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Half-widths (self)

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

Positions

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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).
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"Line positions and intensities for the $\nu_2 + 3\nu_3$ band of $^{16}O_3$ around 2.7 μm," *J.Mol.Spectrosc.* **143,** 381-388 (1990).
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5. C.P. Rinsland, M.A.H. Smith, V.Malathy Devi, A. Perrin, J.-M. Flaud, and C. Camy-Peyret, "The ν_2 bands of $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$: 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 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); J.-M. Flaud, C. Camy-Peyret, V.M. Devi, C.P.Rinsland, M.A.H. Smith, "The ν_1 and ν_3 bands of $^{16}O_3$ 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 $^{16}O_3$ in the 7-μm region.," *J.Mol.Spectrosc.* **134,** 106-112 (1989).
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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.
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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).
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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).
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39. Data taken from the Spectroscopy & Molecular Properties of Ozone (S&MPO) database in January 2012.

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 ($J\leq35$) 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 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).
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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,** 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 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/n2o.html.
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).
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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/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_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/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 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).
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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).
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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)

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Temperature dependence of air-broadened half-width

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Pressure shift (air)

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CH_4 [6] 211, 311, 212, 312

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Half-widths (air)

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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).

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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).

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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 μm," *JQSRT* **96**, 251-270 (2005).

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Pressure shift (air)

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O_2 [7] 66, 68, 67

Positions

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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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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 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 cm^{-1} to be consistent with the (0←0) transitions.

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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) 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) 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) 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.
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Intensities

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Half-widths (air)

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NO_2 [10] 646

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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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NH_3 [11] 4111, 5111

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11. Same as Ref. 5 above, but upper-state level is unassigned due to mixing from perturbations.

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Temperature dependence of air-broadened half-width
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OH [13] 61, 81, 62

Positions

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HF [14] 19

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HCl [15] 15, 17

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HI [17] 17

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ClO [18] 56, 76

Positions

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

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Intensities

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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.

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Shift

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

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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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Pressure shift (air)
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PH_3 [28] 1111

Positions

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COF_2 [29] 269

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SF_6 [30] 29

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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

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Half-widths (self)

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HCOOH [32] 126

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HO_2 [33] 166

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O [34] 6

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 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," private communication; 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 (2006); 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).
2. A.S.Pine, "Tunable laser survey of molecular air poluants," 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 ν_{11}, $\nu_2 + \nu_{12}$, $2\nu_{10} + \nu_{12}$, ν_9 et $\nu_3 + \nu_8 + \nu_{10}$ de $^{12}C_2H_4$," *Can.J.Phys*. **61,** 514-521 (1983).
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).

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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).

CS [46] 22, 23, 24, 32

Positions

1. 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 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_2 Broadening of Carbon Disulfide $^{12}C^{32}S_2$ in the ν_3 and ν_3-ν_1 Bands," *J.Mol.Spectrosc.* **198,** 408-415 (1999). (Estimate obtained from extrapolating CS nitrogen-broadening parameters from CS_2-nitrogen broadening parameters by comparing CO to CO_2 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 ν_3-ν_1 Band of CS_2," *J.Mol.Spectrosc.* **254,** 16-19 (2009). (Estimate obtained from extrapolating CS nitrogen-broadening parameters from CS_2-nitrogen broadening parameters by comparing CO to CO_2 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, $ClONO_2$, 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).

5. J. Ballard, W.B. Johnston, M.R. Gunson, and P.T. Wassell, "Absolute Absorption Coefficients of $ClONO_2$ 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 ν_2 Band Region around 1292 cm^{-1} at Stratospheric Temperatures," *J.Geophys.Res.D* **99,** 14549-14555 (1994).

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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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cm^{-1} to 10000 cm^{-1} (238-1000 nm) at 220 K and 294 K,"*JQSRT* **59,** 171-184 (1997).
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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.
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35. C. Hermans, A.C. Vandaele, and S. Fally, "Fourier Transform measurements of SO_2 absorption cross sections: I. Temperature dependence in the 23 500 - 29 000 cm^{-1} (345-425 nm) region," *JQSRT* **110,** 756-765 (2009); A.C. Vandaele, C. Hermans, and S. Fally, "Fourier Transform measurements of SO_2 absorption cross sections: II. Temperature dependence in the

29 000 – 44 000 cm^{-1} (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_3H_8) in the 3 μm region," *JQSRT* **111**, 1282-1288 (2010).
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Molecules and isotopologues in line-by-line portion of HITRAN (2008 edition, including some updates)

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm^{-1})	Number of lines	Total number
1	H_2O	161	0.9973	0 – 25233	37432	69201
		181	$1.999\ 10^{-3}$	0 – 14519	9753	
		171	$3.719\ 10^{-4}$	10 – 14473	6992	
		162	$3.107\ 10^{-4}$	0 – 22708	13238	
		182	$6.230\ 10^{-7}$	0 – 3825	1611	
		172	$1.158\ 10^{-7}$	1234 – 1599	175	
2	CO_2	626	0.9842	352 – 12785	128170	314919
		636	$1.106\ 10^{-2}$	438 – 12463	49777	
		628	$3.947\ 10^{-3}$	0 – 11423	79958	
		627	$7.339\ 10^{-4}$	0 – 8271	19264	
		638	$4.434\ 10^{-5}$	489 – 6745	26737	
		637	$8.246\ 10^{-6}$	583 – 6769	2953	
		828	$3.957\ 10^{-6}$	491 – 8161	7118	
		827	$1.472\ 10^{-6}$	626 – 5047	821	
		838	$4.446\ 10^{-8}$	4599 – 4888	121	
3	O_3	666	0.9929	0 – 5787	249456	409686
		668	$3.982\ 10^{-3}$	0 – 2768	44302	
		686	$1.991\ 10^{-3}$	1 – 2740	18887	
		667	$7.405\ 10^{-4}$	0 – 2122	65106	
		676	$3.702\ 10^{-4}$	0 – 2101	31935	
4	N_2O	446	0.9903	0 – 7797	33074	47843
		456	$3.641\ 10^{-3}$	5 – 5086	4222	
		546	$3.641\ 10^{-3}$	4 – 4704	4592	
		448	$1.986\ 10^{-3}$	542 – 4672	4250	
		447	$3.693\ 10^{-4}$	550 – 4430	1705	
5	CO	26	0.9865	3 – 8465	917	4477
		36	$1.108\ 10^{-2}$	3 – 6279	780	
		28	$1.978\ 10^{-3}$	3 – 6267	760	
		27	$3.679\ 10^{-4}$	3 – 6339	728	
		38	$2.222\ 10^{-5}$	3 – 6124	712	
		37	$4.133\ 10^{-6}$	1807 – 6197	580	
6	CH_4	211	0.9883	0 – 9200	212061	290091
		311	$1.110\ 10^{-2}$	0 – 6070	28793	
		212	$6.158\ 10^{-4}$	7 – 6511	45024	
		312	$6.918\ 10^{-6}$	959 – 1695	4213	
7	O_2	66	0.9953	0 – 15928	1431	6430
		68	$3.991\ 10^{-3}$	1 – 15852	674	
		67	$7.422\ 10^{-4}$	0 – 14537	4325	

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm^{-1})	Number of lines	Total number
8	NO	46 56 48	0.9940 $3.654\ 10^{-3}$ $1.993\ 10^{-3}$	0 – 9274 1609 – 2061 1602 – 2039	103701 699 679	105079
9	SO_2	626 646	0.9457 $4.195\ 10^{-2}$	0 – 4093 0 – 2501	72460 22661	95121
10	NO_2	646	0.9916	0 – 3075	104223	104223
11	NH_3	446 456	0.9959 $3.661\ 10^{-3}$	0 – 5295 0 – 5180	27994 1090	29084
12	HNO_3	146	0.9891	0 – 1770	487254	487254
13	OH	61 81 62	0.9975 $2.000\ 10^{-3}$ $1.554\ 10^{-4}$	0 – 19268 0 – 329 0 – 332	30769 295 912	31976
14	HF	19	0.9998	41 – 11536	107	107
15	HCl	15 17	0.7576 0.2422	20 – 13459 20 – 10995	324 289	613
16	HBr	19 11	0.5068 0.4931	16 – 9759 16 – 9758	651 642	1293
17	HI	17	0.9998	12 – 8488	806	806
18	ClO	56 76	0.7559 0.2417	0 – 1208 0 – 1200	5721 5780	11501
19	OCS	622 624 632 623 822	0.9374 $4.158\ 10^{-2}$ $1.053\ 10^{-2}$ $7.399\ 10^{-3}$ $1.880\ 10^{-3}$	0 – 4200 0 – 4166 0 – 4056 0 – 4164 0 – 4046	15618 6087 3129 2886 1641	29361
20	H_2CO	126 136 128	0.9862 $1.108\ 10^{-2}$ $1.978\ 10^{-3}$	0 – 3100 0 – 73 0 – 48	36120 563 367	37050
21	HOCl	165 167	0.7558 0.2417	1 – 3800 1 – 3800	8877 7399	16276
22	N_2	44	0.9927	1992 – 2626	120	120
23	HCN	124 134 125	0.9851 $1.107\ 10^{-2}$ $3.622\ 10^{-3}$	0 – 3424 2 – 3405 2 – 3420	2955 652 646	4253
24	CH_3Cl	215 217	0.7489 0.2395	0 – 3173 0 – 3162	100293 95927	196220
25	H_2O_2	1661	0.9950	0 – 1731	126983	126983
26	C_2H_2	1221 1231	0.9776 $2.197\ 10^{-2}$	604 – 9890 613 – 6589	11055 285	11340

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm^{-1})	Number of lines	Total number
27	C_2H_6	1221	0.9770	706 – 3001	28439	28439
28	PH_3	1111	0.9995	770 – 3602	20099	20099
29	COF_2	269	0.9865	725 – 2002	70601	70601
30	**SF_6**	**29**	**0.9502**	**580 – 996**	**2889065**	**2889065**
31	H_2S	121 141 131	0.9499 $4.214\ 10^{-2}$ $7.498\ 10^{-3}$	2 – 4257 5 – 4172 5 – 4099	12330 4894 3564	20788
32	HCOOH	126	0.9839	10 – 1890	62684	62684
33	HO_2	166	0.9951	0 – 3676	38804	38804
34	O	6	0.9976	68 – 159	2	2
35	**$ClONO_2$**	**5646** **7646**	**0.7496** **0.2397**	**763 – 798** **765 – 791**	**21988** **10211**	**32199**
36	NO^+	46	0.9940	1634 – 2531	1206	1206
37	HOBr	169 161	0.5056 0.4919	0 – 316 0 – 316	2177 2181	4358
38	C_2H_4	221 231	0.9773 $2.196\ 10^{-2}$	701 – 3243 2947 – 3181	18097 281	18378
39	CH_3OH	2161	0.9859	0 – 1408	19897	19897
40	CH_3Br	219 211	0.5010 0.4874	794 – 1706 796 – 1697	18692 18219	36911
41	CH_3CN	2124	0.9739	890 – 946	3572	3572
42	**CF_4**	**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^{-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		