Collision-Induced Absorption (CIA) cross-sections in HITRAN

Contact: igordon@cfa.harvard.edu and/or tijs.karman@cfa.harvard.edu

Collision-Induced Absorption (CIA) of infrared radiation contributes appreciably to the total absorption of radiation in planetary atmospheres. This section of the database has undergone substantial update and extension in 2018. This extension is documented in detail in Karman *et al.* [1] As in the original effort described in Richard *et al.* [2], only binary collisions are considered. We continue to provide "Main" and "Alternate" folders. The main folder contains recommended sets of collision-induced absorptions whereas the supplementary folder contains two types of data. One type of data is simply alternative to that in the main folder, in particular where the CIA parameterization is intended to be used in conjunction with a specific line-by-line list. This is the case for O_2−Air absorption in particular. A second type of data in the "Alternate" folder is provided when the data are not generally recommended due to large uncertainties, and should be used with caution, but the data have a clear advantage over the recommended set for specific applications, *e.g.* extended temperature ranges or to account for spin statistics.

Table 1 summarizes the data that are presently available, while Fig. 1 illustrates the format of the headers for each individual data set.

Instructions for accessing the database can be found on the HITRAN website (`www.hitran.org/cia`).

Table 1: Summary of the different bands available in the HITRAN CIA section, including Supplementary folders for all collisional systems. Note that the reference numbers refer only to this readme file and do not coincide with a CIA reference Table provided at **`https://hitran.org/data/CIA/Collision-Induced-Absorption_references.pdf`**.

System	Folder	Spectral range (cm^{-1})	T range (K)	# of sets	Ref.
H_2−H_2	Main	20–10 000	200–3 000	113	[3]
	Alternate	0–2 400	40–400	120	[4]

Continued on next page

Table 1 – *Continued from previous page*

System	Folder	Spectral range (cm^{-1})	T range (K)	# of sets	Ref.
H_2-He	Main	20–20 000	200–9900	334	[5]
H_2-H	Main	100–10 000	1 000–2 500	4	[6]
$He-H$	Main	50–11 000	1 500–10 000	10	[7]
H_2-CH_4	Main	0–1 946	40–400	10	[8]
N_2-He	Main	1–1 000	300	1	[9]
CO_2-He	Main	0–1 000	300	1	[9]
CH_4-He	Main	1–1 000	40–350	10	[10]
CH_4-Ar	Alternate	1–697	70–296	5	[11]
CH_4-CH_4	Alternate	0–990	200–800	7	[12]
CO_2-H_2	Main	0–2 000	200–350	4	[13]
CO_2-CH_4	Main	1–2 000	200–350	4	[13]
CO_2-CO_2	Main	1–750	200–800	10	[14]
		1 000–1 800	200–350	6	[15]
		1 000–1 800	200–350	6	[16]
		2 510–2 850	221–297	3	[17]
N_2-H_2	Main	0–1 886	40–400	10	[18]
N_2-N_2	Main	0–554	200–309	9	[19]
		1 850–3 000	301–363	5	[20]
		2 000–2 698	228–272	5	[21]
		4 300–5 000	200–330	14	[22]
	Alternate	30-300	78–129	4	[23]
O_2-O_2	Main	1 150–1 950	193–353	15	[24]
		7 450–8 491	296	1	[25]
		9 091–9 596	293	1	[26]
		10 512–11 228	293	1	[27]
		12 600–13 839	296	1	[28]
		14 206–14 898	293	1	[29]
		15 290–16 664	203–287	4	[30]
		16 700–29 800	203–293	5	[30]
	Alternate	7 583–8 183	206–346	15	[26]
		9 060–9 960	206–346	15	[26]
		10 525–11 125	206–346	15	[26]
		12 804–13 402	206–346	15	[26]
		14 296–14 806	206–346	15	[26]
O_2-N_2		1 850–3 000	301–363	5	[20, 31]

Continued on next page

Table 1 – *Continued from previous page*

System	Folder	Spectral range (cm^{-1})	T range (K)	# of sets	Ref.
		2 000–2 698	228–272	5	[21, 31]
		7 450–8 488	293	1	[25]
		12 600–13 840	296	1	[28]
	Alternate	7 583–8 183	206–346	15	[26]
		12 804–13 402	206–346	15	[26]
N_2-Air		1 850–3 000	301–363	5	[20, 31]
		2 000–2 698	228–272	5	[21, 31]
		4 300–5 000	200–330	14	[22]
O_2-Air	Main	7 450–8 480	250–296	3	[25]
		9 091–9 596	293	1	[26]
		10 512–11 228	293	1	[27]
		12 600–13 839	300	1	[28]
	Alternate	12 990–13 220	298	1	[32]
		7 583–8 183	206–346	15	[26]
		9 060–9 960	206–346	15	[26]
		10 525–11 125	206–346	15	[26]
		12 1804–13 402	206–346	15	[26]
		14 296–14 806	206–346	15	[26]
N_2-H_2O	Main	1 930–2 830	250–350	11	[33]
N_2-CH_4	Alternate	0–1 379	40–400	10	[34]
O_2-CO_2	Main	12 600–13 839	200–300	1	[35]

1. General definitions

The attenuation of light by a gas with absorption coefficient $k(\nu)$ is given by the Lambert law

$$-\ln\left[T\left(\nu\right)\right] = k(\nu)L, \tag{1}$$

where $T(\nu)$ is the transmittance at wave number ν and L is the optical path length. Leaving aside pressure variations in the line shape of resonant transitions of an individual molecule, the absorption coefficient is given by the virial expansion in the number density ρ

$$k(\nu) = k^{(1)}(\nu)\ \rho + k^{(2)}(\nu)\ \rho^2 + \ldots, \tag{2}$$

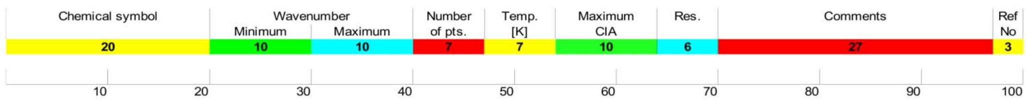

Figure 1: Definition of the HITRAN CIA header. The numbers indicate the length of each block. Reference numbers identify the sources of the data, which are tabulated in a file available from `www.hitran.org/cia`.

which permits discrimination of monomer absorption and absorption by molecular pairs or ternary and larger complexes of colliding molecules. The absorption by collision complexes involving more than two molecules is expected to be insignificant under typical atmospheric conditions, even for planets with dense atmospheres such as Venus, and is thus disregarded here.

In HITRAN units, the density ρ is given in molecule cm^{-3}. The monomer absorption cross section $k^{(1)}(\nu)$ is given in cm^2 molecule^{-1}, and is tabulated in HITRAN for many molecules relevant to planetary atmospheres. The contribution of binary complexes is given by the CIA absorption coefficient, $k^{(2)}(\nu)$, which is tabulated in the HITRAN CIA section discussed in this paper, in units of cm^5 molecule^{-2}. The frequency and absorption coefficient are tabulated in two-column format, where each band and temperature set is preceded by a header, formatted as defined in Fig. 1.

For mixtures containing multiple molecular species, for example A and B, the binary contributions take the form

$$k(\nu) = k^{(A-A)}(\nu)\ \rho_A^2 + k^{(A-B)}(\nu)\ \rho_A \rho_B + k^{(B-B)}(\nu)\ \rho_B^2, \tag{3}$$

where ρ_A and ρ_B are the number densities of both molecular species. The current updated version of the HITRAN CIA database consistently tabulates binary CIA absorption coefficients $k^{(A-A)}(\nu)$, $k^{(A-B)}(\nu)$, and $k^{(B-B)}(\nu)$, separately. By contrast, the previous version of the database also listed coefficients for different mixtures which had to be scaled with the square of the *total* number density $(\rho_A + \rho_B)^2$. This may have been confusing, and lead to deviations from Eq. (3)–especially when combined with interpolation or extrapolation schemes–and it was inconsistent with the tabulation of theoretical results which obtain $k^{(A-A)}(\nu)$, $k^{(A-B)}(\nu)$, or $k^{(B-B)}(\nu)$ directly, without using mixtures. Fortunately, the only system for which results with different mixtures were previously reported was $O_2 - N_2$. This issue has been fixed in the HITRAN 2016 update.[36]

Also introduced in the HITRAN 2016 update was the concept of an $M-$Air CIA section, which aims to combine $M-\mathrm{O}_2$, $M-\mathrm{N}_2$, and $M-$Ar as ready-to-use absorption coefficients for applications for the Earth's atmosphere. To be explicit,

$$-\frac{\ln\left[T(\nu)\right]}{L} = k^{(M-\mathrm{Air})}(\nu)\ \rho_M \rho_{\mathrm{Air}}, \tag{4}$$

with $\rho_{\mathrm{Air}} = \rho_{\mathrm{O}_2} + \rho_{\mathrm{N}_2}$. The $M-$ Air data typically come from three sources:

1. The data may contain the sum of $M-\mathrm{O}_2$, $M-\mathrm{N}_2$, and $M-$ Ar contributions, where these are separately available. These data should be consistent and hence preferably from the same source, which may be either experimental or obtained from calculations.
2. In many cases the 1% $M-$ Ar data will be unavailable. In these cases, we typically provide 21:79 or 22:78 mixtures of $M-\mathrm{O}_2$:$M-\mathrm{N}_2$ contributions, depending on whether O_2 or N_2 is to be considered the better model for Ar, which may depend on the transition considered.
3. The data provided as $M-$Air may also directly come from experiments using either air or a similar mixture, e.g. synthetic air.

In summary: where available, the $M-$ Air CIA section gives the recommended binary absorption coefficient. Users should not double count contributions by explicitly adding the contributions of $M-\mathrm{O}_2$, $M-\mathrm{N}_2$ or $M-$Ar, which are already accounted for.

Unlike the *line-by-line* and *cross-sections* parts of the HITRAN database which are cast into the SQL structure described in Hill *et al.* [37], the CIA files are still provided in static ASCII format accompanied with a reference Table (`https://hitran.org/data/CIA/Collision-Induced-Absorption_references.pdf`). In the near future, CIA parameters will also be cast into SQL structure. Access through the HITRAN Application Programming Interface (HAPI) [38] will also be enabled. Thus, calculations of absorption coefficients, cross-sections, etc using HAPI will be implemented.

[1] T. Karman, I. E. Gordon, A. van der Avoird, Y. I. Baranov, C. Boulet, B. J. Drouin, G. C. Groenenboom, M. Gustafsson, J.-M. Hartmann, R. L. Kurucz, L. S. Rothman, K. Sun, K. Sung, R. Thalman, H. Tran, E. H. Wishnow, R. Wordsworth, A. A. Vigasin, R. Volkamer, W. J. van der Zande, Update of the HITRAN collision-induced absorption section, Icarus (in press). doi:10.1016/J.ICARUS.2019.02.034.

[2] C. Richard, I. Gordon, L. Rothman, M. Abel, L. Frommhold, M. Gustafsson, J.-M. Hartmann, C. Hermans, W. Lafferty, G. Orton, K. Smith, H. Tran, New section of the HITRAN database: Collision-induced absorption (CIA), J. Quant. Spectrosc. Radiat. Transfer 113 (2012) 1276. doi:10.1016/j.jqsrt.2011.11.004.

[3] M. Abel, L. Frommhold, X. Li, K. L. C. Hunt, Collision-induced absorption by H_2 pairs: From hundreds to thousands of Kelvin, J. Phys. Chem. A 115 (25) (2011) 6805–6812. doi:10.1021/jp109441f.

[4] L. N. Fletcher, M. Gustafsson, G. S. Orton, Hydrogen dimers in giant-planet infrared spectra, Astrophys. J. Supplement Series 235 (1) (2018) 24.

[5] M. Abel, L. Frommhold, X. Li, K. L. C. Hunt, Infrared absorption by collisional H_2–He complexes at temperatures up to 9000 K and frequencies from 0 to 20000 cm^{-1}, J. Chem. Phys. 136 (4) (2012) 044319. doi:10.1063/1.3676405.

[6] M. Gustafsson, L. Frommhold, The H_2–H infrared absorption bands at temperatures from 1000 K to 2500 K, Astronomy & Astrophysics 400 (3) (2003) 1161–1162. doi:10.1051/0004-6361:20030100.

[7] M. Gustafsson, L. Frommhold, Infrared absorption spectra of collisionally interacting He and H atoms, Astrophys. J. 546 (2) (2001) 1168.

[8] A. Borysow, L. Frommhold, Theoretical collision-induced rototranslational absorption spectra for the outer planets-H_2–CH_4 pairs, Astrophys. J. 304 (1986) 849–865.

[9] E. Bar-Ziv, S. Weiss, Translational Spectra Due to Collision-Induced Overlap Moments in Mixtures of He with CO_2, N_2, CH_4, and C_2H_6, J. Chem. Phys. 57 (1972) 34. doi:10.1063/1.1677970.

[10] R. H. Taylor, A. Borysow, L. Frommhold, Concerning the rototranslational absorption spectra of He–CH_4 pairs, J. Mol. Spectrosc. 129 (1988) 45. doi:10.1016/0022-2852(88)90257-3.

[11] R. E. Samuelson, N. R. Nath, A. Borysow, Gaseous abundances and methane supersaturation in Titan's troposphere, Planet. Space Sci. 45 (8) (1997) 959–980.

[12] A. Borysow, L. Frommhold, Collision-induced rototranslational absorption spectra of CH_4-CH_4 pairs at temperatures from 50 to 300 K, Astrophys. J. 318 (1987) 940–943.

[13] R. Wordsworth, Y. Kalugina, S. Lokshtanov, A. Vigasin, B. Ehlmann, J. Head, C. Sanders, H. Wang, Transient reducing greenhouse warming on early Mars, Geophys. Res. Lett. 44 (2017) 665. doi:10.1002/2016GL071766.

[14] M. Gruszka, A. Borysow, Roto-translational collision-induced absorption of CO_2 for the atmosphere of Venus at frequencies from 0 to 250 cm^{-1}, at temperatures from 200 to 800 K, Icarus 129 (1997) 172. doi:10.1006/icar.1997.5773.

[15] Y. Baranov, A. Vigasin, Collision-induced absorption by CO_2 in the region of ν_1, $2\nu_2$, J. Mol. Spectrosc. 193 (2) (1999) 319 – 325. doi:10.1006/jmsp.1998.7743.

[16] Y. Baranov, G. T. Fraser, W. J. Lafferty, A. Vigasin, Collision-induced absorption in the CO_2 fermi triad for temperatures from 211 K to 296 K, in: C. Camy-Peyret, A. Vigasin (Eds.), Weakly Interacting Molecular Pairs: Unconventional Absorbers of Radiation in the Atmosphere, Springer, 2003, pp. 149–158.

[17] Y. I. Baranov, Collision-induced absorption in the region of the $\nu_2+\nu_3$ band of carbon dioxide, J. Mol. Spectrosc. 345 (2018) 11 – 16. doi:10.1016/j.jms.2017.11.005.

[18] A. Borysow, L. Frommhold, Theoretical collision-induced rototranslational absorption spectra for modeling Titan's atmosphere-H_2–N_2 pairs, Astrophys. J. 303 (1986) 495–510.

[19] T. Karman, E. Miliordos, K. L. C. Hunt, G. C. Groenenboom, A. van der Avoird, Quantum mechanical calculation of the collision-induced absorption spectra of N_2–N_2 with anisotropic interactions, J. Chem. Phys. 142 (2015) 084306. doi:10.1063/1.4907917.

[20] Y. Baranov, W. Lafferty, G. Fraser, Investigation of collision-induced absorption in the vibrational fundamental bands of O_2 and N_2 at elevated temperatures, J. Mol. Spectrosc. 233 (1) (2005) 160 – 163. doi:10.1016/j.jms.2005.06.008.

[21] W. J. Lafferty, A. M. Solodov, A. Weber, W. B. Olson, J.-M. Hartmann, Infrared collision-induced absorption by N_2 near 4.3 μm for atmospheric applications: measurements and empirical modeling, Applied Optics 35 (30) (1996) 5911. doi:10.1364/AO.35.005911.
URL https://www.osapublishing.org/abstract.cfm?URI=ao-35-30-5911

[22] J.-M. Hartmann, C. Boulet, G. C. Toon, Collision-induced absorption by N_2 near 2.16 μm: Calculations, model, and consequences for atmospheric remote sensing, J. Geophys. Res.: Atmos. 122 (2017) 2419. doi:10.1002/2016JD025677.

[23] E. Wishnow, K. Sung, et al., The far-infrared collision-induced spectrum of nitrogen over the temperature range 78–129 K, J. Quant. Spectrosc. Radiat. Transfer in preparation. (2018).

[24] Y. I. Baranov, W. Lafferty, G. Fraser, Infrared spectrum of the continuum and dimer absorption in the vicinity of the O_2 vibrational fundamental in O_2/CO_2 mixtures, J. Mol. Spectrosc. 228 (2) (2004) 432 – 440, special Issue Dedicated to Dr. Jon T. Hougen on the Occasion of His 68th Birthday. doi:10.1016/j.jms.2004.04.010.

[25] Maté, B. and Lugez, C. and Fraser, G. T. and Lafferty, W. J., Absolute intensities for the O_2 1.27 μm continuum absorption, J. Geophys. Res.: Atmospheres 104 (D23) (1999) 30585–30590. doi:10.1029/1999JD900824.

[26] T. Karman, M. A. J. Koenis, A. Banerjee, D. H. Parker, I. E. Gordon, A. van der Avoird, W. J. van der Zande, G. C. Groenenboom, O_2-O_2 and O_2-N_2 collision-induced absorption mechanisms unravelled, Nature

Chem. 10 (2018) 549. doi:10.1038/s41557-018-0015-x.
URL https://rdcu.be/K2f0

[27] F. R. Spiering, W. J. van der Zande, Collision induced absorption in the $a^1\Delta(\nu{=}2) \leftarrow X^3\Sigma_g^-(\nu{=}0)$ band of molecular oxygen, Phys. Chem. Chem. Phys. 14 (28) (2012) 9923–9928. doi:10.1039/c2cp40961e.

[28] H. Tran, C. Boulet, J.-M. Hartmann, Line mixing and collision-induced absorption by oxygen in the A-band: Laboratory measurements, model, and tools for atmospheric spectra computations, J. Geophys. Res. 111 (2006) D15210. doi:10.1029/2005JD006869.

[29] F. R. Spiering, M. B. Kiseleva, N. N. Filippov, L. van Kesteren, W. J. van der Zande, Collision-induced absorption in the O_2 B-band region near 670 nm, Phys. Chem. Chem. Phys. 13 (2011) 9616–9621. doi:10.1039/C1CP20403C.

[30] R. Thalman, R. Volkamer, Temperature dependent absorption cross-sections of O_2-O_2 collision pairs between 340 and 630 nm and at atmospherically relevant pressure, Phys. Chem. Chem. Phys. 15 (37) (2013) 15371. doi:10.1039/c3cp50968k.

[31] V. Menoux, R. L. Doucen, C. Boulet, A. Roblin, A. M. Bouchardy, Collision-induced absorption in the fundamental band of N_2: temperature dependence of the absorption for N_2-N_2 and N_2-O_2 pairs., Applied optics 32 (3) (1993) 263–268. doi:10.1364/AO.32.000263.

[32] B. J. Drouin, D. C. Benner, L. R. Brown, M. J. Cich, T. J. Crawford, V. M. Devi, A. Guillaume, J. T. Hodges, E. J. Mlawer, D. J. Robichaud, F. Oyafuso, V. H. Payne, K. Sung, E. H. Wishnow, S. Yu, Multispectrum analysis of the oxygen A-band, J. Quant. Spectrosc. Radiat. Transfer 186 (2017) 118. doi:10.1016/j.jqsrt.2016.03.037.

[33] J.-M. Hartmann, C. Boulet, D. D. Tran, H. Tran, Y. Baranov, Effect of humidity on the absorption continua of CO_2 and N_2 near 4 μm: Calculations, comparisons with measurements, and consequences for atmospheric spectra, J. Chem. Phys 148 (5) (2018) 054304. doi:10.1063/1.5019994.

[34] A. Borysow, C. Tang, Far infrared CIA spectra of N_2–CH_4 pairs for modeling of Titan's atmosphere, Icarus 105 (1) (1993) 175–183.

[35] M. Vangvichith, H. Tran, J.-M. Hartmann, Line-mixing and collision induced absorption for O_2–CO_2 mixtures in the oxygen A-band region, J. Quant. Spectrosc. Radiat. Transfer 110 (18) (2009) 2212–2216. doi:10.1016/j.jqsrt.2009.06.002.

[36] I. E. Gordon, L. Rothman, C. Hill, R. Kochanov, Y. Tan, P. Bernath, M. Birk, V. Boudon, A. Campargue, K. Chance, B. Drouin, J.-M. Flaud, R. Gamache, J. Hodges, D. Jacquemart, V. Perevalov, A. Perrin, K. Shine, M.-A. Smith, J. Tennyson, G. Toon, H. Tran, V. Tyuterev, A. Barbe, A. Császár, V. Devi, T. Furtenbacher, J. Harrison, J.-M. Hartmann, A. Jolly, T. Johnson, T. Karman, I. Kleiner, A. Kyuberis, J. Loos, O. Lyulin, S. Massie, S. Mikhailenko, N. Moazzen-Ahmadi, H. Müller, O. Naumenko, A. Nikitin, O. Polyansky, M. Rey, M. Rotger, S. Sharpe, K. Sung, E. Starikova, S. Tashkun, J. V. Auwera, G. Wagner, J. Wilzewski, P. Wcisło, S. Yu, E. Zak, The HITRAN2016 molecular spectroscopic database, J. Quant. Spectrosc. Radiat. Transfer 203 (2017) 3. doi:10.1016/j.jqsrt.2017.06.038.

[37] C. Hill, I. E. Gordon, R. V. Kochanov, L. Barrett, J. S. Wilzewski, L. S. Rothman, HITRANonline: An online interface and the flexible representation of spectroscopic data in the HITRAN database, J. Quant. Spectrosc. Radiat. Transfer 177 (2016) 4–14. doi:10.1016/j.jqsrt.2015.12.012. URL http://www.sciencedirect.com/science/article/pii/S0022407315302375

[38] R. V. Kochanov, I. E. Gordon, L. S. Rothman, P. Wcisło, C. Hill, J. S. Wilzewski, HITRAN Application Programming Interface (HAPI): A comprehensive approach to working with spectroscopic data, J. Quant. Spectrosc. Radiat. Transfer 177 (2016) 15–30. doi:10.1016/j.jqsrt.2016.03.005.
URL http://www.sciencedirect.com/science/article/pii/S0022407315302466