

Collision-induced absorption coefficients of H₂ pairs at temperatures from 60 K to 1000 K

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Abstract. New collision-induced absorption data of H₂ pairs at temperatures between 400 K and 1000 K are presented here for the first time. They are based on a careful interpolation and extension of the existing ‘low’ temperature data, which were suited for use in planetary atmospheric modelling. The new data are aimed to help in modelling the coolest halo white dwarfs, the coolest M dwarfs, the L- and T- type dwarf stars, as well as brown dwarfs and “hot jupiters”. In addition, for the convenience of the future users, the already existing low temperature (60 K to 400 K) data are provided, in a consistent and user friendly tabular form. The data above 1000 K, which already existed, form a continuous sequence with the new data presented here. The total data set from 60 K to 7000 K and frequencies from 0 cm⁻¹ to ≤17 000 cm⁻¹ (computed for every 10 cm⁻¹) is now located at www.astro.ku.dk/~aborysow/programs.

Key words. molecular data – astronomical data bases – stars: atmospheres – stars: low-mass, brown dwarfs – infrared: stars

1. Introduction

Until quite recently atmospheric modelling was divided between planetary atmospheres, which required low temperature data (20 K to max. 500 K), and stellar atmospheres which required high temperature data (1000 K to 7000 K). Two sets of collision-induced absorption (CIA) data have been produced in the past, with the aim to assist the planetary and the stellar efforts. These data have been based on two slightly different inputs, suitable for the task at hand. Whereas the low temperature data were almost “exact”, i.e. matched closely all laboratory results, the input they were based on was not suitable for computing CIA spectra at very high temperatures. As a result, the two sets were not “compatible” to be inter- or extrapolated into each other. They were meant to be used for either one task, or the other.

In 1995 two new kind of objects, on the border between the traditional regions of stars and planets, were discovered: the first brown dwarf (Nakajima et al. 1995) and the first “hot jupiter” extra-solar planet (Mayor & Queloz 1995). As a consequence, the need emerged for analysing spectra at intermediate temperatures between 400 K and 1000 K.

Collision-induced absorption due to hydrogen pairs has been recognised, for many years, to play an important role in the radiative transfer of atmospheres of the outer planets (Conrath et al. 1989; Hanel et al. 1992; Trafton 1995), and

it also plays a decisive role as a dominant opacity source in Saturn’s largest moon Titan (Samuelson et al. 1997). In recent years, interest has increased concerning the impact of CIA on stellar atmospheres of cool stars as well (Borysow 1994; Borysow et al. 1997; Borysow & Jørgensen 1999). Here, CIA is very important for the infrared energy balance. Therefore the missing data now have been computed by the means described below, and have been placed on the Internet, at www.astro.ku.dk/~aborysow/programs. The low- and the high temperature part of the new data (i.e. those below and above 400 K) will be described in Sects. 2, 3, respectively.

The theory of collision-induced absorption in general is described in detail in the extensive monograph by Frommhold (1993) and will not be summarized in this paper.

2. Low temperature CIA data

Although models of the low temperature CIA spectra of hydrogen pairs exist already, they were given in the form of FORTRAN programs, separately for each spectral band. This has turned out to be inconvenient for many users, and has caused unnecessary troubles when the programs refused to work under various compilers or computer platforms. In order to ease the use of the data, the spectra at all bands (ranging from the roto-translational, to the roto-vibrational fundamental, first and second overtone transition) have been consolidated in one block of

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data. It is presented as a table of intensities (in $\text{cm}^{-1}/\text{amagat}^2$)¹ from 0 to approx. $16\,500\text{ cm}^{-1}$. The spacing is chosen to be 10 cm^{-1} which should be sufficient for most applications and which is sufficient for high accuracy interpolation, if necessary. Hydrogen in thermal equilibrium was assumed everywhere.

The combined spectra are based on the following computer models, ν_0 (cm^{-1}) being the vibrational transition wavenumber for the hydrogen molecule:

1. roto-translational band (RT) CIA (40–300 K) (Borysow et al. 1985), ($\nu_0 = 0.0\text{ cm}^{-1}$),
2. fundamental band $\nu_0 = 4162\text{ cm}^{-1} \approx 2.4\text{ }\mu\text{m}$, (20–300 K) (Borysow 1991),
3. first overtone band, $\nu_0 = 8089\text{ cm}^{-1} \approx 1.2\text{ }\mu\text{m}$, (20–500 K) (Zheng & Borysow 1995),
4. second overtone band, $\nu_0 = 11786\text{ cm}^{-1} \approx 0.8\text{ }\mu\text{m}$, (50–500 K) (Borysow et al. 2000).

All these computer models can be found at www.astro.ku.dk/~aborysow/programs. A few of the models provide reliable predictions only up to 300 K, and the use of the models above the designed limits is strongly discouraged. The data combined in the table are all for temperatures up to 350 K. The data for temperatures from 150 to 350 K are shown on Fig. 1. The data for 60 and 100 K can be found in the table on the Internet.

3. New high temperature CIA data from 400 K to 1000 K

The current need of data for modelling objects in-between traditional stellar and planetary temperatures became obvious with the long awaited identification of a brown dwarf in 1995 and with the surprising discovery of the first extrasolar “hot jupiter” planet during the same year. The development of this field has been described in numerous papers and proceedings, for example recently in the proceedings volume “From Giant Planets to Cool Stars” (Griffith & Marley 2000). The variety, and the vast abundance of newly discovered stars with significantly lower effective temperature than the cool M dwarfs, calls for reevaluation of the existing opacity data. In the case of CIA intensities due to hydrogen pairs, only those at temperatures starting at 1000 K were available (Borysow & Jørgensen 2000; Borysow et al. 2001) for stellar atmospheric modelling. Numerous inquiries have been made to the author about the availability of data for temperatures from 500 K to 1000 K. Stars of special interest are those classified as L- and T-dwarfs, as well as brown dwarfs, cool M dwarfs, cool white dwarfs, and hot extrasolar planets. The new classification (L and T types) has been introduced by Kirkpatrick and was also presented at the abovementioned conference (Kirkpatrick 2000). A comprehensive review on the subject of the model atmospheres of the very cool low mass stars and brown dwarfs by Allard et al. (1997) was published recently.

¹ The density is usually expressed in units of amagat. For hydrogen it is very close to the density of the ideal gas at standard temperature and pressure, which is $2.68676 \times 10^{19}\text{ cm}^{-3}$.

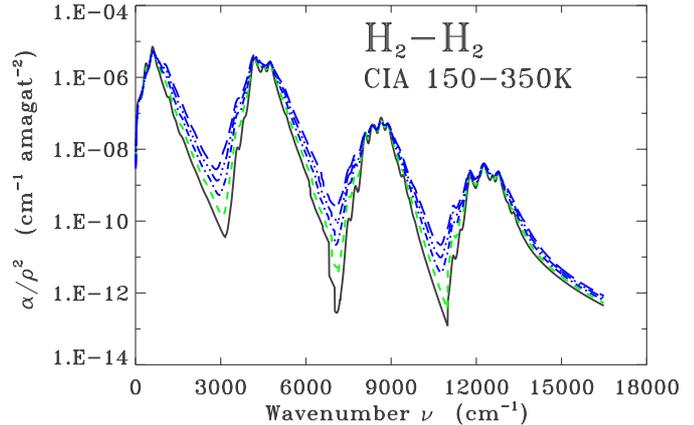


Fig. 1. CIA spectra of hydrogen pairs computed at temperatures 150 K (lowest solid line), 200 K, 250 K, 300 K and 350 K (uppermost line).

3.1. Approach

The data we start with, are the existing low temperature ones. All of them assume the initial state of the H₂ molecule to be the ground ($v = 0$) state. Fortunately, at the highest temperature considered here, $T = 1000\text{ K}$, $v = 0$ is populated with probability 0.997. It is therefore acceptable to ignore higher initial vibrational states even at temperatures as high as 1000 K.

We decided to create, as accurately as possible, the missing intensities, based on the original dipole functions, where possible. The data were computed using the H₂–H₂ intermolecular potential suitable for “low-temperature” computations (Schaefer & Köhler 1989, from now on called SK). After that, a smooth rescaling procedure was designed, in order to join the data, starting from 300 K, with those based on the “high temperature” intermolecular potential (Ross et al. 1983, from now on called RRY).

It needs to be clarified what we mean by the “low-” and the “high-” temperature potentials. The SK potential is an *ab initio* isotropic potential, which has subsequently been adjusted to fit a variety of low temperature experiments. It is therefore an extremely dependable tool for computing low temperature (roughly below $T = 300\text{ K}$) phenomena like CIA, in molecular hydrogen. It is, however, highly uncertain at the very short range of intermolecular interactions, corresponding to the high temperatures (high energy of collisions).

On the other hand, the RRY potential is an empirical isotropic potential. It is based on shock wave experiments with collision energies corresponding to the temperature of 7000 K. It will not be as accurate as the SK potential is at low temperatures, but it has an advantage of being both effective and isotropic, and at the same time it is adequate at very short intermolecular distances.

One needs to be aware of the fact that the real H₂–H₂ interaction potential is not exactly isotropic, even though such an assumption seems to work well at low temperatures. At increasingly smaller distances the potential becomes more and more anisotropic. Until presently, even if an adequate potential existed that could be used at high temperatures, the CIA computations accounting for anisotropy of the interactions were limited to very low temperatures. At increasing temperatures the RRY

Table 1. Ratios $1/A$ of the integrated intensities $G0$ of the quadrupolar terms, at selected temperatures, based on the RRY and SK intermolecular potentials.

$T(K)$	$G0(RRY)/G0(SK)$	$f(T)$
300.	1.161	1.000
350.	1.166	1.012
400.	1.170	1.024
500.	1.180	1.051
600.	1.189	1.081
700.	1.197	1.113
800.	1.206	1.147
900.	1.215	1.184
1000.	1.223	1.223

potential effectively accounts for higher vibrational states of the H₂ molecule. This fact has an impact on the potential shape as well. The effective potential has thus many advantages when used in the region where there exist no reliable computations of the intermolecular interactions and when, even if such existed, computations accounting for the interaction anisotropy would not yet be possible.

It can be safely assumed that the main contributor to the CIA intensities, for each band, is the quadrupole induced term. For this reason, the ratios between the integrated intensities ($G0$) of the quadrupolar term for Ross et al. (1983) and for Schaefer & Köhler (1989) were computed first. These are listed in Table 1 in the second column. Next, an arbitrary function was used to rescale the intensity of the data at various temperatures. We multiplied the results obtained with the SK potential, by the following function of temperature $T(K)$:

$$f(T) = 1/A \times \{a * T + b\},$$

$$\text{with } a = (1 - A)/700, \text{ and } b = 10A/7 - 3/7,$$

$$\text{where } A = G0(SK)/G0(RRY).$$

We assumed that the rescaling will take place beginning at temperature $T = 300$ K and ending at $T = 1000$ K. The results for $f(T)$ are shown in the third column of Table 1. As can be seen, we take the data exact at the lowest temperature considered (300 K) and gradually rescale them to match the data computed with the RRY potential at 1000 K.

4. Computing the RT band, 300–1000 K

Since no easy rescaling was possible, as both the intensity and especially the spectral shapes change with temperature, we computed the new spectra based on the semi-classical moments and using the usual lineshape profiles BC and K0, as in the original paper by Borysow et al. (1988). The test made at 300 K with this slightly simplified approach turned out to be highly satisfactory, so we proceeded in this way at the higher temperatures, where the semi-classical moments are increasingly more suitable. In this way, we obtained entirely new and accurate spectra. The computations were based on the SK potential and

the same dipole moment functions as used by Borysow et al. (1988) for all contributing terms $\lambda_1\lambda_2\Lambda L = 2023, 2021, 2233$ and 4045.

5. The fundamental band, 350–1000 K

We base our approach on the original theoretical paper where the most accurate ab initio dipole moments are computed (Meyer et al. 1989) and the papers describing the computer model of this band at low temperatures (Borysow 1991; Borysow 1993). We used the same model as the one available on the Internet, but with the new lineshape parameters based on the semi-classical moments, now computed at temperatures from 350 to 1000 K for $j_1 = j_2 = j'_1 = j'_2 = 0$. We used all significant induction terms: $\lambda_1\lambda_2\Lambda L = 0001, 0221, 0223, 2021, 2023, 2233$ and the SK potential. We adopted lineshapes BC and K0 instead of the more advanced BB lineshapes used by Borysow (1991). All other parameters are computed by the model internally.

6. The first overtone band, 350–1000 K

We have used the same FORTRAN model program (Zheng & Borysow 1995) as deposited on the Internet. Since the fits of the spectral lineshape parameters extend over a remarkable broad range of temperatures (20–500 K), we estimated that using the same fits up to 1000 K will not cause significant inaccuracies.

7. The second overtone, 400–1000 K

We started with computing the spectra from 600 to 1000 K. We used the “ad hoc” (unpublished) program written for this band and described by Borysow et al. (1997). Since no dipole information was available then, the simplest model has been assumed. Only the quadrupole induced terms were accounted for and the RRY intermolecular potential was used. The comparison of the CIA spectra using this model, with those using the full quantum mechanical approach (Borysow et al. 2001) showed that the “ad hoc” and the most accurate spectra were surprisingly similar to each other. We therefore found it justifiable to use the previous model as a start, and only scale it in accordance with the more accurate results of Borysow et al. (2001), rather than performing a completely new and very time consuming full quantum mechanical computation.

We compared first the results of the old (1997) “ad hoc” program with the far wing of the quantum mechanical results, in the spectral region where the second overtone is important (the maximum appears around $12\,000\text{ cm}^{-1}$). We noticed that the shape of the two spectra is quite similar, but the spectra we produced need to be rescaled by a common factor. It was not a surprise, because the spectra assumed only the 2023 and 0223 terms whereas there are more terms to account for.

After the rescaling there was still a difference in the slope of the very far wing. We adjusted the shape of the slope to match that of the quantum mechanical results. We found this to be the most reliable simple procedure.

Next, we addressed the data for 400 and 500 K. In principle, those data were available from the existing FORTRAN program

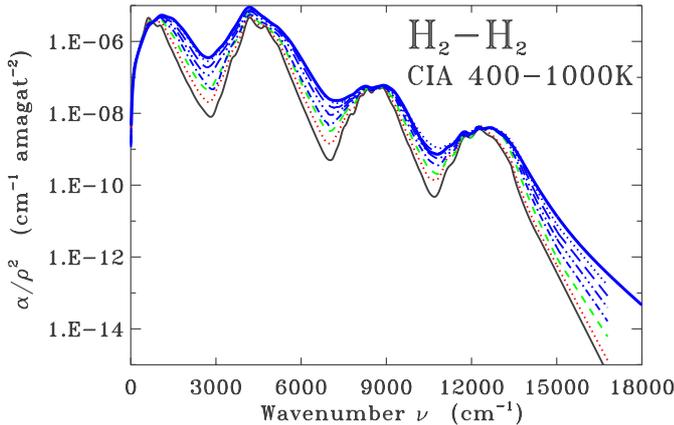


Fig. 2. The CIA spectra of hydrogen pairs computed at temperatures from 400 to 1000 K. Spectra are given at 400 K (lowest lying solid line), 500 K, 600 K, 700 K, 800 K, 900 K and 1000 K (upper dotted line ending at 17000 cm⁻¹). For comparison, the results obtained by Borysow et al. (2001) at 1000 K are also shown (thick, uppermost, solid line).

(Borysow et al. 2000) which works up to 500 K. However, we found out that the width of the spectral lines does not match with that of the high temperature data. We therefore convoluted the spectra with a Gaussian weight function with a halfwidth equal to 40 cm⁻¹ and 50 cm⁻¹ at 400 and 500 K, respectively. Next, since the far wings were not suitable for use at very high wavenumbers, the slope of the far wings was adjusted accordingly, to match the spectra at higher temperatures.

8. Summary of the high temperature results

We have combined the spectra of the three lowest bands (RT, the fundamental band and the 1st overtone) and multiplied them by a function $f(T)$ presented in Sect. 3.1. Next, we assembled the results with the data for the second overtone, which did not need to be rescaled.

The results for the high temperature data are shown in Fig. 2. The spectra are computed for hydrogen at thermal equilibrium. We present here our results from 400 to 1000 K. In addition, we compare our current results with those obtained by Borysow et al. (2001) at 1000 K. The agreement between the two sets is remarkable, when the difference in approach is considered.

9. Conclusions

We presented here the missing data of the H₂–H₂ CIA absorption coefficients at temperatures between 400 and 1000 K. Since the flux maximum of the black body radiation is at 3–6 μm (i.e. 3000–1700 cm⁻¹) for temperatures between 1000 and 500 K, especially this region should be modelled very accurately. This region corresponds, in fact, to the purely roto-translational band and to the fundamental band (see Fig. 2). These two bands were computed exactly, based on the pure theory, and rescaling has not been involved (other than that related to the interaction potential, $f(T)$ factor). The CIA spectra of the two other bands, falling at frequencies beyond 7000 cm⁻¹,

have been modelled by careful rescaling, as described in the previous sections. The continuous set of the 60–1000 K data presented here, together with the 1000–7000 K data presented by Borysow et al. (2001), thus represent the most accurate H₂–H₂ CIA data available. They are suitable for modelling of all types of astrophysical objects known, where CIA plays an important role – ranging all the way from planetary atmospheres, over “hot jupiters” and brown dwarfs, to M-dwarfs and metal poor subgiants.

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