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The H_2–H infrared absorption bands at temperatures from 1000 K to 2500 K

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Abstract. H_2–H collision-induced absorption spectra are computed for temperatures from 1000 K to 2500 K and frequencies from 100 cm^{-1} to 10 000 cm^{-1}. The calculations are quantum mechanical and the isotropic potential approximation has been applied. The computed absorption in the fundamental band agrees roughly with the one determined by Patch (1974). However, the absorption in the translational band, which has not been obtained before, is significantly stronger than in the fundamental band.

Key words. molecular processes – infrared: stars – line: profiles – radiation mechanisms: thermal – scattering – stars: atmospheres

Colliding atoms or molecules acquire a transient electric dipole moment even if the non-interacting (i.e., well separated) individual atoms or molecules are nonpolar. As a consequence, at high enough gas densities, collision-induced infrared absorption is observed, even if at lower densities the corresponding gases and gas mixtures are infrared-inactive (Welsh 1972; Frommhold 1993). Collision-induced absorption of compressed, nonpolar gases and gas mixtures, such as hydrogen, were discovered by Welsh et al. (1949) and their significance for astrophysics was almost instantly recognized (Welsh 1972; Herzberg 1952a; Herzberg 1952b; Trafton 1964). Since then, extensive investigations of collision-induced absorption in planetary atmospheres and, more recently, in the atmospheres of certain cool stars (Borysow et al. 1997; Burrows et al. 1997; Jørgensen et al. 2000) have been carried out.

Whereas for systems such as H_2–H_2 and H_2–He a number of excellent laboratory measurements of the collision-induced spectra exist that permit stringent tests of the quantum chemical computations (Frommhold 1993), no such measurements are known for the H_2–H system and its spectra are obtained from theory. This is similar to the H–He pair, which also has been investigated theoretically (Gustafsson & Frommhold 2001). The absorption due to H_2–H pairs could be important for the dynamics of the atmospheres of stars, when temperatures are such that atomic and molecular hydrogen coexist. Opacities of zero-metallicity gas were thoroughly investigated by Lenzuni et al. (1991). Collision-induced absorption is in general most important at the lowest of the temperatures considered there, namely 3000 K. At higher temperatures there are other strong continuum absorbers, such as ionic hydrogen. It is at temperatures below 3000 K and at relatively low pressures (for significant atomic hydrogen abundance) that we anticipate the H_2–H collision-induced absorption to be important.

We have employed quantum calculations (Frommhold 1993) of the absorption spectra of H_2–H collisional pairs at temperatures from 1000 K to 2500 K. This is a range of temperatures where atomic hydrogen is abundant under pressures which could be of interest. For the modeling of stellar atmospheres, the maximum of the Planck distribution of black body radiation should be considered, or rather at what frequency $\nu_{\max}$ this maximum appears. According to Wien's displacement law $\nu_{\max} \approx 1.96T$ cm^{-1} and in order to have a significant amount of radiation intensity within our frequency range we need to extend the calculation to frequencies which are larger than $\nu_{\max}$ at each temperature.

An ab initio interaction-induced dipole moment was reported recently by Gustafsson et al. (2003). Three vibrational matrix elements of the dipole, $B^{vv'}_{\lambda L}(R)$, were obtained, namely $B^{00}_{\lambda L}$, $B^{11}_{\lambda L}$, and $B^{01}_{\lambda L}$. At temperatures above 1000 K, which we have considered in the present work, vibrational hot-bands will contribute to the absorption. In order to obtain dipole matrix elements with v and v' greater than one we have assumed that the dipole's dependence of the H_2 separation r is a quadratic polynomial. This yields three independent coefficients which can be determined since we know three vibrational matrix elements, $B^{vv'}_{\lambda L}$, and the matrix elements $\langle v|\, r^n \,|v'\rangle$ with $n = 0, 1$, and 2. The j dependence of the H_2 vibrational wave functions is neglected and they are determined for $j = 0$ using the potential by Kolos et al. (1986). This approximation is expected to be good to a few percent, which is acceptable

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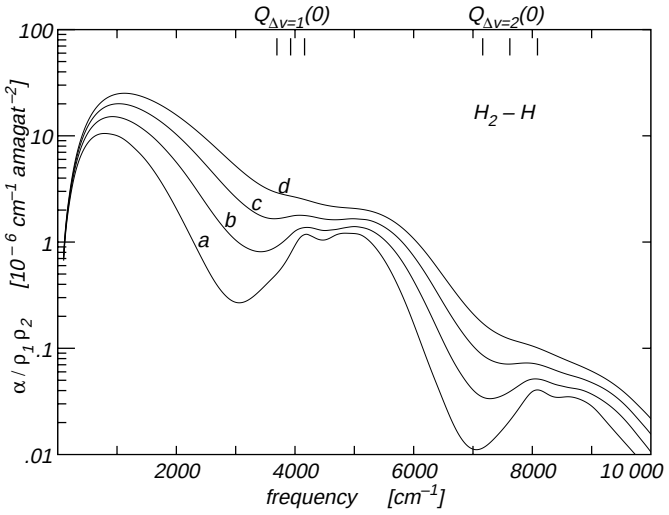

Fig. 1. The absorption coefficient, α, normalized by the atomic and molecular hydrogen gas densities, ρ_1 and ρ_2, respectively, as function of frequency in the rototranslational band. The temperatures are: (a) 1000 K, (b) 1500 K, (c) 2000 K, and (d) 2500 K. The positions of the Q transitions for initial vibrational quantum numbers, v, of 0, 1, and 2 are indicated.

considering the overall uncertainty of the dipole surface. For the intermolecular potential we used the isotropic part of the ab initio surface by Partridge et al. (1993). The influence of the anisotropy was investigated in Gustafsson et al. (2003) and turned out to be negligible at temperatures below 1000 K. It is expected to be small at the temperatures considered here as well.

At sufficiently high kinetic energies collisions between atomic and molecular hydrogen produce exchange reactions, namely $H_2 + H \rightarrow H + H_2$. The cross section of that reaction has been investigated experimentally by Nieh & Valentini (1990). They showed that hydrogen molecules, in their rotovibrational groundstate, colliding with hydrogen atoms at a kinetic energy of about .7 eV give cross sections on the order of 1 Å^2 for exchange reactions. Now, in the present calculations the particles have kinetic energies on the order of only .2 eV, but they also have a significant amount of rotovibrational energy. There is no attempt to model collision-induced absorption including exchange reactions here. At a temperature of 2500 K we believe that this is not a serious approximation. However, for higher temperatures reaction channels most likely have to be included in the H_2–H scattering process.

A numerical accuracy on the 1% level is desired, although the dipole and potential input are expected to be less accurate than that. Vibrational hotbands up to an initial vibration, v, of 1 and 2 are included for the two lowest and the two highest temperatures considered, respectively. Initial rotational levels up to $j = 13$ and partial waves up to $l = 58$ are included in the calculation at 2500 K. Five dipole components, $\lambda L = 01, 21, 23, 43, 45$, are taken into account.

Figure 1 shows the calculated spectra at four temperatures, from 1000 K to 2500 K, covering the translational, the H_2 fundamental, and the first H_2 overtone bands. A comparison of the translational and the first overtone bands shows more than two orders of magnitude difference in absorption. Accordingly, at the temperatures considered, most of the black body radiation falls in the high absorption part of the spectrum. The fundamental band absorption was modeled by Patch (1974) and we note that the absorption calculated here is of similar intensity. However, the translational band absorption is about one order of magnitude stronger than that of the fundamental band and appears to be important to include in modeling of star atmospheres.

A table with the data presented in Fig. 1 is accessible online (Borysow 2002).

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