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

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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).
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.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).
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
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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).

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Intensities

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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).

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(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).

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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

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Intensities

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5. H.S.P. Müller, F. Schloder, J. Stutzki, and G. Winnewisser, "The Cologne Database for Molecular Spectroscopy, CDMS: a useful tool for astronomers and spectroscopists," *J.Mol.Struct.* **742,** 215-227 (2005). Data adopted in June 2010.
6. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung, L.R. Brown, and A.Predoi-Cross, "Spectral line parameters including temperature dependences of self- and air-broadening in the 2←0 band of CO at 2.3 μm," *JQSRT* **113**, 1013-1033 (2012).
7. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung and L.R. Brown, "Spectral line parameters including temperature dependences of air-broadening in the 2←0 bands of $^{13}C^{16}O$ and $^{12}C^{18}O$ at 2.3 μm," *J.Mol.Spectrosc.* **276**, 33-48 (2012).

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).
3. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung, L.R. Brown, and A.Predoi-Cross, "Spectral line parameters including temperature dependences of self- and air-broadening in the 2←0 band of CO at 2.3 μm," *JQSRT* **113**, 1013-1033 (2012).
4. V. Malathy Devi, D.Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung, and L.R. Brown, "Spectral line parameters including temperature dependences of air-broadening in the 2←0 bands of $^{13}C^{16}O$ and $^{12}C^{18}O$ at 2.3 μm," *J.Mol.Spectrosc.* **276**, 33-48 (2012).

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).
3. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung, L.R. Brown, and A.Predoi-Cross, "Spectral line parameters including temperature dependences of self- and air-broadening in the 2←0 band of CO at 2.3 μm," *JQSRT* **113**, 1013-1033 (2012).
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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).
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3. V. Malathy Devi, D. Chris Benner, M.A.H. Smith, A.W. Mantz, K. Sung, and L.R. Brown, "Spectral line parameters including temperature dependences of air-broadening in the 2←0 bands of $^{13}C^{16}O$ and $^{12}C^{18}O$ at 2.3 μm," *J.Mol.Spectrosc.* **276**, 33-48 (2012).

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).

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$$\delta_{0-0}(\mathbf{m}) = \delta_{(2-0)\text{asymmetric}} = \frac{\delta_{2-0}(\mathbf{m}) - \delta_{2-0}(-\mathbf{m})}{2}.$$

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$\delta_{v'-v''}(\mathbf{m}) = 0.5 \times (v' - v'') \times \delta_{(2-0)\text{symmetric}} + \delta_{(2-0)\text{asymmetric}}$, where

$$\delta_{(2-0)symmetric} = \frac{\delta_{2-0}(\mathbf{m}) + \delta_{2-0}(-\mathbf{m})}{2}, \quad \delta_{(2-0)\text{asymmetric}} = \frac{\delta_{2-0}(\mathbf{m}) - \delta_{2-0}(-\mathbf{m})}{2}.$$

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.

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Half-widths (self)
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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).
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Pressure shift (air)

1. L.R. Brown, D.C. Benner, J.-P. Champion, V.M. Devi, L. Fejard, R.R. Gamache, T. Gabard,

J.C. Hilico, B. Lavorel, M. Loëte, G.C. Mellau, A. Nikitin, A.S. Pine, A. Predoi-Cross, C.P. Rinsland, O. Robert, R.L. Sams, M.A.H. Smith, S.A. Tashkun, and V.G. Tyuterev, "Methane Line Parameters in HITRAN," *JQSRT* **82,** 219-238 (2003).
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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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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.

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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.

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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.

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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.
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Intensities

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Halfwidths (self)
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Temperature dependence of air-broadened half-width
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NO_2 [10] 646

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Positions

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Intensities
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OH [13] 61, 81, 62

Positions

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HF [14] 19, 29

Positions

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Pressure shift (air)

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HCl [15] 15, 17, 25, 27

Positions

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Half-widths (air)

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($\Delta v = 0$ bands)

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ClO [18] 56, 76

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

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HOCl [21] 165, 167

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HCN [23] 124, 134, 125

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CH_3Cl [24] 215, 217

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Shift

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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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Half-widths (self)

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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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Half-widths (self)

1. J. Vander Auwera, N. Moazzen-Ahmadi, and J.-M. Flaud, "Toward an accurate database for the 12 μm region of the ethane spectrum," *Ap.J.* **662**, 750-757 (2007).
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Temperature dependence of air-broadened half-width

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

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PH_3 [28] 1111

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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COF_2 [29] 269

Positions

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SF_6 [30] 29

Positions

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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); K. Fox, *Opt.Comm.* **19,** 397-400 (1976); B. Bobin, private communication (1990).
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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

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6. Experimental values from A.A.A. Azzam, S.N. Yurchenko, J. Tennyson, M.-A. Martin, O. Pirali, "Terahertz spectroscopy of hydrogen sulphide," *JQSRT* (in press) (2013) DOI: 10.1016/j.jqsrt.2013.05.035.
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11. O. Naumenko and A. Campargue, "Local mode effects in the absorption spectrum of H_2S between 10780 and 11330 cm^{-1}," *J.Mol.Spectrosc.* **209**, 242-253 (2001).

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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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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).
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); 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).

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

Intensities

1. M.S. Zahniser, K.E. McCurdy, and A.C. Stanton, "Quantitative Spectroscopic Studies of the HO_2 Radical: Band Strength Measurements for the ν_1 and ν_2 Vibrational Bands," *J.Phys.Chem.* **93,** 1065-1070 (1989).
2. K. Chance, K.W. Jucks, D.G. Johnson, and W.A. Traub, "The Smithsonian Astrophysical Observatory Database SAO92," *JQSRT* **52,** 447-457 (1994).

Half-widths (air)

1. D.D. Nelson and M.S. Zahniser "Air broadening measurements for the 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. Matsushima, T. Nelis, and R. L. Robinson, "Atomic oxygen fine-structure 108hermosph 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 110hermosphere," *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] 2211, 2311

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).

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).

C_4H_2 [43] 2211

Positions

1. L. Bizzocchi,C. Degli Esposti, and L. Dore. "Submillimetre-wave spectrum of diacetylene and diacetylene-d2," *Mol.Phys.* **108**, 2315-2323 (2010).

2. L. Bizzocchi, F. Tamassia, C.D. Esposti, L. Fusina, E Canè, and L. Dore, "High-resolution infrared spectroscopy of diacetylene below 1000 cm^{-1}," *Mol.Phys.* **109**, 2181-2190 (2011).

3. A. Jolly, A. Fayt, Y. Benilan, D. Jacquemart, C.A. Nixon, and D.E. Jennings, "The ν_8 bending mode of diacetylene: from laboratory spectroscopy to the detection of ^{13}C isotopologues in Titan's atmosphere," *Ap.J.* **714**, 852-859 (2010).

Intensities

1. K. Matsumura and T. Tanaka, "Microwave vibration rotation spectrum of diacetylene," *J.Mol.Spectr.* **96,** 219-233(1982). (Integrated band intensity); L. Bizzocchi,C.D. Esposti, and L. Dore. "Submillimetre-wave spectrum of diacetylene and diacetylene-d2," *Mol.Phys.* **108,** 2315-2323 (2010). (Relative rotational line intensities).

2. L. Bizzocchi, F. Tamassia, C.D. Esposti, L. Fusina, E Canè and L. Dore, "High-resolution infrared spectroscopy of diacetylene below 1000 cm^{-1}," *Mol.Phys.* **109**, 2181-2190 (2011). (Relative rotational line intensities). Integrated band intensities are taken from Ref. [3].

3. A. Jolly, A. Fayt, Y. Benilan, D. Jacquemart, C.A. Nixon, and D.E. Jennings, "The ν_8 bending mode of diacetylene: from laboratory spectroscopy to the detection of ^{13}C isotopologues in Titan's atmosphere," *Ap.J.* **714**, 852-859 (2010).

HC_3N [44] 1224

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).

2. A. Jolly, Y. Benilan, and A. Fayt, "New infrared integrated band intensities for HC_3N and extensive line list for the ν_5 and ν_6 bending modes," *J.Mol.Spectrosc.* **242**, 46-54 (2007).

Intensities

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).

2. A. Jolly, Y. Benilan, and A. Fayt, "New infrared integrated band intensities for HC_3N and extensive line list for the ν_5 and ν_6 bending modes," *J.Mol.Spectrosc.* **242**, 46-54 (2007).

Halfwidths (air)

1. A. Jolly, Y. Benilan, and A. Fayt, "New infrared integrated band intensities for HC_3N and extensive line list for the ν_5 and ν_6 bending modes," *J.Mol.Spectrosc.* **242**, 46-54 (2007).

Halfwidths (self)

1. A. Jolly, Y. Benilan, and A. Fayt, "New infrared integrated band intensities for HC_3N and extensive line list for the ν_5 and ν_6 bending modes," *J.Mol.Spectrosc.* **242**, 46-54 (2007).

Temperature dependence of air-broadened half-width

1. A. Jolly, Y. Benilan, and A. Fayt, "New infrared integrated band intensities for HC_3N and extensive line list for the ν_5 and ν_6 bending modes," *J.Mol.Spectrosc.* **242**, 46-54 (2007).

H_2 [45] 11, 12

Positions

1. J. Komasa, K. Piszczatowski, G. Lach, M. Przybytek, B. Jeziorski, and K. Pachucki, "Quantum Electrodynamics Effects in Rovibrational Spectra of Molecular Hydrogen," *J.Chem.Theory.Comput.* **7**, 3105-3115 (2011).
2. K. Pachucki and J. Komasa, "Rovibrational levels of HD," *Phys.Chem.Chem.Phys.* **12**, 9188-9196 (2010).

Intensities

1. L. Wolniewicz, I. Simbotin, and A. Dalgarno, "Quadrupole Transition Probabilities for the Excited Rovibrational States of H_2," *Astrophys.J.Suppl.Ser.* **115**, 293-313 (1998).
2. K. Pachucki and J. Komasa, "Electric dipole rovibrational transitions in the HD molecule," *Phys.Rev.A* **78**, 052503 (2008).

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.

SO_3 [47] 26

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Molecules and isotopologues in line-by-line portion of HITRAN 2012 edition

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm^{-1})	Number of lines	Total number
1	H_2O	161	0.9973	0 – 25711	142 045	224 515
		181	$1.999\ 10^{-3}$	0 – 19918	39 903	
		171	$3.719\ 10^{-4}$	0 – 19946	27 544	
		162	$3.107\ 10^{-4}$	0 – 22708	13 237	
		182	$6.230\ 10^{-7}$	0 – 3825	1611	
		172	$1.158\ 10^{-7}$	1234 – 1599	175	
2	CO_2	626	0.9842	345 – 12785	169 292	471 847
		636	$1.106\ 10^{-2}$	406 – 12463	70 611	
		628	$3.947\ 10^{-3}$	0 – 9558	116 482	
		627	$7.339\ 10^{-4}$	0 – 9600	72 525	
		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	
		727	$1.368\ 10^{-7}$	535 – 5933	5187	
		838	$4.446\ 10^{-8}$	4599 – 4888	121	
3	O_3	666	0.9929	0 – 6997	261 886	422 116
		668	$3.982\ 10^{-3}$	0 – 2768	44 302	
		686	$1.991\ 10^{-3}$	1 – 2740	18 887	
		667	$7.405\ 10^{-4}$	0 – 2122	65 106	
		676	$3.702\ 10^{-4}$	0 – 2101	31 935	
4	N_2O	446	0.9903	0 – 7797	33 074	47 843
		456	$3.641\ 10^{-3}$	5 – 5086	4 222	
		546	$3.641\ 10^{-3}$	4 – 4704	4 592	
		448	$1.986\ 10^{-3}$	542 – 4672	4 250	
		447	$3.693\ 10^{-4}$	550 – 4430	1 705	
5	CO	26	0.9865	3 – 8465	1 019	4 606
		36	$1.108\ 10^{-2}$	3 – 6274	797	
		28	$1.978\ 10^{-3}$	3 – 6267	770	
		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 – 11502	336 830	468 013
		311	$1.110\ 10^{-2}$	0 – 11319	72 420	
		212	$6.158\ 10^{-4}$	7 – 6511	54 550	
		312	$6.918\ 10^{-6}$	959 – 1695	4 213	
7	O_2	66	0.9953	0 – 15928	1 787	13 975
		68	$3.991\ 10^{-3}$	1 – 15853	875	
		67	$7.422\ 10^{-4}$	0 – 14537	11 313	

Molecule Number	Molecule	Isotopologue (AFGL notation)	Fractional Abundance	Spectral Coverage (cm^{-1})	Number of lines	Total number
8	NO	46	0.9940	0 – 9274	103 701	105 079
		56	$3.654\ 10^{-3}$	1609 – 2061	699	
		48	$1.993\ 10^{-3}$	1602 – 2039	679	
9	SO_2	626	0.9457	0 – 4093	72 460	95 121
		646	$4.195\ 10^{-2}$	0 – 2501	22 661	
10	NO_2	646	0.9916	0 – 3075	104 223	104 223
11	NH_3	4111	0.9959	0 – 7000	45 302	46 392
		5111	$3.661\ 10^{-3}$	0 – 5180	1 090	
12	HNO_3	146	0.9891	0 – 1770	903 854	961 962
		156	$3.636\ 10^{-3}$	0 – 923	58 108	
13	OH	61	0.9975	0 – 19268	30 772	31 979
		81	$2.000\ 10^{-3}$	0 – 329	295	
		62	$1.554\ 10^{-4}$	0 – 332	912	
14	HF	19	0.9998	24 – 46985	10 073	34 376
		29	$1.557\ 10^{-4}$	13 – 47365	24 303	
15	HCl	15	0.7576	8 – 13459	11 879	83 691
		17	0.2422	8 – 10995	11 907	
		25	$1.180\ 10^{-4}$	5 – 33284	29 994	
		27	$3.774\ 10^{-5}$	5 – 33258	29 911	
16	HBr	19	0.5068	13 – 16034	3 039	8 980
		11	0.4931	13 – 16032	3 031	
		29	$7.894\ 10^{-5}$	7 – 8781	1 455	
		21	$7.680\ 10^{-5}$	7 – 8778	1 455	
17	HI	17	0.9998	10 – 13908	3 161	4 751
		27	$1.557\ 10^{-4}$	5 – 7625	1 590	
18	ClO	56	0.7559	0 – 1208	5 721	11 501
		76	0.2417	0 – 1200	5 780	
19	OCS	622	0.9374	0 – 4200	15 618	29 361
		624	$4.158\ 10^{-2}$	0 – 4166	6 087	
		632	$1.053\ 10^{-2}$	0 – 4056	3 129	
		623	$7.399\ 10^{-3}$	0 – 4164	2 886	
		822	$1.880\ 10^{-3}$	0 – 4046	1 641	
20	H_2CO	126	0.9862	0 – 3100	40 670	44 601
		136	$1.108\ 10^{-2}$	0 – 117	2 309	
		128	$1.978\ 10^{-3}$	0 – 191	1 622	
21	HOCl	165	0.7558	1 – 3800	8 877	16 276
		167	0.2417	1 – 3800	7 399	
22	N_2	44	0.9927	11 – 9355	1 107	1 268
		45	$7.478`\ 10^{-3}$	11 – 2578	161	

23	HCN	124 134 125	0.9851 $1.107\ 10^{-2}$ $3.622\ 10^{-3}$	0 – 3424 2 – 3405 2 – 3420	2 955 652 646	4 253
24	CH_3Cl	215 217	0.7489 0.2395	0 – 3198 0 – 3198	107 642 104 854	212 496
25	H_2O_2	1661	0.9950	0 – 1731	126 983	126 983
26	C_2H_2	1221 1231 1222	0.9776 $2.197\ 10^{-2}$ $3.046\ 10^{-4}$	604 – 9890 613 – 6589 1 – 789	12 613 285 7 512	20 410
27	C_2H_6	1221 1231	0.9770 $2.195\ 10^{-2}$	706 – 3001 725 – 919	43 592 6 037	49 629
28	PH_3	1111	0.9995	0 – 3602	22 189	22 189
Molecule Number	**Molecule**	**Isotopologue (AFGL notation)**	**Fractional Abundance**	**Spectral Coverage (cm^{-1})**	**Number of lines**	**Total number**
29	COF_2	269 369	0.9865 $1.108\ 10^{-2}$	696 – 2002 686 – 815	168 793 15 311	184 104
30	**SF_6**	**29**	**0.9502**	**580 – 996**	**2 889 065**	**2 889 065**
31	H_2S	121 141 131	0.9499 $4.214\ 10^{-2}$ $7.498\ 10^{-3}$	2 – 11330 5 – 11227 5 – 11072	36 561 11 352 6 322	54 325
32	HCOOH	126	0.9839	10 – 1890	62 684	62 684
33	HO_2	166	0.9951	0 – 3676	38 804	38 804
34	O	6	0.9976	68 – 159	2	2
35	**$ClONO_2$**	**5646** **7646**	**0.7496** **0.2397**	**763 – 798** **765 – 791**	**21 988** **10 211**	**32 199**
36	NO^+	46	0.9940	1634 – 2531	1 206	1 206
37	HOBr	169 161	0.5056 0.4919	0 – 316 0 – 316	2 177 2 181	4 358
38	C_2H_4	221 231	0.9773 $2.196\ 10^{-2}$	701 – 3243 2947 – 3181	18 097 281	18 378
39	CH_3OH	2161	0.9859	0 – 1408	19 897	19 897
40	CH_3Br	219 211	0.5010 0.4874	794 – 1706 796 – 1697	18 692 18 219	36 911
41	CH_3CN	2124	0.9739	890 – 946	3 572	3 572
42	**CF_4**	**29**	**0.9889**	**594 – 1313**	**60 033**	**60 033**
43	C_4H_2	2211	0.9560	0 – 758	124 126	124 126
44	HC_3N	1224	0.9633	0 – 760	180 332	180 332

45	H_2	11 12	0.9997 $3.114\ 10^{-4}$	15 – 36024 3 – 36406	4 017 5 129	9 146
46	CS	22 24 32 23	0.9396 $4.168\ 10^{-2}$ $1.056\ 10^{-2}$ $7.417\ 10^{-3}$	1 – 2586 1 – 1359 1 – 1331 1 – 156	1 088 396 396 198	2 078
47	SO_3	26	0.9434	0 – 2825	10 881	10 881

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	Better than 0.00000001		