

H₂CO ROTATIONAL EXCITATION BY H₂

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Abstract. Since its discovery in 1969, the abnormal absorption of H₂CO in dark clouds has remained an open problem owing to the lack of accurate collisional rates. We aim to assess the influence of H₂CO-H₂ collisional rates on the pumping scheme of Townes & Cheung (1969). Full converged close-coupling calculation based on a high accuracy potential energy surface have been performed for H₂CO colliding with para(J=0,2)- and ortho(J=1)-H₂. Rotational rates for transitions among the five lowest doublets of ortho-H₂CO and for kinetic temperatures between 5 K and 50 K are obtained and discussed.

1 Introduction

In the end of the sixties, astronomers discovered a large amount of formaldehyde in space (e.g. Buhl et al. 1969), always detected in emission until Palmer et al. (1969) discovered the absorption of the $1_{11} \rightarrow 1_{10}$ transition (4.8 GHz) against the CMB in molecular clouds. In 1969, Townes and Cheung proposed a classical collisional scheme which was able to explain this abnormal absorption. This work investigate the impact of accurate collisional cross sections between H₂CO and H₂. We first present the *ab initio* Potential energy surface used for our calculations (section 2), the cross sections we obtained and a comparison with the former rates of Green (1991) (section 3), and the implication of these new rates on the abnormal absorption (section 4).

2 The *ab-initio* Potential Energy Surface

The *ab initio* Potential Energy Surface was computed at the CCSD(T) level of theory using basis set extrapolations. The accuracy of the extrapolation scheme was checked against explicitly correlated CCSD(T)+R12 calculations and was found to be within a few cm⁻¹. At each intermolecular distance, the interaction potential was least-square fitted over a set of 146 terms angular expansion using the procedure described in Faure et al. (2005).

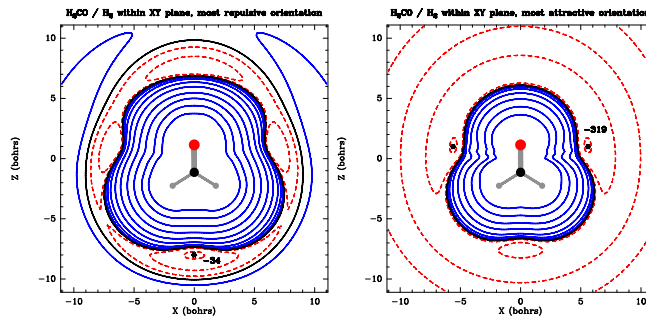


Fig. 1. Potential energy surface of H₂CO-H₂ for two configurations: the most repulsive relative orientation (left), the most attractive orientation (right). Colour: blue: repulsive interaction, red: attractive interaction. Distance are in Bohrs.

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3 Rotational cross sections and rates

We present in Fig.2 the rotationally inelastic cross section between H₂CO and ortho-H₂ ($J = 1$) for the transition $2_{12} \rightarrow 2_{11}$. The cross section falls steeply as the collisional energy increases. Moreover, our energy grid is fine enough to properly describe the resonances that arise at low energies.

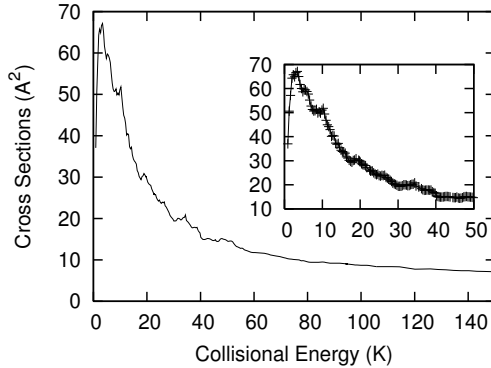


Fig. 2. Cross sections of the $2_{12} \rightarrow 2_{11}$ transition with a zoom on the resonances region.

Fig.3 shows comparisons between the H₂CO-He results of Green (1991), currently used by astronomers, and the present rates calculated for temperatures ranging from 5 to 50 K obtained by integrating the cross sections over Maxwell-Boltzmann distribution of collision energy. We see that our rates are about twice as large as those of Green (1991), suggesting a significant impact on radiative transfer studies.

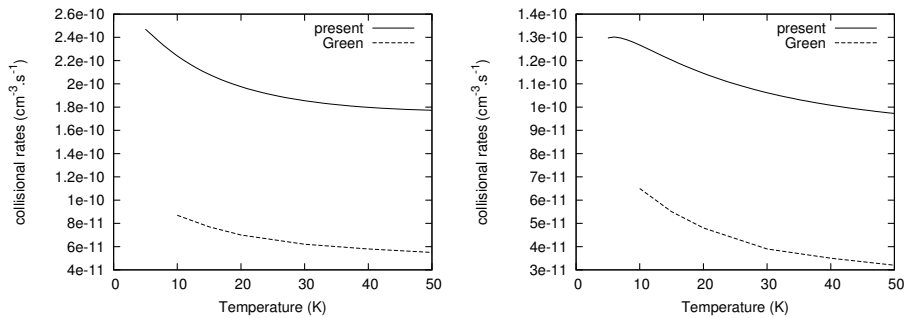


Fig. 3. Comparison between the Green rotational rates (1991) and ours for the $1_{10} \rightarrow 1_{11}$ (first K-doublet, left curves) and $2_{11} \rightarrow 2_{12}$ (second K-doublet, right curves) transitions

4 The abnormal absorption

In 1975, Garrison et al. described qualitatively the abnormal absorption in molecular clouds by a ratio R (Eq.4.1) obtained by solving the (4 level) statistical equilibrium equations with the following assumption: the radiative decays between $J=2$ and $J=1$ is infinitely faster than the collision processes and the radiative processes between the levels of same rotational number are negligible:

$$R = \frac{\sigma(1_{10} \rightarrow 2_{11}) + \sigma(1_{10} \rightarrow 1_{11})}{\sigma(1_{11} \rightarrow 2_{12}) + \sigma(1_{11} \rightarrow 1_{10})} \quad (4.1)$$

Relating this ratio to the excitation temperature : $R = \exp(\Delta E/kT_{ex})$, they found that R must be around 1.13 to account for an excitation temperature of the $1_{11} \rightarrow 1_{10}$ transition around 1.8 K, as observed by Palmer

et al. (1969).

Our values of R (Fig.4) are in good agreement with the expected value in the temperature range 5-25 K, although irregularities due to resonances appear. However, these values are smoothed if the ratio is calculated with rates instead of cross sections.

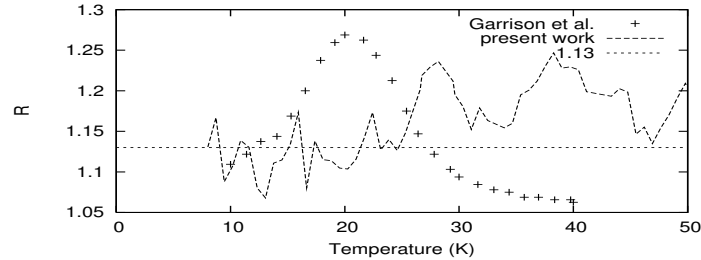


Fig. 4. Ratio R as a function of temperature. The dotted line is the expected $R = 1.13$.

5 Conclusion

Thanks to an accurate ab initio potential energy surface and precise calculations for the cross sections, we have computed inelastic collisional cross sections for the rotational excitation of ortho-H₂CO by ortho-H₂. The propensity rules that we obtain are similar to those of Garrison et al. (1975), which were shown to explain the abnormal absorption of formaldehyde in the CMB. Collision calculations with para-H₂ are currently in progress.

References

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