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

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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]

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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]
CO_2-Ar	Main	0–300	200–400	21	[10]
CH_4-He	Main	1–1 000	40–350	10	[11]
CH_4-Ar	Alternate	1–697	70–296	5	[12]
CH_4-CH_4	Alternate	0–990	200–800	7	[13]
CO_2-H_2	Main	0–2 000	200–350	4	[14]
CO_2-CH_4	Main	1–2 000	200–350	4	[14]
CO_2-CO_2	Main	1–750	200–800	10	[15]
		1 000–1 800	200–350	6	[16]
		1 000–1 800	200–350	6	[17]
		2 510–2 850	221–297	3	[18]
		2 850–3 250	298	1	[18]
N_2-H_2	Main	0–1 886	40–400	10	[19]
N_2-N_2	Main	0–450	70–200	14	[20]
		0–550	210–300	10	[20]
		0–650	310–400	10	[20]
		1 850–3 000	301–363	5	[21]
		2 000–2 698	228–272	5	[22]
		4 300–5 000	200–330	14	[23]
	Alternate	30-300	78–129	4	[24]
O_2-O_2	Main	1 150–1 950	193–353	15	[25]
		7 450–8 491	296	1	[26]
		9 091–9 596	293	1	[27]
		10 512–11 228	293	1	[28]
		12 600–13 839	296	1	[29]
		14 206–14 898	293	1	[30]
		15 290–16 664	203–287	4	[31]
		16 700–29 800	203–293	5	[31]
	Alternate	1300–1850	193–356	7	[32, 33]
		7 583–8 183	206–346	15	[27]

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Table 1 – *Continued from previous page*

System	Folder	Spectral range (cm^{-1})	T range (K)	# of sets	Ref.
		9 060–9 960	206–346	15	[27]
		10 525–11 125	206–346	15	[27]
		12 804–13 402	206–346	15	[27]
		14 296–14 806	206–346	15	[27]
O_2-N_2	Main	1 300–1 850	193–356	7	[32, 33]
		1 850–3 000	301–363	5	[21, 34]
		2 000–2 698	228–272	5	[22, 34]
		7 450–8 488	293	1	[26]
		12 600–13 840	296	1	[29]
	Alternate	7 583–8 183	206–346	15	[27]
		12 804–13 402	206–346	15	[27]
N_2-Air		1 850–3 000	301–363	5	[21, 34]
		2 000–2 698	228–272	5	[22, 34]
		4 300–5 000	200–330	14	[23]
O_2-Air	Main	1 300–1 850	193–356	7	[32, 33]
		7 450–8 480	250–296	3	[26]
		9 091–9 596	293	1	[27]
		10 512–11 228	293	1	[28]
		12 600–13 839	300	1	[29]
	Alternate	12 990–13 220	298	1	[35]
		7 583–8 183	206–346	15	[27]
		9 060–9 960	206–346	15	[27]
		10 525–11 125	206–346	15	[27]
		12 1804–13 402	206–346	15	[27]
		14 296–14 806	206–346	15	[27]
N_2-H_2O	Main	1 930–2 830	250–350	11	[36]
N_2-CH_4	Alternate	0–1 379	40–400	10	[37]
O_2-CO_2	Main	12 600–13 839	200–300	1	[38]

1. General definitions

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

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

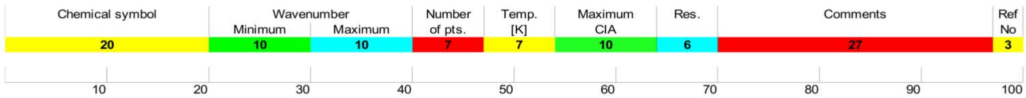

Figure 1: Definition of the HITRAN CIA header. The numbers indicate the length of each block. Reference numbers identify the sources of the data, which are tabulated in a file available from `www.hitran.org/cia`.

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

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

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.[39]

Also introduced in the HITRAN 2016 update was the concept of an $M-$Air CIA section, which aims to combine $M-O_2$, $M-N_2$, 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 $M - O_2$, $M - N_2$, 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 $M-O_2$:$M-N_2$ 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 $M-O_2$, $M-N_2$ 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.* [40], 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) [41] will also be enabled. Thus, calculations of absorption coefficients, cross-sections, etc using HAPI will be implemented.

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