

Theoretical Predictions of Collision-Induced Absorption spectra from first principles at 300 K by molecular H₂ pairs

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Synopsis We report the current extension of our opacity data base of H₂-H₂ CIA spectra to frequencies up to 20,000 cm⁻¹ at temperatures in the broader vicinity of 300 K (work in progress). The work is based on a recent quantum chemical computations by Hunt and associates of the potential energy surface (PES) and induced dipole surface (IDS) of two H₂ molecules, which interact through van der Waals forces.

It is well known that dense gases of infrared inactive molecules such as H₂ absorb infrared radiation with range from the microwave and far infrared regions of the spectrum to near infrared, and possibly into the visible. The reason for these absorption continua are collisionally interacting pairs of hydrogen molecules, which in contrast to the non-interacting molecules in general possess transient electric dipole moments [1, 2]. Since molecular hydrogen is the most abundant species of the universe in order to get a deeper understanding of the universe as a whole it is important to study the properties of hydrogen. In this work the main focus is on the low absorption by collisional hydrogen complexes in the frequency range of 0 to 20,000 cm⁻¹ for H₂ pairs for temperature at 300 K. CIA spectra are composed of a great number of very diffuse, strongly overlapping lines, the bands of the rovibrational transitions of the (unperturbed) molecules of the collisional complex, and bands at sum and differences of these when simultaneous transitions in both molecules take place $\nu_1'j_1'\nu_2'j_2' \leftarrow \nu_1j_1\nu_2j_2$. The CIA spectrum of a diatomic gas, such as hydrogen, is given by [6,60]: $\alpha(\omega, T) = \frac{2\pi^2 N_a^2}{3\hbar} \rho^2 \omega [1 - \exp(-\frac{\hbar\omega}{kT}) Vg(\omega, T)]$. The function $Vg(\omega, T)$ is the sum over all optical transitions [10]. For the calculation of collision-induced absorption spectra for this work Fortran program codes and the Intel Fortran compiler were used. Figure 1 shows the calculation CIA spectrum for H₂ pairs at 300 K. From left to right, the structures correspond roughly to the H₂ pure rotational band, the H₂ fundamental band, and the first, second, third and fourth H₂ overtone bands. All of these bands are of course

dipole-forbidden in an unperturbed (noninteracting) H₂ molecule. For our present purpose, we compare our computations to laboratory measurements at the highest available temperatures ($\simeq 300$ K). The comparison with laboratory measurements are not shown. The normalized absorption coefficient varies over a range of nearly six orders of magnitude. Between the six bands just mentioned are deep minima.

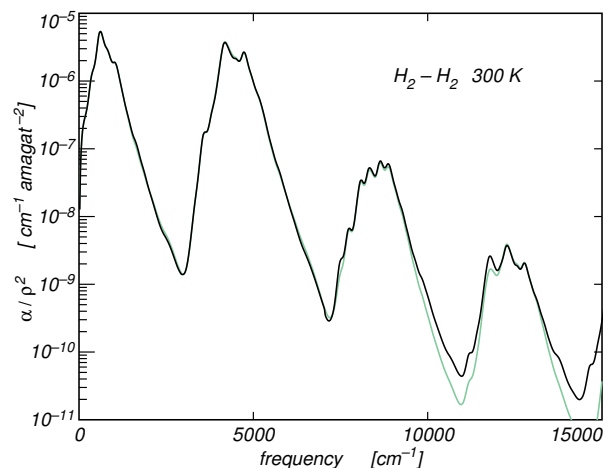


Figure 1. Calculated binary CIA coefficients, α , normalized by gas density square (ρ^2) of hydrogen gas at 300 K. Also shown is an earlier calculation [2] (green line).

References

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- [2] Abel, M.; Frommhold, L.; Li, X.; Hunt, K.L. 2011 *The J. Phys. Chem. A* **115** 6805.

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