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Collisional excitation of sulfur dioxide by molecular hydrogen in warm molecular clouds

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ABSTRACT

Interpretation of SO₂ line emission in warm environments requires a detailed knowledge of collisional rate coefficients for a wide range of levels and temperatures. Using an accurate theoretical interaction potential for SO₂–H₂, rate coefficients for collisions of SO₂ with para and ortho-H₂ for the 31 first SO₂ rotational levels are calculated for temperatures up to 500 K using the coupled states (CS) approximation. From a comparison with previously published close-coupling (CC) results, it was shown that the two sets of data agree within 20–30 per cent for both para- and ortho-H₂ collisions. As previously found within the CC approach, the CS rate coefficients with ortho and para-H₂ differ by a factor of 2 in average, the largest being mainly the rates for collisions with ortho-H₂. For higher levels and temperatures, rate constants were computed within the infinite order sudden (IOS) approximation. Rate coefficients were obtained for the lowest 410 rotational levels of SO₂ in the 100–1000 K temperature range. A comparison at 30, 100 and 300 K of the IOS data with the corresponding para-H₂ CS results indicates that the IOS approximation systematically underestimates the CS results by a factor up to 2 at the lowest temperatures. As expected, IOS and CS rates are in a better agreement at higher temperatures. Considering that the IOS theory was developed for collisions with para-H₂, this approach cannot describe with the same accuracy collisions with ortho-H₂. So, our IOS data may be considered as quite reliable for collisions with para-H₂ and less accurate for collisions with ortho-H₂.

Key words: molecular data – molecular processes.

1 INTRODUCTION

Since its detection by Snyder et al. (1975), SO₂ has been found to be very abundant in a large variety of objects. It has been observed towards cold dark clouds with an abundance of a few 10^{−9} (Irvine, Good & Schloerb 1983; Dickens et al. 2000). It has also been observed in warm molecular clouds in which lines involve energy levels of several hundred K. SO₂ as well as other sulphur-bearing molecules are very good tracers of the physical and chemical properties of the hot core phase of high-mass star formation (Schloerb et al. 1983; Schilke et al. 2001).

According to recent studies (Hatchell et al. 1998; Viti et al. 2001), the abundances of these species are strongly time-dependent giving constraints on the evolution of the different phases of the star formation, the hot core, the surrounding molecular outflows and the associated shocked gas. Many observations (Bachiller 1996; Esplugues et al. 2013 and references therein) have shown that SO and SO₂ molecules present increased column densities (by factors up to 10³) in shocked regions so that these species could be

considered as very good tracers of shocks. Orion Kleinmann–Low nebula Orion (Orion KL), the closest high-mass-forming region, is one of the most studied regions owing to its chemical complexity and to the presence of several components characterized by different physical and chemical conditions (Tercero et al. 2010, and references therein). In the recent broad-band spectral line survey of Orion KL (Crockett et al. 2014), obtained using the Heterodyne Instrument for Far-Infrared (HIFI) instrument on board the *Herschel Space Observatory*, transitions with levels up to 1100 K were observed for the main isotopologue of SO₂, rarer isotopologues ³³SO₂ and ³⁴SO₂ were also detected.

Detailed non-local thermodynamic equilibrium (LTE) modelling is a powerful tool for investigating the physical and chemical conditions of these objects. This requires a precise knowledge of the state-to-state collisional rates between the molecule under study and the main collider in the cloud, i.e. molecular hydrogen. To the best of our knowledge, no experimental data are available for SO₂–H₂. Green (1995) has computed SO₂–He rate coefficients for temperatures between 25 and 125 K for the first 50 rotational levels of SO₂ (i.e. for levels with energy below 90 K). From a state-of-the-art accurate 5D potential energy surface, Spielfiedel et al. (2009) and Cernicharo et al. (2011) have provided full close-coupling (CC)

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collisional rates for the first 31 levels of SO₂ and temperatures from 5 to 30 K, suitable for cold dark cloud modelling. To date, however, for warm molecular clouds where high j -levels are observed, non-LTE analysis cannot be performed due to the lack of collisional rates (Esplagues et al. 2014). It is the purpose of the present paper to provide such rate coefficients for high temperatures and for a large number of rotational levels.

Scattering calculations based on CC method provide rate coefficients with the best accuracy. Unfortunately, converged scattering calculations that consider the rotational structure of both molecules grow dramatically in size with the energy, in particular when high j -levels are involved, thus CC calculations at high temperatures would be prohibitive in terms of memory and CPU time. Approximate quantum dynamics treatments of rotation by the coupled state (CS) and infinite sudden order (IOS) approaches should provide a reasonable estimate at high energies and for higher levels (Green 1976, 1979).

Our current objective is to obtain a set of rotational state-to-state rate coefficients for large temperatures and high rotational j -levels. For that purpose, we used two different quantum approaches in order to provide two sets of state-to-state rate coefficients: (i) the CC calculations among the 31 first rotational levels were extended at temperatures up to 500 K using the CS approximation; (ii) IOS calculations provide state-to-state rate coefficients for temperatures up to 1000 K and among all the rotational levels until the 41_{1,41} level (410 levels), i.e. all levels lower than the $v = 1$ vibrational level. This data are expected to enable accurate non-LTE modelling of the *Herschel*/HIFI and Institut de Radioastronomie Millimétrique 30 m recent observations (Tercero et al. 2011; Esplagues et al. 2014).

The paper is organized as follows: Section 2 provides a brief description of the potential energy surface (PES) and describes some theoretical aspects of the scattering calculations. Section 3 displays a comparison of the rate coefficients obtained with the different quantum approaches, CC, CS and IOS. Rate coefficients are presented in Section 4 and concluding remarks are drawn in Section 5.

2 COMPUTATIONAL METHODOLOGY

2.1 Potential energy surface

All calculations presented below were performed with rigid molecules using the expansion of the 5D-PES described in Spielfiedel et al. (2009) where full details can be found. Here, we just describe the main features of the PES.

This PES involves an angular expansion over 129 angular functions $\bar{t}_{l_1 m_1 l_2 l}(\theta, \phi, \theta', \phi')$ according to the conventions in Phillips, Maluendes & Green (1996). Extensive calculations of a reference PES were performed including Complete Basis Set extrapolation. The global minimum was found to be $V_{\min} = -192.723\,758\text{ cm}^{-1}$ for $R = 6.147\,979\text{ bohr}$, $\theta = 91^\circ 721\,778$, $\phi = 90^\circ 0$, $\theta' = 90^\circ 0$ and $\phi' = 0^\circ$. The angular expansion of the PES was obtained from the final very accurate set as a least square fit of the ab initio values. The selection was found to reproduce the ab initio values within 1 cm^{-1} for internuclear distances R larger than 6.5 a_0 .

At short distances, severe steric hindrance problems had been encountered as found previously for the HC₃N–H₂ system. So a regularization of the SO₂–H₂ PES was performed by introducing a scaling function S_f (see details in Spielfiedel et al. 2009). The final PES can easily be expanded over angular functions with an excellent accuracy. A threshold value of $10\,000\text{ cm}^{-1}$ was selected

for S_f , high enough for applications where both molecules can be kept rigid.

2.2 Collisional dynamics

Previous CC calculations have provided collisional para- and ortho-H₂ rate coefficients for temperatures ranging from 5 to 30 K for the 31 lowest SO₂ rotational levels (Cernicharo et al. 2011). CC calculations are computationally very expensive, so different approximate methods (CS and IOS approximations) are tested and used in the present work. The CS method, computationally less expensive than CC, is expected to be reliable for low-lying levels at energies far from the energy thresholds. As the IOS approximation neglects the energy structure of the levels, it is expected to be very poor at low energies, however, it was found to give a correct estimate of the rates among high j -levels at high energies (Lique, Cernicharo & Cox 2006).

These two methods approximate the centrifugal scattering potential and IOS further ignores rotational energy spacings compared to the collision energy (Green 1976, 1979).

As a result, the IOS state-to-state cross-sections are factorized into dynamical factors which contain information about the collisional system and spectroscopic factors that include information about rotational levels and angular momentum coupling. For asymmetric top rotors, the wave functions $|j\tau m\rangle$ (with $\tau = K_a - K_c$ in the usual notation) can be expanded in terms of symmetric top wave functions as (Green 1979):

$$|j\tau m\rangle = \sum_{k \geq 0} \alpha_{\tau k}^j (1 + \delta_{k,0})^{-1} (|jkm\rangle + \epsilon_{j,\tau} |j - km\rangle), \quad (1)$$

where j is the total rotor angular momentum, m is its projection on a space-fixed axis, k is the projection on the molecule-fixed axis, $\delta_{k,0}$ is a Kronecker delta function and the $\alpha_{\tau k}^j$ are the expansion coefficients. $|jkm\rangle$ are symmetric top wave functions. The state-to-state inelastic cross-sections are obtained from the generalized IOS cross-sections, $Q(L, M_a, M_b)$, as:

$$\begin{aligned} \sigma(j\tau \rightarrow j'\tau') &= (2j' + 1) \\ &\times \sum_{L M_a M_b} Q(L, M_a, M_b) C(j\tau, j'\tau' | L, M_a, M_b), \end{aligned} \quad (2)$$

with

$$\begin{aligned} C(j\tau, j'\tau' | L, M_a, M_b) &= \sum_{k_a k'_a k_b k'_b} \alpha_{\tau' k'_a}^{j'} \alpha_{\tau k_a}^j \alpha_{\tau' k'_b}^{j'} \alpha_{\tau k_b}^j \times (-1)^{k'_a + k'_b} \\ &\times \begin{pmatrix} j' & L & j \\ k'_a & M_a & -k_a \end{pmatrix} \begin{pmatrix} j' & L & j \\ k'_b & M_b & -k_b \end{pmatrix}. \end{aligned}$$

The SO₂ energy levels and wave functions were obtained from spectroscopic constants describing the SO₂ Hamiltonian up to the fourth order. These data, provided by the MADEX code (Cernicharo 2012), result from a fit of SO₂ spectra including levels up to $j = 92$ and $K = 28$. However, the coordinate system used in MADEX, with the SO₂ molecule lying in the x - z plane and with the z -axis along the a -axis of SO₂ (Watson's reduced Hamiltonian, reduction A representation I' ; Watson 1977), is different from the one required by the MOLSCAT scattering program for an asymmetric rotor in collision with H₂. As a consequence, the MADEX Hamiltonian matrix was converted to the MOLSCAT coordinate system where the SO₂ molecule lies in the x - z plane with the a -axis of SO₂ along

Table 1. SO₂-calculated energy levels (in cm⁻¹).

Level	j_{K_a, K_c}	This work
1	0 _{0,0}	0.0000
2	2 _{0,2}	1.9120
3	1 _{1,1}	2.3208
4	2 _{1,1}	3.6975
5	3 _{1,3}	5.3820
6	4 _{0,4}	6.3601
7	4 _{1,3}	8.3356
8	2 _{2,0}	8.7469
9	3 _{2,2}	10.6590
10	5 _{1,5}	10.8864
11	4 _{2,2}	13.2258
12	6 _{0,6}	13.3134
13	6 _{1,5}	15.6140
14	5 _{2,4}	16.3950
15	7 _{1,7}	18.8247
16	3 _{3,1}	19.1968
17	6 _{2,4}	20.2941
18	4 _{3,1}	21.7502
19	8 _{0,8}	22.7267
20	7 _{2,6}	24.6713
21	5 _{3,3}	24.9425
22	8 _{1,7}	25.5183
23	6 _{3,3}	28.7760
24	9 _{1,9}	29.1848
25	8 _{2,6}	29.9882
26	7 _{3,5}	33.2472
27	4 _{4,0}	33.6930
28	10 _{0,10}	34.5495
29	9 _{2,8}	35.4777
30	5 _{4,2}	36.8845
31	10 _{1,9}	38.0265

ox. This conversion corresponds to the rotation of (0, $\Pi/2$, Π) Euler angles between the two coordinate systems. Using the rotated Hamiltonian, our calculated rotational levels of SO₂ are identical to those given in MADEX and agree very well with values deduced from the JPL molecular spectroscopy catalogue of Pickett et al. (1998). The calculated energies of the lowest 31 rotational levels of SO₂ are given in Table 1.

The state-to-state rotational inelastic rates are the Boltzmann thermal average at temperature T of state-to-state inelastic cross-sections:

$$R(\beta \rightarrow \beta') = \left(\frac{8kT}{\pi\mu}\right)^{\frac{1}{2}} \left(\frac{1}{kT}\right)^2 \int_0^\infty \sigma_{\beta \rightarrow \beta'}(E_c) E_c e^{-E_c/kT} dE_c, \quad (3)$$

where k is the Boltzmann constant, E_c is the kinetic energy, $\beta = j_{K_a, K_c}$. Rate coefficients obey the detailed balance relation:

$$R(\beta' \rightarrow \beta) = \frac{(2j+1)}{(2j'+1)} \exp\left[\frac{E_{\beta'} - E_\beta}{kT}\right] R(\beta \rightarrow \beta') \quad (4)$$

3 TESTS OF ACCURACY OF CS AND IOS DATA

3.1 Comparison of CS coefficients with CC data

In this section, the accuracy of the CS approximation is studied by comparing the resulting rate coefficients with the CC values (Cernicharo et al. 2011). These CC results showed that inclusion of H₂($j_{H_2=2}$) has a negligible contribution to para-H₂ rate coefficients,

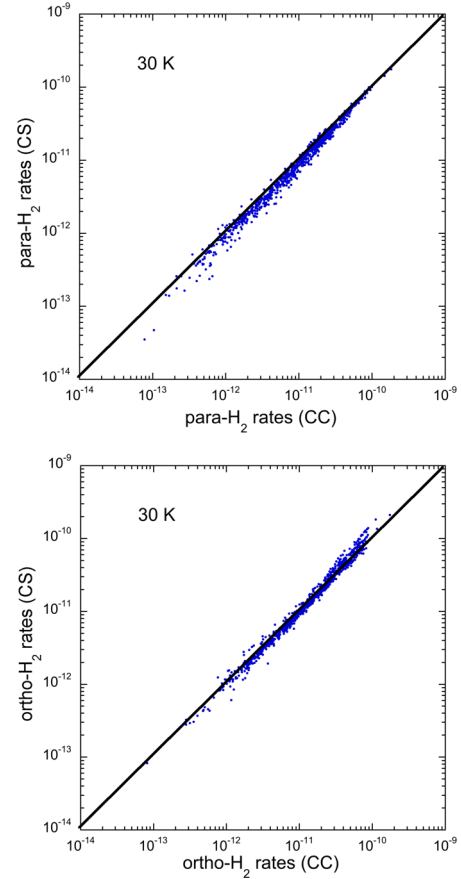


Figure 1. Rate coefficients for SO₂ in collision with para- and ortho-H₂, calculated with the CS approximation as function of full CC rate coefficients. The black line indicates equal rate coefficients. Units are cm³ s⁻¹.

both sets of rates agree within a few per cent at the considered temperatures. This confirms that, for heavy molecules with a high density of rotational states, rotation–rotation processes are not efficient with H₂ and calculations could be restricted to para-H₂($j_{H_2=2}$) and ortho-H₂($j_{H_2=1}$) (Daniel, Dubernet & Grosjean 2011). It was also found that ortho-para-H₂ differences are about a factor of 2 in average. This can be explained by analysing the angular expansion of the PES. It was found (Spielfiedel et al. 2009) for $R = 7.0$ bohr (near the minimum of the isotropic term) that, except for the isotropic term (0000), the dominant terms are the (2202) and (3003) terms that are included for collisions with para-H₂($j_{H_2=0}$). The dipole–quadrupole (1023) and quadrupole–quadrupole (2224) terms, that are excluded for collisions with para-H₂($j_{H_2=0}$), are large but not dominant.

From the same PES, basis set and energy grid, we have calculated cross-sections and rate coefficients within the CS approximation. Calculations performed with a larger SO₂ basis set ($j_{\max} = 17$ and $E_{\max} = 200$ cm⁻¹, i.e. 120 SO₂ rotational levels) have shown that the inclusion of 72 SO₂ levels in the basis set (as used in the CC calculations) is sufficient to obtain convergence better than 5 per cent on the collisional rate coefficients.

Fig. 1 compares the CC and CS rate coefficients at 30 K for collisions of SO₂ with para-H₂($j_{H_2=0,2}$) and ortho-H₂($j_{H_2=1}$). One can observe that, for collision with para-H₂ as well as for ortho-H₂, the CC and CS sets of rates agree within a few up to 20 per cent, according to the transition. This relatively good agreement is confirmed for other temperatures as shown in Fig. 2, which displays the

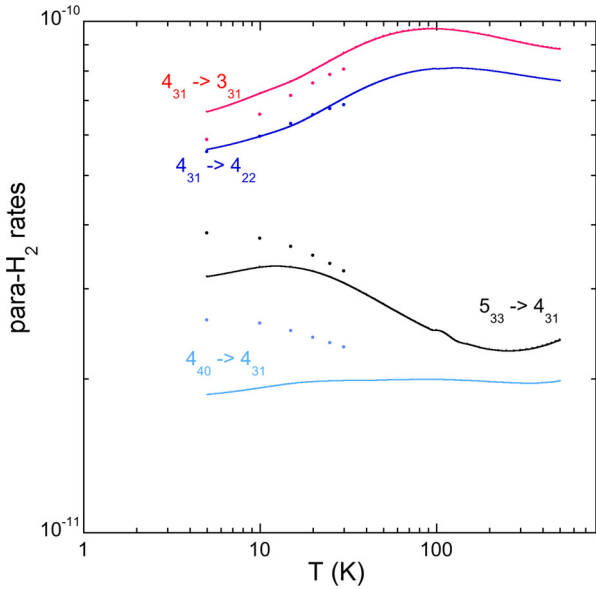


Figure 2. Temperature variation of SO_2 -para- H_2 CS rate coefficients for (from top to bottom) the $4_{31} \rightarrow 3_{31}$ (red line), $4_{31} \rightarrow 4_{22}$ (dark blue line), $5_{33} \rightarrow 4_{31}$ (black line) and the $4_{40} \rightarrow 4_{31}$ (light blue line) transitions compared with CC results (dots). Units are rates in $\text{cm}^3 \text{s}^{-1}$, temperatures in K.

temperature variation of the CC and CS para- H_2 and ortho- H_2 rate coefficients for a selection of $\Delta K_a = 0$ and $\Delta J = 0$ transitions. We also observe the temperature variation to be weak for temperatures larger than 200 K. As previously found in CC calculations, we note that $\Delta K_a = 0$ are the largest rates.

The comparison at $T = 30$ and 100 K between the CS ortho- and para- H_2 rates (see Fig. 3) shows the same trend as previously found in the full CC approach: ortho- H_2 rate coefficients are larger than para rates by a factor smaller than 2 in average. However, factors up to 8 are found for some transitions identified mainly as $\Delta K_a = 1$ transitions. The same trend is found at higher temperatures.

3.2 Towards high temperatures: comparison between CS and IOS rates

CS calculations were extended for energies up to 3000 cm^{-1} in order to provide CS rate coefficients for temperatures up to 500 K. In Figs 4(a,b,c), the SO_2 IOS de-excitation rate coefficients are compared to the corresponding CS para- H_2 coefficients for $T = 30, 100$ and 300 K . From these results, it appears clearly that the IOS approximation leads to a systematic underestimation of para- H_2 rates by a factor of 3 to 4 in average at low temperatures, with a better agreement (less than a factor of 2 in average) for increasing temperatures as can be seen in Fig. 5 that displays the temperature variation of the rate coefficients for a selection of transitions. As expected, the agreement is not so good for collisions with ortho- H_2 , the IOS approximation leading to a systematic underestimation of the rates by a factor of 3 to 4 in average compared to CS ortho- H_2 values.

These comparisons show that: (i) the CS approximation gives reliable rate coefficients even at relatively large temperatures for the transitions relevant to the first levels, (ii) the IOS approximation is a possible alternative to obtain rate coefficients at high temperatures and for high j -levels transitions for collisions with para- H_2 . As the IOS approximation only describes collisions with para- H_2 ($j_{\text{H}_2} = 0$),

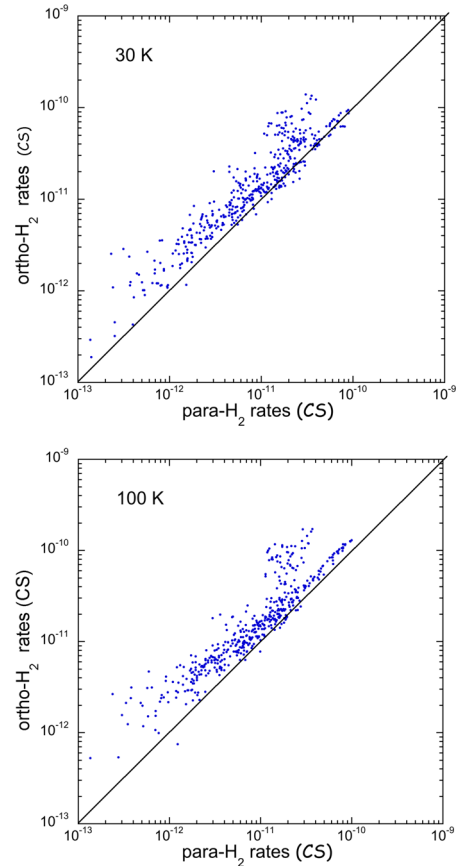


Figure 3. Comparison of ortho- H_2 and para- H_2 rate coefficients, calculated using the CS approximation. Units are $\text{cm}^3 \text{s}^{-1}$.

the IOS data are believed to be less accurate for collisions with ortho- H_2 .

With a bending mode at 518 cm^{-1} and symmetric and antisymmetric stretching modes at 1151 and 1362 cm^{-1} , respectively, one can question the validity at high energies of the ‘rigid-body’ approach used in this study when SO_2 vibrational levels could be excited. In recent works on He in collision with C_3 (Stoecklin, Denis-Alpizar & Halvick 2015) and HCN (Stoecklin et al. 2013), Stoecklin and his colleagues investigate the effect of the coupling between vibrational (bending) and rotational excitations. For the very floppy C_3 molecule, the coupling was shown to be important. On the contrary, for the HCN molecule with a bending vibration frequency relatively small but still large compared to the rotational constant, the effect is almost negligible as long as the vibrational modes are not excited (Stoecklin et al. 2013). In the case of SO_2 with a very small rotational constant, one can consider that the coupling with the bending mode does not affect the CS rate coefficients at temperatures lower than 100 K as the maximum of the Boltzmann velocity distribution does not focus on high kinetic energies. However, the coupling with the bending channels may deteriorate the accuracy of the results at higher temperatures.

4 INELASTIC RATE COEFFICIENTS FOR EXCITATION OF SO_2 BY H_2 AT HIGH TEMPERATURES

State-to-state inelastic rate coefficients for excitation of SO_2 by para- and ortho- H_2 were calculated within the CS approach for all

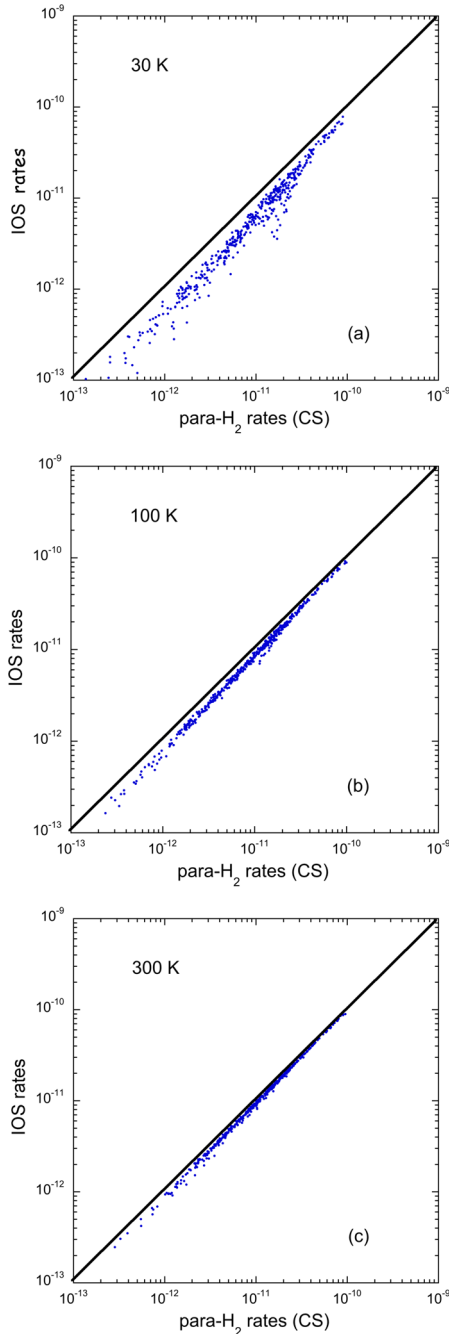


Figure 4. SO_2 de-excitation rate coefficients in collision with para- H_2 calculated with the IOS approximation as function of para- H_2 CS-rate coefficients at 30, 100 and 300 K. The black line indicates equal rate coefficients. Units are $\text{cm}^3 \text{s}^{-1}$.

transitions involving the 31 lowest SO_2 levels and temperatures up to 500 K. As discussed above, those data may be considered as accurate within 20–30 per cent.

For higher temperatures and high-energy levels, IOS data are provided for all the transitions involving the lowest 410 levels and temperatures up to 1000 K. Those data give accurate rate coefficients for collisions with para- H_2 within a factor better than 50 per cent. It is important to underline that the temperature variation of these rate coefficients is weak as can be seen in Fig. 6 that displays the rate coefficients at 100 and 500 K for 100 transitions among the lowest levels.

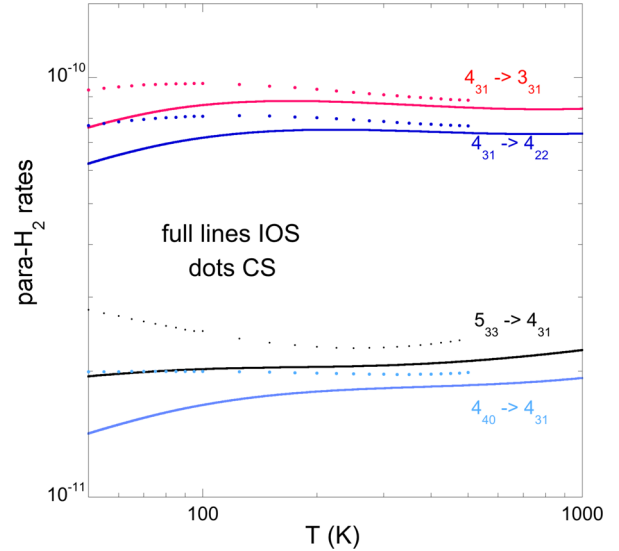


Figure 5. Temperature variation of SO_2 -para- H_2 IOS de-excitation rate coefficients for (from top to bottom) the $4_{31} \rightarrow 3_{31}$ (red line), $4_{31} \rightarrow 4_{22}$ (dark blue line), $5_{33} \rightarrow 4_{31}$ (black line) and the $4_{40} \rightarrow 4_{31}$ (light blue line) transitions compared with CS results (dotted lines). Units are rates in $\text{cm}^3 \text{s}^{-1}$, temperatures in K.

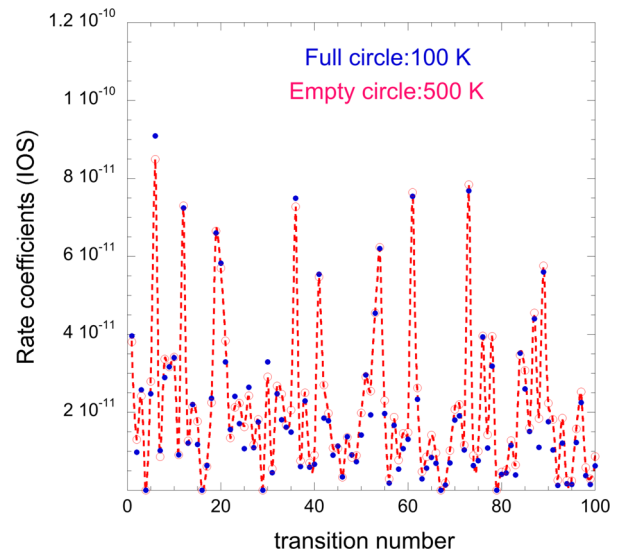


Figure 6. De-excitation IOS rate coefficients at $T = 100$ K (full circles) and 500 K (empty circles, dashed line) for the first hundred transitions as function of the labelling of the de-excitation transitions. Units are rates in $\text{cm}^3 \text{s}^{-1}$.

The situation is not as good for collisions with ortho- H_2 as the IOS approximation describes collisions with para- H_2 ($j_{\text{H}_2} = 0$) and does not take into account all the angular couplings involved in collisions with ortho- H_2 . However, it was found that the temperature variation of ortho- H_2 rate coefficients is very similar to that obtained for para- H_2 rates.

The complete sets of CS para and ortho- H_2 as well as IOS para- H_2 (de-)excitation rate coefficients will be made available online from the LAMDA¹ and BASECOL² data bases.

¹ <http://www.strw.leidenuniv.nl/~moldata/> (Schöier F. L. et al. 2005).

² <http://basecol.obspm.fr/> (Dubernet et al. 2013).

The Quasi Classical Trajectory (QCT) method could be an alternative to investigate very high rotational levels as this approach can describe at the same level collisions by para and ortho-H₂ (Faure et al. 2007). A comparison at $T = 30$ K between the CC para-H₂ and QCT rates (Feautrier et al. 2012) shows a relatively good agreement between both results. The temperature variation of the rate coefficients obtained through QCT calculations was also found to be relatively flat, as suggested by the present CS and the IOS results. Moreover, the ortho/para H₂ effects are found to be relatively small (within error bars) at the QCT level, as shown within the present CS data. These initial results need to be confirmed by extensive calculations to come in future works.

5 SUMMARY – CONCLUSION

Using a very accurate SO₂-H₂ 5D-PES, we have computed rate coefficients for rotational excitation of SO₂ colliding with H₂ at high temperatures. Two approximate quantum approaches were used: (i) the CS approximation for collisions with both para and ortho-H₂ in the temperature range 20–500 K; (ii) the IOS approximation to provide rate coefficients at high temperatures (up to 1000 K) and high j -levels. The first set of data (CS) gives state-to-state rate coefficients for the lowest 31 levels of SO₂ and the second set of data (IOS) provides de-excitation rates for all transitions involved among the lowest 410 SO₂ levels.

From a comparison with previously published full CC rates, the present CS rate coefficients agree with the CC data within 20–30 per cent in average. By comparing CS and IOS data for collisions with para-H₂, it is shown that the IOS approximation underestimates rate coefficients by a factor of 2 in average at low temperatures (30 K) but leads to a good estimate of the rate coefficients at higher temperatures. As the IOS theory does not take into account all the angular momenta couplings present in collisions with ortho-H₂, this approach cannot describe these collisions. The comparison between ortho and para-H₂ CS rate coefficients shows that ortho-H₂ rate coefficients are systematically larger than para-H₂ rates by a factor of 2 in average. However, the temperature variation of both rate coefficients is very similar. The present rates should be useful in any detailed population model of SO₂ in warm and hot environments.

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REFERENCES

- Bachiller R., 1996, *ARA&A*, 34, 111
 Cernicharo J., 2012, in Stehlé C., Joblin C., d’Hendecourt L., eds, *EAS Publ. Ser. Vol. 58, Laboratory Astrophysics and Astrochemistry in the Herschel/ALMA Era*. Cambridge Univ. Press, Cambridge, p. 251
 Cernicharo J. et al., 2011, *A&A*, 531, A103
 Crockett N. R. et al., 2014, *ApJ*, 787, 112
 Daniel F., Dubernet M.-L., Grosjean A., 2011, *A&A*, 536, A76
 Dickens J. E., Irvine W. M., Snell R. L., Bergin E. A., Schloerb F. P., Pratap P., Miralles M. P., 2000, *ApJ*, 542, 870
 Dubernet M.-L. et al., 2013, *A&A*, 553, A50
 Esplugues G. B., Tercero B., Cernicharo J., Goicoechea J. R., Palau A., Marcelino N., Bell T. A., 2013, *A&A*, 556, A143
 Esplugues G. B., Viti S., Goicoechea J. R., Cernicharo J., 2014, *A&A*, 567, A95
 Faure A., Crimier N., Ceccarelli C., Valiron P., Wiesenfeld L., Dubernet M. L., 2007, *A&A*, 472, 1029
 Feautrier N., Balança C., Dayou F., Spielfiedel A., Cressiot-Vincent L., Faure A., Wiesenfeld L., Senent M.-L., 2012, in Ceccarelli C., Faure A., Wiesenfeld L., eds, *EPJ Web Conf.*, 34, 03003
 Green S., 1976, *J. Chem. Phys.*, 64, 3463
 Green S., 1979, *J. Chem. Phys.*, 70, 816
 Green S., 1995, *ApJS*, 100, 213
 Hatchell J., Thompson M. A., Millar T. J., MacDonald G. H., 1998, *A&A*, 338, 713
 Irvine W. M., Good J. C., Schloerb F. P., 1983, *A&A*, 127, L10
 Lique F., Cernicharo J., Cox P., 2006, *ApJ*, 653, 1342
 Phillips T. R., Maluendes S., Green S., 1996, *ApJS*, 107, 467
 Pickett H. M., Poynter R., Cohen E., Delitsky M., Pearson J., Muller H., 1998, *J. Quant. Spectrosc. Radiat. Transfer*, 60, 883
 Schilke P., Benford D. J., Hunter T. R., Lis D. C., Phillips T. G., 2001, *ApJS*, 132, 281
 Schloerb F. P., Irvine W. M., Friberg P., Hjalmarson A., Hoglund B., 1983, *ApJ*, 264, 161
 Schöier F. L., van der Tak F. F. S., van Dishoeck E. F., Black J. H., 2005, *A&A*, 432, 369
 Snyder L. E., Hollis J. M., Ulich B. L., Lovas F. J., Johnson D. R., Buhl D., 1975, *ApJ*, 198, L81
 Spielfiedel A., Senent M.-L., Dayou F., Balança C., Cressiot-Vincent L., Faure A., Wiesenfeld L., Feautrier N., 2009, *J. Chem. Phys.*, 131, 014305
 Stoecklin T., Denis-Alpizar O., Halvick P., Dubernet M.-L., 2013, *J. Chem. Phys.*, 139, 124317
 Stoecklin T., Denis-Alpizar O., Halvick P., 2015, *MNRAS*, 449, 3420
 Tercero B., Cernicharo J., Pardo J. R., Goicoechea J. R., 2010, *A&A*, 517, A96
 Tercero B., Vincent L., Cernicharo J., Viti S., Marcelino N., 2011, *A&A*, 528, A26
 Viti S., Caselli P., Hartquist T. W., Williams D. A., 2001, *A&A*, 370, 1017
 Watson J. K. G., 1977, *Vibration Spectra and Structure*. Elsevier, Amsterdam

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