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CO_2 [2] 626, 636, 628, 627, 638, 637, 828, 827, 838, 837

Positions

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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 $^{16}O_3$," *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, Vl.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 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, Vl.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 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 $^{16}O_3$*," 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.

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25. S.N. Mikhailenko and A. Barbe, private communication (2008). Line intensities were calculated with transition moment parameters from S.N. Mikhailenko, A. Barbe, Vl.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).
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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, Vl.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, Vl.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, Vl.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, Vl.G. Tyuterev, "Extended analysis of line positions and intensities of ozone bands in the 2900-3400 cm^{-1} region," *J.Mol.Spectrosc.* **215**, 29-41 (2002).
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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 Insitute of Atmosperic 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 N_2-broadened halfwidths of $^{16}O_3$," *Appl.Opt.* **24,** 1651-1655 (1985) scaled by 0.90 (N_2/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.G.R.* **107,** D22 (2002).
5. Use of values obtained for the ν_3 band from Ref. 4.
6. Use of values obtained for the ν_1/ ν_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-μm 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 $^{16}O^{16}O^{17}O$ and $^{16}O^{17}O^{16}O$ 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_2-broadened halfwidths of ozone," *J.Mol.Spectrosc.* **114,** 114-131 (1985).
2. G. Wagner, M. Birk, F. Schreier, and J.-M. Flaud, "Spectroscopic database for ozone in the fundamental spectral regions," *J.G.R.* **107,** D22 (2002).
3. Use of values obtained for the ν_3 band from Ref. 2.
4. Use of values obtained for the ν_1/ ν_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_3 lines in the ν_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_3 lines in the ν_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_3 lines in the 3-μm 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_3 lines in the 3-μm region" by M.A.H. Smith, C.P. Rinsland, V. Malathy Devi, and E.S. Prochaska," *J.Mol.Spectrosc.* **165,** 596 (1994).

N_2O [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_2O between 900 and 4700 cm^{-1}," *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 ν_2 fundamental of N_2O at 17 μm," *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 $^{14}N_2{}^{16}O$: the 10 micrometers region revisited," *JQSRT* **72,** 37-55 (2002).
6. R.A. Toth, "Linelist of N_2O parameters from 500 to 7500 cm^{-1}," see http://mark4sun.jpl.nasa.gov/data/spec/N2O.
7. L. Daumont, J. Vander Auwera, J.-L. Teffo, V.I. Perevalov, and S.A. Tashkun, "Line Intensity Measurements in $^{14}N_2{}^{16}O$ 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 ν_2 fundamental of N_2O at 17 μm," *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 $^{14}N_2{}^{16}O$: 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 $^{14}N_2{}^{16}O$ and their Treatment using the Effective Dipole Moment Approach," *J.Mol.Spectrosc.* **208,** 281-291 (2001).
5. R.A. Toth, "Linelist of N_2O parameters from 500 to 7500 cm^{-1}," see http://mark4sun.jpl.nasa.gov/data/spec/N2O.

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_2-, and

O_2-broadening of N_2O 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_2-, and O_2-broadening of N_2O lines: temperature dependence of linewidths," *Appl.Opt.* **23,** 425-434 (1984); R.A. Toth, "N_2- and air-broadened linewidths and frequency-shifts of N_2O," *JQSRT* **66**, 285-304 (2000); and V. Nemtchinov, C. Sun, and P. Varanasi, "Measurements of Line Intensities and Line Widths in the ν_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^{-1}), self-broadened linewidths, and frequency shifts (1800-2660 cm^{-1}) of N_2O," *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_2-, and O_2-broadening of N_2O 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 ν_3-fundamental Band of Nitrous Oxide at Atmospheric Temperatures," *JQSRT* **83,** 267-284 (2004).

Pressure shift (air)
1. R.A. Toth, "Linelist of N_2O parameters from 500 to 7500 cm^{-1}," see http://mark4sun.jpl.nasa.gov/data/spec/N2O.

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 μm; 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).

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 $^{12}C^{16}O$ line shapes in the v = 2 ← 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 $^{12}C^{16}O$" *JQSRT* **83,** 445-458 (2004).

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 cm^{-1}/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 cm^{-1}/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 $^{12}C^{16}O$ 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 cm^{-1}/atm). For the 2-0 band, values for transitions having $-23 \geq m \geq 24$ are assumed to be constant (-0.0055 cm^{-1}/atm).

2. K. Sung and P. Varanasi, "Intensities, collision-broadened half-widths, and collision-induced line shifts in the second overtone band of $^{12}C^{16}O$," *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 cm^{-1}/atm).

CH_4 [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 ν_2/ν_4 dyad of $^{12}CH_4$ and $^{13}CH_4$," *J.Mol.Spectrosc.* **133,** 256-272 (1989).

9. L.R. Brown, "Methane line parameters from 3700 to 4136 cm^{-1}," *Appl.Opt.* **27,** 3275-3279 (1988).

10. J.S. Margolis, "Measured line positions and strengths of methane between 5500 and 6180 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 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 Spectroscopyu of Rovibrational Transitions in the ν_2 - ν_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).

15. G. Tarrago, M. Delaveau, L. Fusina, and G. Guelachvili, "Absorption of $^{12}CH_3D$ at 6-10 μm: triad ν_3, ν_5, ν_6," *J.Mol.Spectrosc.* **126,** 149-158 (1987); for ν_2, C. Chackerian, NASA Ames Research Center, unpublished (1990).

18. L.R. Brown and L.S. Rothman, "Methane line parameters for the 2.3-μm region," *Appl.Opt.* **21,** 2425-2427 (1982).

19. L.R. Brown, "Empirical Lower State Energies of Methane at 2.5-μm," 3rd International Conference on Laboratory Research for Planetary Atmospheres (1991).

20. G.S. Orton and A.G. Robiette, "A Line Parameter List for the ν_2 and ν_4 Bands of $^{12}CH_4$ and $^{13}CH_4$, 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 cm^{-1}," *Appl.Opt.* **20,** 932-935 (1981).

22. B. Bobin and K. Fox, "New analysis of ν_3 of $^{12}CH_4$," *J.Chem.Phys.* **58,** 1771-1773 (1973).

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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←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←0) band.

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Half-widths (air)

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Half-widths (self)

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Temperature dependence of air-broadened half-width

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Half-widths (air)

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NO_2 [10] 646

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NH_3 [11] 4111, 5111

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Positions

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15. Intensities have been rescaled by multiplying by a factor of 1.067, Ref. 7

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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_3 line parameters using MIPAS satellite measurements," *Atmos. Chem. Phys. Discuss.* **6,** 4251-4272 (2006).

OH [13] 61, 81, 62

Positions

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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).

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Temperature dependence of air-broadened half-width

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HF [14] 19

Positions

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HCl [15] 15, 17

Positions

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Half-widths (air)

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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

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Pressure shift (air)

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HBr [16] 19, 11

Positions

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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

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Intensities

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ClO [18] 56, 76

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OCS [19] 622, 624, 632, 623, 822

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Half-widths (air)

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H_2CO [20] 126, 136, 128

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Half-widths (air)

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HOCl [21] 165, 167

Positions

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N_2 [22] 44

Positions

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Halfwidths (self)

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HCN [23] 124, 134, 125

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Pressure shift (air)
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C_2H_6 [27] 1221

Positions

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Half-widths (air)

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Half-widths (self)

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Pressure shift (air)

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PH_3 [28] 1111

Positions

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Half-widths (air)

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Half-widths (self)

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Temperature dependence of air-broadened half-width

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COF_2 [29] 269

Positions

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5. C.P. Rinsland, NASA Langley Research Center, private communication (1992).
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Half-widths (air)

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SF_6 [30] 29

Positions

1. C.P. Rinsland, L.R. Brown, and C.B. Farmer, "Infrared Spectroscopic Detection of Sulfur Hexafluoride (SF_6) 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 (ν_3=1) States of $^{32}SF_6$ from Saturated Absorption Spectroscopy," *J.Mol.Spectrosc.* **121,** 91-127 (1987); B. Bobin, private communication (1990).
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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).
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Half-widths (air)

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Half-widths (self)

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Temperature dependence of air-broadened half-width

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H_2S [31] 121,141,131

Positions

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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).
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5. B. Sumpf, A. Kissel, and H.-D. Kronfeldt, "Line-Broadening and Line-Shift in the ν_1, ν_3, and $2\nu_2$ bands of H_2S," in preparation.
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Half-widths (self)

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Pressure shift (air)

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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).

HCOOH [32] 126

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 cm^{-1} ν_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 ν_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 μm 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 ν_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 cm^{-1} ν_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 ν_6 region of HCOOH and its measurement in the infrared tropospheric spectrum," *J.Geophys.Res.* **104,** 18,661-18,666 (1999).
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4. A. Perrin and J. Vander Auwera, "An improved database for the 9 μm 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 ν_3 fundamental band of *trans*-formic acid," *JQSRT* **110,** 743-755 (2009).

Intensities

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 μm 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 ν_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 μm 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_2 [33] 166

Positions

1. C. Yamada, Y. Endo, and E. Hirota, "Difference frequency laser spectroscopy of the ν_1 band of the HO_2 radical," *J.Chem.Phys.* **78,** 4379-4384 (1983).
2. K. Nagai, Y. Endo, and E. Hirota, "Diode Laser Spectroscopy of the HO_2 ν_2 Band," *J.Mol.Spectrosc.* **89,** 520-527 (1981).
3. D.D. Nelson, Jr., and M.S. Zahniser, "Diode Laser Spectroscopy of the ν_3 Vibration of the HO_2 Radical," *J.Mol.Spectrosc.* **150,** 527-534 (1991).
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Intensities

1. M.S. Zahniser, K.E. McCurdy, and A.C. Stanton, "Quantitative Spectroscopic Studies of the HO_2 Radical: Band Strength Measurements for the ν_1 and ν_2 Vibrational Bands," *J.Chem.Phys.* **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 ν_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).

O [34] 6

Positions

1. L.R. Zink, K.M. Evenson, F. Matsuchima, T. Nelis, and R. L. Robinson, "Atomic oxygen fine-structure splittings with tunable far-infrared spectroscopy," *Astrophys.J.* **371,** L85 (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 cm^{-1}/atm was appended.

$ClONO_2$ [35] 5646, 7646

Positions

1. W. Bell, G. Duxbury, and D.D. Stuart, "High-Resolution Spectra of the ν_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 NOy 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 NOy 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 NOy Molecules in Atmospheric Spectra," *JQSRT* **52,** 367-377 (1994).

NO^+ [36] 46

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^+ from Atmospheric Emission Spectra," in preparation; D.R. Smith, E.R. Huppi, and J.O. Wise, "Observation of highly rotationally excited NO^+ 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^+," *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^+ fundamental and first hot ro-vibrational line frequencies from MIPAS/Envisat atmospheric spectra," *J.Mol.Spectrosc.* **237,** 218-224 (1996); W.C. Bowman, E. Herbst, and F.C. De Lucia, "Millimeter and submillimeter spectrum of NO^+," *J.Chem.Phys.* **77,** 4261–4262 (1982); E. Miescher, "Rotationsanalyse der NO^+-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 $X^1\Sigma^+$ Ground State of the NO^+ Ion," *J.Mol.Spectrosc.* **96,** 362-367 (1982).

Half-widths (air)

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

C_2H_4 [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 ν_{10}, ν_7, and ν_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_2H_4 Using a CO_2 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 ν_7 band of C_2H_4 with a CO_2 Laser Sideband Spectrometer," *J.Mol.Spectrosc.* 189, 64-73 (1998).

2. A.S. Pine, "Tunable laser survey of molecular air poluants," 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 ν_{12} band of ethylene near 1450 cm^{-1}: 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 ν_{10}, ν_7, and ν_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 ν_7 band of ethylene: tunable laser measurements used to calibrate FTS broadband spectra," *JQSRT* **68,** 467-472 (2001).

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3. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the ν_{12} band of ethylene near 1450 cm^{-1}: 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^{-1} Line of $^{12}C_2H_4$ at Planetary Atmospheric Temperatures," *JQSRT* **47,** 237-242 (1992).

2. M. Rotger, V. Boudon, and J. Vander Auwera, "Line positions and intensities in the ν_{12} band of ethylene near 1450 cm^{-1}: 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 ν_{12} band of ethylene near 1450 cm^{-1}: 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^{-1}

Line of $^{12}C_2H_4$ at Planetary Atmospheric Temperatures," *JQSRT* **47,** 237-242 (1992).

CH_3OH [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_3OH at 10 μm," *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_3OH at 10 μm," *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_3OH at 10 μm," *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_3OH at 10 μm," *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_3OH at 10 μm," *J.Mol.Spectrosc.* **228,** 453-470 (2004).

CH_3Br [40] 219, 211

Positions

1. D. Jacquemart, F. Kwabia Tchana, N. Lacome, and I. Kleiner, "A complete set of line parameters for CH_3Br in the 10-μm 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 ν_2 and ν_5 bands of $CH_3{}^{79}Br$ and $CH_3{}^{81}Br$," *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_3Br in the 10-μm 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-μm 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_3Br in the 10-μm 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_3Br in the 10-μm 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_2-broadening coefficients for CH_3Br in the 10-μm spectral region," *JQSRT* **109**, 569-579 (2008).

CH_3CN [41] 2124

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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-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 ν_4 band of CH_3CN: Positions, intensities, self- and N_2-broadening, and pressure-induced shifts," *JQSRT* **109**, 974-994 (2008).

CF_4 [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 ν_3 Band of CF_4," *J.Mol.Spectrosc.* **178**, 139-142 (1996).

Half-widths (self)

1. Estimate (0.08 $cm^{-1}atm^{-1}$).

Temperature dependence of air-broadened half-width

1. S. Höjer and R.D. May, "Air-Broadening Coefficients for the ν_3 Band of CF_4," *J.Mol.Spectrosc.* **178**, 139-142 (1996).

** Cross-section files **

1. S.T. Massie, A. Goldman, D.G. Murcray, and J.C. Gille, "Approximate absorption cross sections of F12, F11, $ClONO_2$, N_2O_5, HNO_3, CCl_4, CF_4, F21, F113, F114, and HNO_4," *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_2O_5," *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).

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6. J. Orphal, M. Morillon-Chapey, and G. Guelachvili, "High-Resolution Absorption Cross Sections of Chlorine Nitrate in the ν_2 Band Region around 1292 cm^{-1} 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_2O 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_2 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_6 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).

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15. P. Varanasi, private communication (2000).

16. Q. Zou, C. Sun, V. Nemtchinov, and P. Varanasi, "Thermal infrared absorption cross-sections of C_2F_6 at atmospheric temperatures," *JQSRT* **83,** 215-221 (2004).

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Isotopic Abundances Used for HITRAN

[based on P. De Bievre, M. Gallet, N.E. Holden, and I.L. Barnes, "Isotopic Abundances and Atomic Weights of the Elements," *J.Phys.Chem.Ref.Data* **13,** 809-891 (1984)]

Molecule	Isotopologue	Abundance
H_2O (1)	161	0.997317
	181	0.00199983
	171	0.000372
	162	0.00031069
	182	0.000000623
	172	0.000000116
CO_2 (2)	626	0.98420
	636	0.01106
	628	0.0039471
	627	0.000734
	638	0.00004434
	637	0.00000825
	828	0.0000039573
	728	0.00000147
	838	0.0000000445
O_3 (3)	666	0.992901
	668	0.00398194
	686	0.00199097
	667	0.000740
	676	0.000370
N_2O (4)	446	0.990333
	456	0.0036409
	546	0.0036409
	448	0.00198582
	447	0.000369

Molecule	Isotopologue	Abundance
CO (5)	26	0.98654
	36	0.01108
	28	0.0019782
	27	0.000368
	38	0.00002222
	37	0.00000413
CH_4 (6)	211	0.98827
	311	0.01110
	212	0.00061575
	312	0.000006918
O_2 (7)	66	0.995262
	68	0.00399141
	67	0.000742
NO (8)	46	0.993974
	56	0.0036543
	48	0.00199312
SO_2 (9)	626	0.94568
	646	0.04195
NO_2 (10)	646	0.991616
NH_3 (11)	4111	0.9958715
	5111	0.0036613
HNO_3 (12)	146	0.989110
OH (13)	61	0.997473
	81	0.00200014
	62	0.00015537

Molecule	Isotopologue	Abundance
HF (14)	19	0.99984425
HCl (15)	15	0.757587
	17	0.242257
HBr (16)	19	0.50678
	11	0.49306
HI (17)	17	0.99984425
ClO (18)	56	0.75591
	76	0.24172
OCS (19)	622	0.93739
	624	0.04158
	632	0.01053
	623	0.007399
	822	0.001880
H_2CO (20)	126	0.98624
	136	0.01108
	128	0.0019776
HOCl (21)	165	0.75579
	167	0.24168
N_2 (22)	44	0.9926874
HCN (23)	124	0.98511
	134	0.01107
	125	0.0036217
CH_3Cl (24)	215	0.74894
	217	0.23949
H_2O_2 (25)	1661	0.994952

Molecule	Isotopologue	Abundance
C_2H_2 (26)	1221	0.97760
	1231	0.02197
C_2H_6 (27)	1221	0.97699
	1231	0.02195
PH_3 (28)	1111	0.99953283
COF_2 (29)	269	0.98654
SF_6 (30)	29	0.95018
H_2S (31)	121	0.94988
	141	0.04214
	131	0.007498
HCOOH (32)	126	0.983898
HO_2 (33)	166	0.995107
O (34)	6	0.997628
$ClONO_2$ (35)	5646	0.74957
	7646	0.23970
NO^+ (36)	46	0.993974
HOBr (37)	169	0.5056
	161	0.4919
C_2H_4 (38)	221	0.9773
	231	0.02196
CH_3OH (39)	2161	0.98593
CH_3Br (40)	219	0.50099
	211	0.48743
CH_3CN (41)	2124	0.98481
CF_4 (42)	29	0.98889

Uncertainty Codes used in HITRAN Database

Line position and Pressure shift (cm^{-1})		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		