

ROTATIONAL EXCITATION OF CS AND SiO BY COLLISIONS WITH HELIUM

F. Dayou¹, C. Balanca¹, F. Lique¹, A. Spielfiedel¹ and N. Feautrier¹

Abstract. The modelisation of line intensities as a result of molecular excitation calculations requires accurate values of the radiative transfer coefficients and collisional excitation rates, corresponding to collisional processes with the most abundant neutral species, He and H₂. We present new sets of rotational excitation rate coefficients for the SiO-He and CS-He colliding systems, calculated among the 31 (CS) and 26 (SiO) first rotational states for temperatures ranging from 5 to 300 K. These data were obtained from reliable quantum chemical calculations, using 2D SiO-He and CS-He potential energy surfaces and close-coupling calculations of the collisional excitation cross sections. Features of the obtained excitation cross sections, such as their associated propensity rules, were further analyzed.

1 Introduction

The analysis of molecular line surveys of interstellar and circumstellar environments provides crucial information about the chemical and physical conditions of the observed astrophysical objects. A proper modelling of the relative emission line intensities through molecular excitation calculations allows to infer information such as the molecular abundances, the main colliding partner volume density as well as the temperature of the astrophysical objects under study. To this end one needs to account for the radiative and collisional processes that contribute to modify the steady-state population in a given ro-vibrational state of the observed molecule. The aim of the present work is to characterize the rotational (de)excitation processes corresponding to the SiO and CS molecules, taken in their ground vibrational state $v = 0$, in collisions with He. The latter molecules are a good tool to probe the physical conditions of shocked regions (SiO), star-forming regions (CS) or circumstellar environments of AGB stars (SiO and CS). A fully quantum approach of the SiO-He and CS-He colliding systems was chosen to determine the rotational excitation rate coefficients for temperatures ranging from 5 to 300 K.

2 Potential energy surface

Reliable 2D potential energy surfaces (PES) for the SiO-He and CS-He molecular systems were computed by means of highly correlated *ab initio* calculations using the coupled-cluster method at the RCCSD(T) level of theory. The internuclear distance of each diatom was kept fixed at its experimental equilibrium value. The analytic representation of the angular dependance of the PESs was constructed as an expansion into a basis of Legendre polynomials $P_\lambda(\cos\theta)$. Given the strong anisotropy associated with both PESs, it was found necessary to include anisotropic terms up to $\lambda=12$ in the polynomial expansion to correctly reproduce the angular dependance of the potentials.

3 Collisional dynamics

For the SiO-He and CS-He colliding systems, rotational excitation cross sections among the 31 (CS) and 26 (SiO) first rotational states were determined from Close-Coupling quantum scattering calculations in a collisional energy range from 0.1 up to 3000 cm⁻¹. The collisional rate coefficients $k_{j_i-j_f}(T)$ were obtained from a Boltzmann average of the cross sections over a velocity distribution of temperatures ranging from 5 to 300 K.

¹ LERMA, CNRS and Observatoire de Paris-Meudon (UMR 8112), 5 place Jules Janssen, 92195 Meudon Cedex, France

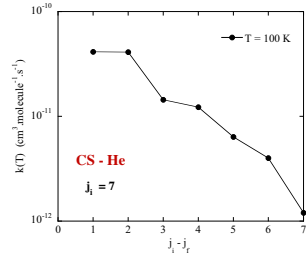


Fig. 1. Rotational de-excitation rate coefficients for collision of CS with He from an initial state $j_i=7$ at $T=100\text{K}$ as a function of $\Delta j=j_i-j_f$

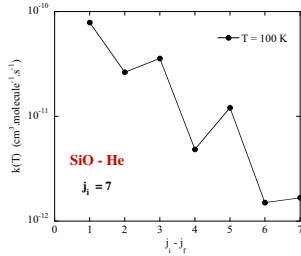


Fig. 2. Rotational de-excitation rate coefficients for collision of SiO with He from an initial state $j_i=7$ at $T=100\text{K}$ as a function of $\Delta j=j_i-j_f$

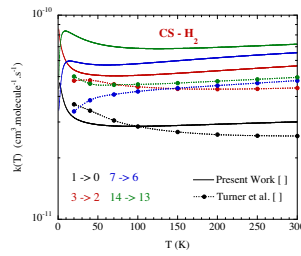


Fig. 3. Comparison of the rotational de-excitation rate coefficients of the present work [1] with those of Turner et al. [3] for the system CS-para- $\text{H}_2(j=0)$

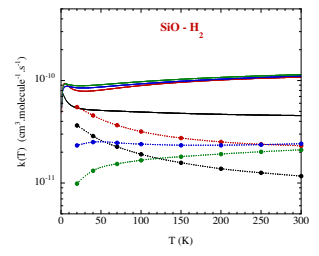


Fig. 4. Comparison of the rotational de-excitation rate coefficients of the present work [2] with those of Turner et al. [3] for the system SiO-para- $\text{H}_2(j=0)$

We report on Fig. 1 and 2 the de-excitation rate coefficients for the CS and SiO molecule, respectively, in collision with He from a given initial rotational state ($j_i = 7$) at a kinetic temperature of 100 K. For both colliding systems it is clearly seen a strong propensity rule for low Δj transitions. Furthermore, for a given Δj transition, the rate coefficients were found increasing with j_i . These features are related to the anisotropy of the two PESs considered. In the particular case of SiO-He, the odd Δj transitions are strongly favored due to the large asymmetry of the PES.

A first order correction can be made to provide collisional rate coefficients with para- $\text{H}_2(j = 0)$, applying a scaling factor close to 1.4 to the rate coefficients with He to account for the reduced mass ratio between the two colliding systems. Our rate coefficients calculated in such a way for the CS [1] and SiO [2] molecules in collision with para- $\text{H}_2(j = 0)$ were compared to the values of Turner et al. [3], obtained using the above approximation together with CS-He and SiO-He PESs computed from a gas-electron model. The two sets of rate coefficients for CS-para- $\text{H}_2(J=0)$ and SiO-para- $\text{H}_2(J=0)$ are compared in Figs. 3 and 4, respectively, for several frequently observed transitions. For each colliding system, large differences are readily seen between the two sets of rate coefficients, which can rise up to a factor 5 for given transitions. Moreover, in the case of the SiO molecule the two set of rate coefficients were found to display opposite propensity rules for even/odd Δj transitions. Since both results rest upon identical approximations, the present comparison emphasises the need for a proper description of the PES to achieve accurate values of collisional rate coefficients. Hence, given the improved accuracy of the present *ab initio* PESs compared to the gas-electron ones, our sets of rate coefficients are thought to be the most appropriate for an astrophysical purpose until the colliding systems with H_2 be explicitly considered.

4 Conclusion

Rotational excitation rate coefficients for the CS-He and SiO-He colliding systems were calculated using new 2D *ab initio* potential energy surfaces and quantum mechanical coupled-channel method for the dynamics. The rate coefficients between the 31 (CS) and 26 (SiO) first rotational states were computed (Lique et al. 2006a, Dayou & Balana 2006) for temperatures ranging from 5 to 300 K. For each molecular system, the comparison with the results previously obtained by Turner et al. (1992) points out that significant differences, up to a factor 5 for selected transitions, exist between the two sets of rate coefficients. Such quite large discrepancies may have an important impact on the diagnostic derived from molecular lines modelling (Lique et al. 2006 b).

References

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