

ROTATIONAL EXCITATION OF SULFUR MONOXIDE BY COLLISIONS WITH HELIUM AT LOW TEMPERATURE

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Abstract. We present cross sections and collisional rates calculated with a new 2D potential energy surface for the SO-He system. Close coupling calculations of the collisional excitation cross sections of the fine structure levels of SO by He are calculated at low energies. The propensity rules for cross sections between fine-structure levels are studied and it is shown that $\Delta N = \Delta j$ cross sections are always much larger than the other cross sections, especially for high- N rotational levels. The use of IOS recoupling techniques from spin-free cross sections is also investigated and we have shown that this method is not valid for our system at low temperature, especially for collisions involving low fine-structure levels. Excitation rates among fine-structure levels are given at low temperatures (5-50K). Finally, we show that the use of our new rate coefficients compared to the use of Green's rate coefficients can significantly change the diagnostics of the SO abundance in dark clouds.

1 Introduction

Observations of molecular emission at millimeter and infrared wavelengths are powerful tools to investigate the physical and chemical conditions of astrophysical objects. Sulfur monoxide has been used extensively to study shocked molecular gas in various environments. The modeling of the line intensities requires comparison with model excitation calculations using radiative and collisional rates. Here, the collisional excitation cross sections of the fine-structure levels of SO are calculated at low energies using a full close coupling (CC) treatment and a new potential energy surfaces (PES). Then, the validity of a recoupling approximation is discussed and we give the rate coefficients among fine-structure levels for temperatures ranging from 5 K to 50 K. Finally, we analyse the impact of these new rate coefficients on astrophysical modeling in comparison with previous data.

2 Potential energy surface

The PES was calculated at the RCCSD(T) level. The SO r-distance was frozen at its experimental minimum energy distance ($r_e = 2.80$ bohr). The *ab initio* surface was calculated using the MOLPRO2002 package. The three atoms were described by the AVQZ basis set, augmented by the (3s3p2d2f1g) bond functions. For this van der Waals system, the global minimum of the interaction energy is found to be $-159.1127 \mu\text{hartree}$ i.e. -34.921 cm^{-1} ($R=7.29 a_0$, $\theta=180$ degree).

3 Fine structure of SO

In the SO ($^3\Sigma^-$) electronic ground state, the rotational levels are split by spin-rotation coupling. In the intermediate coupling scheme, the rotational wave function of SO can be written for $j \geq 1$ as:

$$\begin{aligned}
 |F_{1jm}\rangle &= \cos\alpha|N = j - 1, Sjm\rangle + \sin\alpha|N = j + 1, Sjm\rangle \\
 |F_{2jm}\rangle &= |N = j, Sjm\rangle \\
 |F_{3jm}\rangle &= -\sin\alpha|N = j - 1, Sjm\rangle + \cos\alpha|N = j + 1, Sjm\rangle
 \end{aligned}
 \tag{3.1}$$

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where $|N, Sjm\rangle$ denotes pure Hund's case (b) basis functions and the mixing angle α is obtained by diagonalisation of the molecular hamiltonian. In the pure case (b) limit, $\alpha \rightarrow 0$, the F_1 level corresponds to $N = j - 1$ and the F_3 level to $N = j + 1$. For SO, the case (b) limit becomes valid beyond $N = 5$. All calculations were carried out with the exact energy levels including the fine structure interaction. However, we will use in the following the usual level labeling N_j where $N=j-1$, $N=j$, $N=j+1$ corresponds to the F_1 , F_2 and F_3 levels as defined in equation 3.1.

4 Results

4.1 Cross sections

The dynamics calculations were carried out using the exact CC approach with the MOLSCAT code. The results show (Lique et al. 2005) strong propensity for the $\Delta N = \Delta j$ transitions. This propensity rule, previously noted by Green (1994) for SO and by Corey et al. (1986) for the O_2 , becomes stronger as N increases.

We have explored the validity of the recoupling approximation used by Green (Green 1994). Approximate cross sections among fine-structure levels were obtained in the Hund's case (b) limit from close coupling spin-free cross sections using the infinite order sudden (IOS) approximation scaling relationship to recouple the angular momenta:

$$\sigma(NSj \rightarrow N'Sj') = \frac{\sigma^{IOS}(NSj \rightarrow N'Sj')}{\sigma^{IOS}(N \rightarrow N')} \sigma^{CC}(N \rightarrow N') \quad (4.1)$$

Figure 1 compares these approximate cross sections with the corresponding CC cross sections calculated in the intermediate coupling scheme. As expected, the recoupling approximation seems acceptable for $\Delta N = \Delta j$ transitions. Conversely large differences occur, even at relatively high energies, for the other transitions.

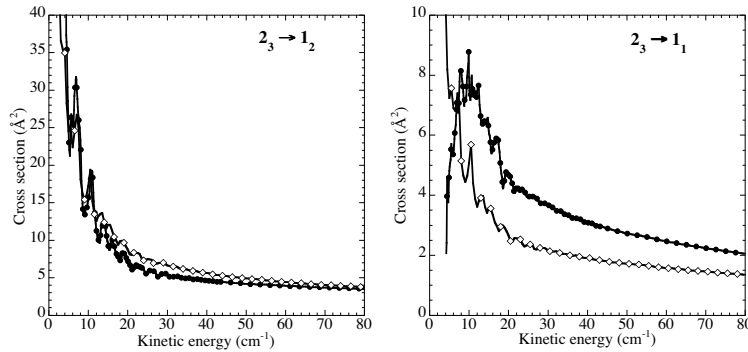


Fig. 1. Comparison between results obtained with the recoupling technique (empty diamonds) with CC results (filled circles).

4.2 Rate coefficients

CC calculations of the cross sections were carried out up to a total energy of 300 cm^{-1} that allows us to determine rate coefficients up to 50 K. Comparison was made with the results obtained at 50 K by Green (1994), by transforming his SO- H_2 rate coefficients into SO-He rate coefficients by a ratio of the reduced mass of the different systems. Figure 2 compares these rate coefficients for different $N_j \rightarrow N'_j$ transitions as a function of N . As seen in Fig. 2, large differences up to a factor ten exist. Two factors may contribute to these differences: (i) the difference between the two potential energy surfaces, as Green adopted the PES calculated obtained for CS- H_2 with an electron-gas model (ii) the recoupling approximation used by Green, that is not valid at low energies and particularly for low N -values and for $\Delta N \neq \Delta j$ transitions.

5 Astrophysical applications

We have analysed the effect of the new rates on the excitation of SO by modeling this excitation through a LVG non local radiative transfer code. We have compared the brightness temperature T_B at $T_K=10 \text{ K}$ for recently

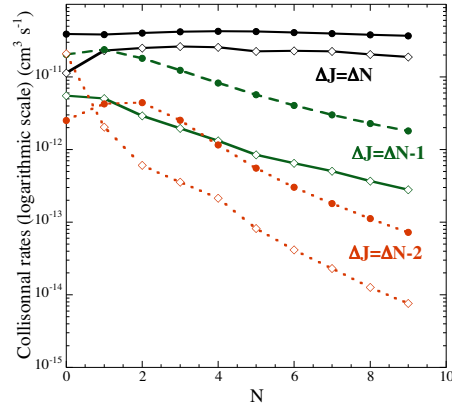


Fig. 2. Our calculated rate coefficients at 50 K for $\Delta N=N^i-N^f=1$ (filled circles) compared with results obtained by Green(1994) (empty diamonds).

observed SO lines obtained by using the present collisional rates and those of Green (1994) extrapolated to 10K (assuming a dependence following the root square of T_K). The corresponding T_B values are plotted in Fig. 3 as functions of the H_2 density and of the SO column density N_{SO} .

We can see that the differences are important, especially for $\Delta N \neq \Delta j$ transitions. These results are not surprising in view of the differences in the collisional rates discussed above.

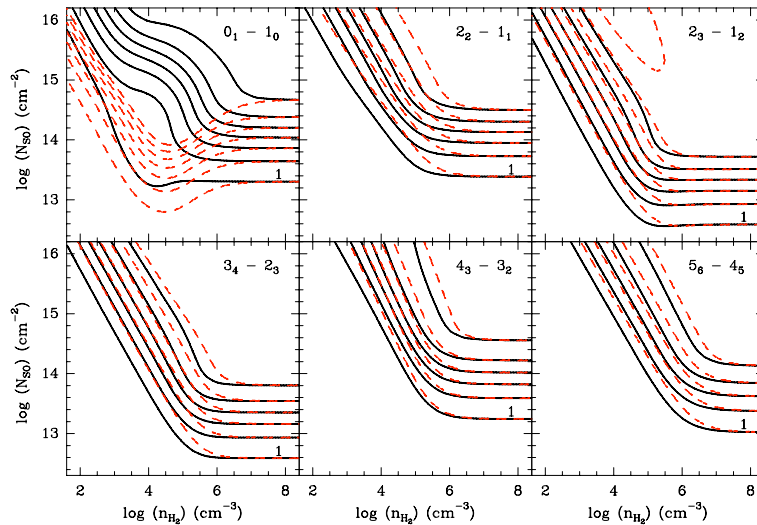


Fig. 3. T_B using our (solid line) and Green (1994) (dashed line) collisional rates at 10K. The T_B values vary from 1K by step of 1K.

References

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