<sub>2</sub> at 213K in the Wavelength Region 172-240 nm," *Planet. Space Sci.* **32**, 1125-1134 (1984).
9. Z.H. Li and P. Varanasi, "Measurement of the Absorption Cross-Sections of CFC-11 at Conditions Representing Various Model Atmospheres," *JQSRT* **52**, 137-144 (1994).
10. P. Varanasi, V. Nemtchinov, Z. Li, and A. Cherukuri, "Spectral Absorption-coefficient Data on HCFC-22 and SF<sub>6</sub> for Remote Sensing Applications," *JQSRT* **52**, 323-332 (1994).
11. P. Varanasi and V. Nemtchinov, "Thermal Infrared Absorption Coefficients of CFC-12 at Atmospheric Conditions," *JQSRT* **51**, 679-687 (1994).
12. K. Smith, D. Newnham, M. Page, J. Ballard, and G. Duxbury, "Infrared Absorption Cross-sections and Integrated Absorption Intensities of HCF-134 and HCF-143a Vapour," *JQSRT* **59**, 437-451 (1998).
13. K. Smith, D. Newnham, M. Page, J. Ballard, and G. Duxbury, "Infrared Band Strengths and Absorption Cross-Sections of HFC-32 Vapour," *JQSRT* **56**, 73-82 (1996).
14. C. Clerbaux, R. Colin, P.C. Simon, and C. Granier, "Infrared Cross Sections and Global Warming Potentials of 10 Alternative Hydrohalocarbons," *J. Geophys. Res.* **98**, 10491-10497 (1993).
15. P. Varanasi, private communication (2000).
16. Q. Zou, C. Sun, V. Nemtchinov, and P. Varanasi, "Thermal infrared absorption cross-sections of C<sub>2</sub>F<sub>6</sub> at atmospheric temperatures," *JQSRT* **83**, 215-221 (2004).
17. A.C. Vandaele, C. Hermans, P.C. Simon, M. Carleer, R. Colin, S. Fally, M.F. Mérienne, A. Jenouvrier, and B. Coquart, "Measurements of the NO<sub>2</sub> absorption cross-section from 42000

- cm<sup>-1</sup> to 10000 cm<sup>-1</sup> (238-1000 nm) at 220 K and 294 K,” *JQSRT* **59**, 171-184 (1997).
18. G. Wagner and M. Birk, “New infrared spectroscopic database for chlorine nitrate,” *JQSRT* **82**, 443-460 (2003).
  19. A.M. Bass and R.J. Paur, “UV absorption cross-sections for ozone: The temperature dependence,” *J.Photochem.* **17**, 141 (1981); A.M. Bass and R.J. Paur, “The ultraviolet cross-sections of ozone: I The measurements,” *Atmospheric Ozone*, edited by C.S. Zerefos and A. Ghazi, pp. 606-610, D. Reidel, Dordrecht, 1985; R.J. Paur and A.M. Bass, “The ultraviolet cross-sections of ozone: II Results and temperature dependence,” *Atmospheric Ozone*, edited by C. S. Zerefos and A. Ghazi, pp. 611-616, D. Reidel, Dordrecht, 1985.
  21. V. Nemtchinov and P. Varanasi, “Absorption cross-sections of HFC-134a in the spectral region between 7 and 12 μm,” *JQSRT* **83**, 285-294 (2004).
  22. V. Nemtchinov and P. Varanasi, “Thermal Infrared Absorption Cross-sections of CCl<sub>4</sub> needed for Atmospheric Remote-Sensing,” *JQSRT* **82**, 473-482 (2003).
  23. V. Nemtchinov and P. Varanasi, “Thermal infrared absorption cross-sections of CF<sub>4</sub> for atmospheric applications,” *JQSRT* **82**, 461-472 (2003).
  24. C.P. Rinsland, S.W. Sharpe, and R.L. Sams, “Temperature-dependent cross-sections in the thermal infrared bands of SF<sub>5</sub>CF<sub>3</sub>,” *JQSRT* **82**, 483-490 (2003).
  25. C.A. Cantrell, J.A. Davidson, A.H. McDaniel, R.E. Shetter, and J.G. Calvert, “Temperature-dependent formaldehyde cross sections in the near-ultraviolet spectral region,” *J.Phys.Chem.* **94**, 3902-3908 (1990).
  26. D.M. Wilmouth, T.F. Hanisco, N.M. Donahue, and J.G. Anderson, “Fourier Transform Ultraviolet Spectroscopy of the A <sup>2</sup>Π<sub>3/2</sub> - X <sup>2</sup>Π<sub>3/2</sub> Transition of BrO,” *J.Phys.Chem.* **103**, 8935-8945 (1999).
  27. R.D. May and R.R. Friedl, “Integrated band intensities of HO<sub>2</sub>NO<sub>2</sub> at 220 K,” *JQSRT* **50**, 257-266 (1993).
  28. G.D. Greenblatt, J.J. Orlando, J.B. Burkholder, and A.R. Ravishankara, “Absorption measurements of oxygen between 330 and 1140 nm,” *J.Geo.Res.* **95**, 18577-18582 (1990).
  29. H. Kromminga, J. Orphal, P. Spietz, S. Voigt, and J.P. Burrows, “The temperature dependence (213-293 K) of the absorption cross-sections of OClO in the 340-450 nm region measured by Fourier-transform spectroscopy,” *J.Photochemistry and Photobiology A: Chemistry* **157**, 149-160 (2003).
  30. J. Orphal, C.E. Fellows, and P.-M. Flaud, “The visible absorption spectrum of NO<sub>3</sub> measured by high-resolution Fourier-transform spectroscopy,” *J.Geo.Res.* **108 (D3)**, 4077 (2003).
  31. G. Allen, J.J. Remedios, D.A. Newnham, K.M. Smith, and P.S. Monks, “High resolution mid-infrared cross-sections for peroxyacetyl nitrate (PAN) vapour,” *Atmos. Chem. Phys. Discuss.* **4**, 5656-5681 (2004).
  32. C.P. Rinsland, S.W. Sharpe, and R.L. Sams, “Temperature-dependent infrared absorption cross-sections of methyl cyanide (acetonitrile)” *JQSRT* **96**, 271-280 (2005).
  33. C.P. Rinsland, V.M. Devi, T.A. Blake, R.L. Sams, S. Sharpe, and L. Chiou, “Quantitative measurement of integrated band intensities of benzene vapor in the mid-infrared at 278, 298, and 323 K,” *JQSRT* **109**, 2511-2522 (2008).
  34. S. Fally, M. Carleer, and A.C. Vandaele, “UV Fourier transform absorption cross sections of benzene, toluene, meta-, ortho-, and para-xylene,” *JQSRT* **110**, 766-782 (2009).
  35. C. Hermans, A.C. Vandaele, and S. Fally, “Fourier Transform measurements of SO<sub>2</sub> absorption cross sections: I. Temperature dependence in the 23 500 - 29 000 cm<sup>-1</sup> (345-425 nm) region,” *JQSRT* **110**, 756-765 (2009); A.C. Vandaele, C. Hermans, and S. Fally, “Fourier

Transform measurements of SO<sub>2</sub> absorption cross sections: II. Temperature dependence in the 29 000 – 44 000 cm<sup>-1</sup> (227-345 nm) region,” *JQSRT* **110**, 2115-2126 (2009).

**36.** G. Di Lonardo and G. Masciarelli, “Infrared cross-sections and integrated absorption intensities of HFC-125 and HFC-143a,” *JQSRT* **66**, 129-142 (2000).

**37.** J.J. Harrison and P.F. Bernath, “Infrared absorption cross sections for propane (C<sub>3</sub>H<sub>8</sub>) in the 3 μm region,” *JQSRT* **111**, 1282-1288 (2010).

**38.** J.J. Harrison, N.D.C. Allen, and P.F. Bernath, “Infrared absorption cross sections for ethane (C<sub>2</sub>H<sub>6</sub>) in the 3 μm region,” *JQSRT* **111**, 357-363 (2010).

**39.** J.J. Harrison, N.D.C. Allen, and P.F. Bernath, “Infrared absorption cross sections for acetone (propanone) in the 3 μm region,” *JQSRT* **112**, 53-58 (2011).

**40.** K.A. Tereszchuk and P.F. Bernath, “Infrared absorption cross sections for acetaldehyde (CH<sub>3</sub>CHO) in the 3 μm region,” *JQSRT* **112**, 990-993 (2011).

**41.** J.J. Harrison, N. Humpage, N.D.C. Allen, A.M. Waterfall, P.F. Bernath, and J.J. Remedios, “Mid-infrared absorption cross sections for acetone (propanone),” *JQSRT* **112**, 457-464 (2011).

**42.** Data originally from A.M. Waterfall, “Measurement of organic compounds in the upper troposphere using infrared remote sensing,” D.Phil. thesis, University of Oxford, 2004, is scaled in Ref. 41 above.

**43.** N.D.C. Allen, J.J. Harrison, and P.F. Bernath, “Acetonitrile (CH<sub>3</sub>CN) infrared absorption cross sections in the 3 μm region,” *JQSRT* **112**, 1961-1966 (2011).

**44.** K. Chance and J. Orphal, “Revised ultraviolet absorption cross sections of H<sub>2</sub>CO for the HITRAN database,” *JQSRT* **112**, 1509-1510 (2011).

**45.** K. Le Bris and K. Strong, “Temperature-dependent absorption cross-sections of HCFC-142b,” *JQSRT* **111**, 364-371 (2010).

**\*\* Collision Induced Absorption (CIA) files \*\***

1. K. Smith K and D. Newnham, "Near-infrared absorption cross sections and integrated absorption intensities of molecular oxygen ( $O_2$ ,  $O_2$ - $O_2$ , and  $O_2$ - $N_2$ )," *J.Geophys.Res.* **105**, 7383-7396 (2000).
2. G. Orton, Jet Propulsion Laboratory, private communication (2011).
3. Y.I. Baranov, W.J. Lafferty, and G.T. Fraser, "Investigation of collision-induced absorption in the vibrational fundamental bands of  $O_2$  and  $N_2$  at elevated temperatures," *J.Mol.Spectrosc.* **233**, 160-163 (2005).
4. W.J. Lafferty, A.M. Solodov, A. Weber, W.B. Olson, and J.-M. Hartmann, "Infrared collision-induced absorption by  $N_2$  near 4.3  $\mu m$  for atmospheric applications: measurements and empirical modeling," *Appl.Opt.* **35**, 5911-5917 (1996).
5. H. Tran, C. Boulet, and J.-M. Hartmann, "Line mixing and collision-induced absorption by oxygen in the A band: Laboratory measurements, model, and tools for atmospheric spectra computations," *J.Geophys.Res.* **111**, D15210 (2006).
6. M. Vangvichith, H. Tran, and J.-M. Hartmann, "Line-mixing and collision induced absorption for  $O_2$ - $CO_2$  mixtures in the oxygen A-band region," *JQSRT* **110**, 2212-2216 (2009).
7. M. Abel, L. Frommhold, X. Li, and K.L.C. Hunt, "Collision-Induced Absorption by  $H_2$  Pairs: From Hundreds to Thousands of Kelvin," *J.Phys.Chem. A* (2011).
8. M. Abel, L. Frommhold, X. Li, and K. Hunt, "Infrared absorption by collisional  $H_2$ -He complexes at temperatures up to 9,000 K and frequencies from 0 to 20,000  $cm^{-1}$ ," *J.Chem.Phys.* in press (2011).
9. G.D. Greenblatt, J.J. Orlando, J.B. Burkholder, and A.R. Ravishankara, "Absorption measurements of oxygen between 330 and 1140 nm," *J.Geophys.Res.* **95**, 18577-18582 (1990).
10. Christian Hermans, *et al.*, Belgian Institute of Space Aeronomy, see <http://spectrolab.aeronomie.be/o2.htm> (downloaded April, 2011).

## Molecules and isotopologues in line-by-line portion of HITRAN

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm <sup>-1</sup> )	Number of lines	Total number
1	H <sub>2</sub> O	161	0.9973	0 – 25233	37432	69201
		181	1.999 10 <sup>-3</sup>	0 – 14519	9753	
		171	3.719 10 <sup>-4</sup>	10 – 14473	6992	
		162	3.107 10 <sup>-4</sup>	0 – 22708	13238	
		182	6.230 10 <sup>-7</sup>	0 – 3825	1611	
		172	1.158 10 <sup>-7</sup>	1234 – 1599	175	
2	CO <sub>2</sub>	626	0.9842	352 – 12785	128170	314919
		636	1.106 10 <sup>-2</sup>	438 – 12463	49777	
		628	3.947 10 <sup>-3</sup>	0 – 11423	79958	
		627	7.339 10 <sup>-4</sup>	0 – 8271	19264	
		638	4.434 10 <sup>-5</sup>	489 – 6745	26737	
		637	8.246 10 <sup>-6</sup>	583 – 6769	2953	
		828	3.957 10 <sup>-6</sup>	491 – 8161	7118	
		827	1.472 10 <sup>-6</sup>	626 – 5047	821	
		838	4.446 10 <sup>-8</sup>	4599 – 4888	121	
3	O <sub>3</sub>	666	0.9929	0 – 5787	249456	409686
		668	3.982 10 <sup>-3</sup>	0 – 2768	44302	
		686	1.991 10 <sup>-3</sup>	1 – 2740	18887	
		667	7.405 10 <sup>-4</sup>	0 – 2122	65106	
		676	3.702 10 <sup>-4</sup>	0 – 2101	31935	
4	N <sub>2</sub> O	446	0.9903	0 – 7797	33074	47843
		456	3.641 10 <sup>-3</sup>	5 – 5086	4222	
		546	3.641 10 <sup>-3</sup>	4 – 4704	4592	
		448	1.986 10 <sup>-3</sup>	542 – 4672	4250	
		447	3.693 10 <sup>-4</sup>	550 – 4430	1705	
5	CO	26	0.9865	3 – 8465	917	4477
		36	1.108 10 <sup>-2</sup>	3 – 6279	780	
		28	1.978 10 <sup>-3</sup>	3 – 6267	760	
		27	3.679 10 <sup>-4</sup>	3 – 6339	728	
		38	2.222 10 <sup>-5</sup>	3 – 6124	712	
		37	4.133 10 <sup>-6</sup>	1807 – 6197	580	
6	CH <sub>4</sub>	211	0.9883	0 – 9200	212061	290091
		311	1.110 10 <sup>-2</sup>	0 – 6070	28793	
		212	6.158 10 <sup>-4</sup>	7 – 6511	45024	
		312	6.918 10 <sup>-6</sup>	959 – 1695	4213	
7	O <sub>2</sub>	66	0.9953	0 – 15928	1431	6430
		68	3.991 10 <sup>-3</sup>	1 – 15852	674	
		67	7.422 10 <sup>-4</sup>	0 – 14537	4325	



Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm <sup>-1</sup> )	Number of lines	Total number
8	NO	46	0.9940	0 – 9274	103701	105079
		56	3.654 10 <sup>-3</sup>	1609 – 2061	699	
		48	1.993 10 <sup>-3</sup>	1602 – 2039	679	
9	SO <sub>2</sub>	626	0.9457	0 – 4093	72460	95121
		646	4.195 10 <sup>-2</sup>	0 – 2501	22661	
10	NO <sub>2</sub>	646	0.9916	0 – 3075	104223	104223
11	NH <sub>3</sub>	446	0.9959	0 – 5295	27994	29084
		456	3.661 10 <sup>-3</sup>	0 – 5180	1090	
12	HNO <sub>3</sub>	146	0.9891	0 – 1770	487254	487254
13	OH	61	0.9975	0 – 19268	30769	31976
		81	2.000 10 <sup>-3</sup>	0 – 329	295	
		62	1.554 10 <sup>-4</sup>	0 – 332	912	
14	HF	19	0.9998	41 – 11536	107	107
15	HCl	15	0.7576	20 – 13459	324	613
		17	0.2422	20 – 10995	289	
16	HBr	19	0.5068	16 – 9759	651	1293
		11	0.4931	16 – 9758	642	
17	HI	17	0.9998	12 – 8488	806	806
18	ClO	56	0.7559	0 – 1208	5721	11501
		76	0.2417	0 – 1200	5780	
19	OCS	622	0.9374	0 – 4200	15618	29361
		624	4.158 10 <sup>-2</sup>	0 – 4166	6087	
		632	1.053 10 <sup>-2</sup>	0 – 4056	3129	
		623	7.399 10 <sup>-3</sup>	0 – 4164	2886	
		822	1.880 10 <sup>-3</sup>	0 – 4046	1641	
20	H <sub>2</sub> CO	126	0.9862	0 – 3100	36120	37050
		136	1.108 10 <sup>-2</sup>	0 – 73	563	
		128	1.978 10 <sup>-3</sup>	0 – 48	367	
21	HOCl	165	0.7558	1 – 3800	8877	16276
		167	0.2417	1 – 3800	7399	
22	N <sub>2</sub>	44	0.9927	1992 – 2626	120	120
23	HCN	124	0.9851	0 – 3424	2955	4253
		134	1.107 10 <sup>-2</sup>	2 – 3405	652	
		125	3.622 10 <sup>-3</sup>	2 – 3420	646	
24	CH <sub>3</sub> Cl	215	0.7489	0 – 3173	100293	196220
		217	0.2395	0 – 3162	95927	
25	H <sub>2</sub> O <sub>2</sub>	1661	0.9950	0 – 1731	126983	126983
26	C <sub>2</sub> H <sub>2</sub>	1221	0.9776	604 – 9890	11055	11340
		1231	2.197 10 <sup>-2</sup>	613 – 6589	285	

27	C <sub>2</sub> H <sub>6</sub>	1221	0.9770	706 – 3001	28439	28439
28	PH <sub>3</sub>	1111	0.9995	770 – 3602	20099	20099
Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm <sup>-1</sup> )	Number of lines	Total number
29	COF <sub>2</sub>	269	0.9865	725 – 2002	70601	70601
30	SF <sub>6</sub>	29	0.9502	580 – 996	2889065	2889065
31	H <sub>2</sub> S	121	0.9499	2 – 4257	12330	20788
		141	4.214 10 <sup>-2</sup>	5 – 4172	4894	
		131	7.498 10 <sup>-3</sup>	5 – 4099	3564	
32	HCOOH	126	0.9839	10 – 1890	62684	62684
33	HO <sub>2</sub>	166	0.9951	0 – 3676	38804	38804
34	O	6	0.9976	68 – 159	2	2
35	ClONO <sub>2</sub>	5646	0.7496	763 – 798	21988	32199
		7646	0.2397	765 – 791	10211	
36	NO <sup>+</sup>	46	0.9940	1634 – 2531	1206	1206
37	HOBr	169	0.5056	0 – 316	2177	4358
		161	0.4919	0 – 316	2181	
38	C <sub>2</sub> H <sub>4</sub>	221	0.9773	701 – 3243	18097	18378
		231	2.196 10 <sup>-2</sup>	2947 – 3181	281	
39	CH <sub>3</sub> OH	2161	0.9859	0 – 1408	19897	19897
40	CH <sub>3</sub> Br	219	0.5010	794 – 1706	18692	36911
		211	0.4874	796 – 1697	18219	
41	CH <sub>3</sub> CN	2124	0.9739	890 – 946	3572	3572
42	CF <sub>4</sub>	29	0.9889	594 – 1313	60033	60033

Note: Rows highlighted in pink are for molecules that have been relegated to a sub-folder since they do not have sufficient hot bands included.

### Uncertainty Codes used in HITRAN Database

Line position and Pressure shift (cm <sup>-1</sup> )		Intensity, Halfwidths, and Temperature-dependence	
Code	Uncertainty Range	Code	Uncertainty Range
0	≥1. or Unreported	0	Unreported or Unavailable
1	≥0.1 and <1.	1	Default or Constant
2	≥0.01 and <0.1	2	Average or Estimate
3	≥0.001 and <0.01	3	≥ 20%
4	≥0.0001 and <0.001	4	≥ 10% and < 20%
5	≥0.00001 and <0.0001	5	≥ 5% and < 10%
6	≥0.000001 and <0.00001	6	≥ 2% and < 5%
7	≥0.0000001 and <0.000001	7	≥ 1% and < 2%
8	≥0.00000001 and <0.0000001	8	< 1%
9	≥0.000000001		