

Rotational excitation of sulfur monoxide in collision with helium at high temperature

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Received 15 November 2005 / Accepted 15 December 2005

ABSTRACT

Context. Over the next few years, ALMA and Herschel missions will open the universe to high spatial and spectral resolution studies at infrared and sub-millimeter wavelengths. This will allow investigators to study in much greater detail the composition and evolution of molecules in space. Modeling of the spectra will require accurate radiative and collisional rates of species of astrophysical interest.

Aims. We calculate new rates coefficients for the 91 first rotational levels of the SO molecule in collision with He for temperatures ranging from 50 to 300 K.

Methods. Different levels of approximations (IOS, IOS scaling relationship) are tested in comparison with the exact full close coupling approach. From the analysis of the validity range of each method, we define a hybrid approach combining the accuracy of the full close coupling method and the less time consuming approximations (IOS, IOS scaling relationship).

Results. The new rate coefficients are calculated up to 300 K. These coefficients differ significantly from previously published ones.

Key words. ISM: molecules – molecular processes – molecular data

1. Introduction

Observations of molecular emission at millimeter and infrared wavelengths, supplemented by careful and detailed modeling, are powerful tools to investigate the physical and chemical conditions of astrophysical objects. First observed by Gottlieb & Ball (1973) in the interstellar gas, sulfur monoxide has been used extensively to study shocked molecular gas in various environments (Turner et al. 1992; Van Dishoeck et al. 1998; Blake et al. 1987). SO is a good probe since the fine structure in its $^3\Sigma^-$ electronic ground state gives many relatively close transitions. The modeling of the line intensities requires comparison with model excitation calculations using radiative as well as collisional rates. It is thus of a great importance to provide accurate collisional rates for a large temperature range. Collisional excitation in the interstellar medium is dominated by collisions with the most abundant neutral species, He and H₂.

Excitation rates by collision among fine structure levels of SO with H₂ were provided some time ago by Green (1994), using coupled states and recoupling approximations of collision dynamics and the potential energy surface (PES) obtained for CS-H₂ with an electron-gas model (Green & Chapman 1978). Spin-free rates were obtained for temperatures from 50 to 350 K and rates of fine structure levels were obtained from the spin-free rates using the recoupling method described by Neufeld & Green (1994). In Paper I (Lique et al. 2005),

we calculated collisional rates among the 31 first fine structure levels of SO for temperatures ranging from 5 to 50 K. The dynamics calculations were performed using a new accurate potential energy surface for the SO-He system. The full close coupling approach was used for the dynamics. The tested approximate approaches are not accurate for calculations at low temperatures involving low energy levels where the fine structure splitting is large compared to the rotational splitting. However, it was shown that the recoupling technique from IOS cross sections should provide a reasonable estimate of cross sections for high-*N* levels and at large energies.

As the number of open rotational channels increases rapidly with energy, we propose here a hybrid approach combining full close coupling for the first levels and different levels of approximations for the higher levels and at high energy. In the next section, we briefly describe the computation methodology, including close coupling, infinite order sudden (IOS) and IOS scaling relationships (hereafter IOSR) scattering techniques. A comparison between these different approaches is discussed in Sect. 3, and results are given in Sect. 4 where a comparison with earlier calculations is also provided. Section 5 summarizes the conclusions.

2. Computation methodology

The PES was calculated at the RCCSD(T) level (Knowles et al. 1993, 2000). The SO *r*-distance was fixed at its experimental

Table 1. Energy in cm^{-1} of the fine structure levels.

Level	N	j	Energy	Level	N	j	Energy	Level	N	j	Energy
1	1	0	0.000	32	11	12	97.963	63	21	20	335.742
2	0	1	1.001	33	11	10	99.302	64	21	21	340.566
3	1	2	3.100	34	11	11	103.865	65	22	23	366.396
4	2	3	6.412	35	12	13	115.221	66	22	21	367.272
5	1	1	10.552	36	12	11	116.746	67	22	22	372.107
6	2	1	10.987	37	12	12	121.088	68	23	24	399.372
7	3	4	11.021	38	13	14	133.906	69	23	22	400.234
8	2	2	13.424	39	13	12	135.091	70	23	23	405.078
9	3	2	14.632	40	13	13	139.745	71	24	25	433.777
10	4	5	16.979	41	14	15	154.021	72	24	23	434.625
11	3	3	17.731	42	14	13	155.147	73	24	24	439.477
12	4	3	19.933	43	14	14	159.835	74	25	26	469.607
13	4	4	23.474	44	15	16	175.565	75	25	24	470.455
14	5	6	24.316	45	15	14	176.641	76	25	25	475.303
15	5	4	26.811	46	15	15	181.358	77	26	27	506.864
16	5	5	30.653	47	16	17	198.538	78	26	25	507.693
17	6	7	33.050	48	16	15	199.571	79	26	26	512.557
18	6	5	35.211	49	16	16	204.314	80	27	28	545.547
19	6	6	39.268	50	17	18	222.941	81	27	26	546.368
20	7	8	43.193	51	17	16	223.938	82	27	27	551.238
21	7	6	45.102	52	17	17	228.701	83	28	29	585.654
22	7	7	49.318	53	18	19	248.774	84	28	27	586.367
23	8	9	54.751	54	18	17	249.739	85	28	28	591.343
24	8	7	56.467	55	18	18	254.521	86	29	30	627.187
25	8	8	60.802	56	19	20	276.036	87	29	28	627.996
26	9	10	67.731	57	19	18	276.974	88	29	29	632.874
27	9	8	69.293	58	19	19	281.772	89	30	31	670.143
28	9	9	73.722	59	20	21	304.727	90	30	29	670.947
29	10	11	82.135	60	20	19	305.642	91	30	30	675.829
30	10	9	83.574	61	20	20	310.454	92	31	32	714.521
31	10	10	88.077	62	21	22	334.847	93	31	30	715.323

minimum energy distance ($r_e = 2.80$ bohr). The ab initio surface was calculated using the MOLPRO package 2002. The three atoms were described by the aug-cc-pVQZ basis set (Woon & Dunning 1994), augmented by the (3s3p2d2f1g) bond functions optimized by Cybulski & Toczyłowski (1999). Details of computations and plots of the PES are given in Paper I. 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).

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:

$$\begin{aligned}
|F_1 jm\rangle &= \cos \alpha |N = j - 1, S jm\rangle \\
&\quad + \sin \alpha |N = j + 1, S jm\rangle \\
|F_2 jm\rangle &= |N = j, S jm\rangle \\
|F_3 jm\rangle &= -\sin \alpha |N = j - 1, S jm\rangle \\
&\quad + \cos \alpha |N = j + 1, S jm\rangle
\end{aligned} \tag{1}$$

where $|N, S jm\rangle$ 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 present paper the usual level labeling N_j where $N = j - 1$, $N = j$, $N = j + 1$ correspond to the F_1 , F_2 and F_3 levels as defined in Eq. (1). The energies of the fine structure levels considered in the calculations were computed with the same effective Hamiltonian as in Paper I. The experimental spectroscopic constants of Bogey et al. (1982) were used. Energies of the 93 first fine structure levels are given in Table 1.

The detailed description of the CC calculations is given in Paper I. The quantal coupled equations were solved in the intermediate coupling scheme using the MOLSCAT code (Hutson & Green 1995) modified to take into account the fine structure of the energy levels. The propagation parameters were tested in order to obtain convergence of the cross sections. The calculations included all the open channels at each energy

corresponding to energetically accessible levels. Several energetically inaccessible levels were included to obtain convergence of the collisional cross sections

Approximate cross sections among fine structure levels can be obtained in the Hund's case (b) limit using the IOS approximation (Corey & Mc Court 1983):

$$\sigma^{\text{IOS}}(NSj \rightarrow N'Sj') = \sum_L (2N+1)(2N'+1)(2j'+1) \begin{pmatrix} N' & N & L \\ 0 & 0 & 0 \end{pmatrix}^2 \left\{ \begin{matrix} L & j & j' \\ S & N' & N \end{matrix} \right\}^2 \sigma^{\text{IOS}}(0 \rightarrow L) \quad (2)$$

where $\begin{pmatrix} \end{pmatrix}$ and $\left\{ \begin{matrix} \end{matrix} \right\}$ are respectively the “3-j” and “6-j” symbols.

$\sigma^{\text{IOS}}(0 \rightarrow L)$ are the “fundamental IOS cross sections” obtained from the L_{th} expansion of the angle dependent S-matrix elements in terms of Legendre polynomials (Goldflam et al. 1977). As the IOS approximation neglects the energy structure of the levels, it is expected to be very poor near the level thresholds.

The way to obtain more reliable cross sections is to derive rates among fine structure levels from spin-free cross sections using the IOS approximation scaling relationship (hereafter IOSR) to recouple the angular momenta. This approximate recoupling method was described in detail by Neufeld & Green (1994) for calculations of rate coefficients among hyperfine structure levels of HCl and used by Green (1994) for collisional excitation of SO by H₂ molecules. In our case, we apply the scaling to downward cross sections:

$$\sigma(NSj \rightarrow N'Sj') = \frac{\sigma^{\text{IOS}}(NSj \rightarrow N'Sj')}{\sigma^{\text{IOS}}(N \rightarrow N')} \sigma^{\text{CC}}(N \rightarrow N') \quad (3)$$

where:

$$\sigma^{\text{IOS}}(N \rightarrow N') = \sum_L (2N'+1) \begin{pmatrix} N' & N & L \\ 0 & 0 & 0 \end{pmatrix}^2 \sigma^{\text{IOS}}(0 \rightarrow L) \quad (4)$$

$\sigma^{\text{IOS}}(NSj \rightarrow N'Sj')$ is given by Eq. (2) and $\sigma^{\text{CC}}(N \rightarrow N')$ are the spin-free close coupling cross sections.

For the IOSR and IOS methods, the number of L values considered in the summation is $0 < L < N + N'$ since the “3-j” and “6-j” coefficients are equal to 0 for the other L .

The MOLSCAT (Hutson & Green 1995) code was also used for all the calculations with the IOS methods.

The downward rate coefficients are the Boltzmann thermal average of collision cross sections σ_{ul} :

$$k_{ul}(T) = \left(\frac{8k_B T}{\pi\mu} \right)^{\frac{1}{2}} \left(\frac{1}{k_B T} \right)^2 \times \int_0^\infty E_k \sigma_{ul}(E_k) e^{-\frac{E_k}{k_B T}} dE_k \quad (5)$$

where u and l are respectively the upper and the lower states, μ is the reduced mass of the system, E_k is the kinetic energy and k_B is the Boltzmann constant.

The upward rate coefficients are obtained through detailed balance:

$$k_{lu} = k_{ul} \frac{g_u}{g_l} \exp(-h\nu/k_B T) \quad (6)$$

where $g = 2j + 1$ is the statistical weight.

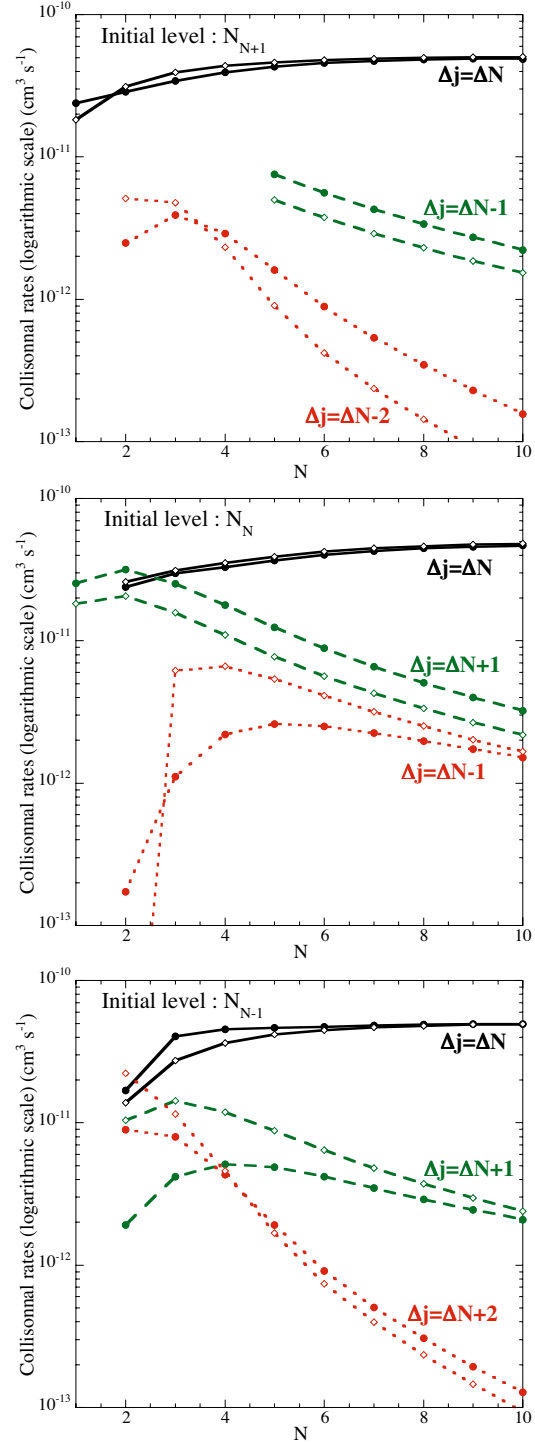


Fig. 1. CC rate coefficients (filled circles) compared with IOSR rate coefficients (empty diamonds) at 50 K for $\Delta N = N' - N = -1$.

3. Scattering calculations: comparison between CC and IOS methods

As discussed in Paper I, the recoupling approximation IOSR is not expected to give accurate results due to the large fine structure splitting in SO. However, it is found to give a correct estimate of the rates among high N levels and at high energy. Figure 1 compares the de-excitation CC rate coefficients with the approximate IOSR coefficients at 50 K for transitions

$N_j \rightarrow N'_j$ with $\Delta N = N' - N = -1$. It is clear that the IOSR approximation is not valid among low lying levels ($N, N' < 5$). However, when the upper level is higher than $N = 5$, a good agreement is found for $\Delta j = \Delta N$ transitions. For transitions with $\Delta j \neq \Delta N$ (except $N_{N+1} \rightarrow N'_{N-1}$, $\Delta j = \Delta N - 2$), the difference between the methods decreases as N increases and the IOSR approximation becomes reasonable. An important difference remains for the small rate coefficients of the $N_{N+1} \rightarrow N'_{N-1}$ ($\Delta j = \Delta N - 2$) transitions. This can be explained by the selection rules imposed by the $\{6j\}$ coefficient in Eq. (2): the two first L values corresponding to large $\sigma^{\text{IOS}}(0 \rightarrow L)$ cross sections are excluded in the IOSR whereas such selection rules do not occur in full close coupling equations. However, as seen in Fig. 2, the difference becomes smaller with increasing energies so that we can expect to have a good agreement for the rate coefficients at high temperature ($T > 100$ K). We also note in Fig. 1 the strong propensity rule $\Delta j = \Delta N$ transitions. This propensity rule, previously noted by Green (1994) for SO and by Corey et al. (1986) for $\text{O}_2(^3\Sigma^-) - \text{He}$ collisions, becomes stronger as N increases.

The validity of the recoupling approximation IOSR compared to IOS is well analysed in Fig. 2 where a comparison between cross sections obtained with the CC, IOS and IOSR approaches is performed. For such cross sections between relatively high- N levels, the agreement of IOSR results with the close coupling occurs at relatively low energy whereas the IOS approximation gives very poor results at low energies. This is due to a better description of the threshold in the IOSR approach. As expected, the difference between IOS and IOSR results decreases when the energy increases and we have found an excellent agreement between them at high energies. Rate coefficients were calculated using the energy grid and propagation parameters defined in Sect. 4.1. The coefficients obtained with the two methods are quite similar for temperature larger than 100 K. This is due to the fact that spin-free CC and IOS cross sections are almost equal at high energies.

4. Results

4.1. "Hybrid" cross sections and rate coefficients

Cross sections were obtained for the 91 first levels of SO (see Table 1) and total energies up to 2000 cm^{-1} that allow us to obtain rate coefficients for temperature up to 300 K. The reduced mass of the system is 3.694 amu . The propagation parameters were tested in order to obtain convergence of the cross sections for energies up to 2000 cm^{-1} . Typically, the minimum and maximum integration distances are respectively $R_{\text{min}} = 2.75 a_0$ and $R_{\text{max}} = 40 a_0$. We carefully spanned the energy ranges to take into account the presence of resonances. The energy steps are 0.1 cm^{-1} below 30 cm^{-1} , 0.2 cm^{-1} from 30 to 50 cm^{-1} , 0.5 cm^{-1} from 50 to 100 cm^{-1} , 1 cm^{-1} from 200 to 800 cm^{-1} , 2 cm^{-1} from 800 to 1200 cm^{-1} , 4 cm^{-1} from 1200 to 2000 cm^{-1} . According to the previous discussion, we used the following hybrid procedure: exact close coupling calculations were done for the 16 first levels ($N \leq 5$) and total energies up to 2000 cm^{-1} . The calculations included at each energy 43 levels in order to obtain convergence of the cross sections.

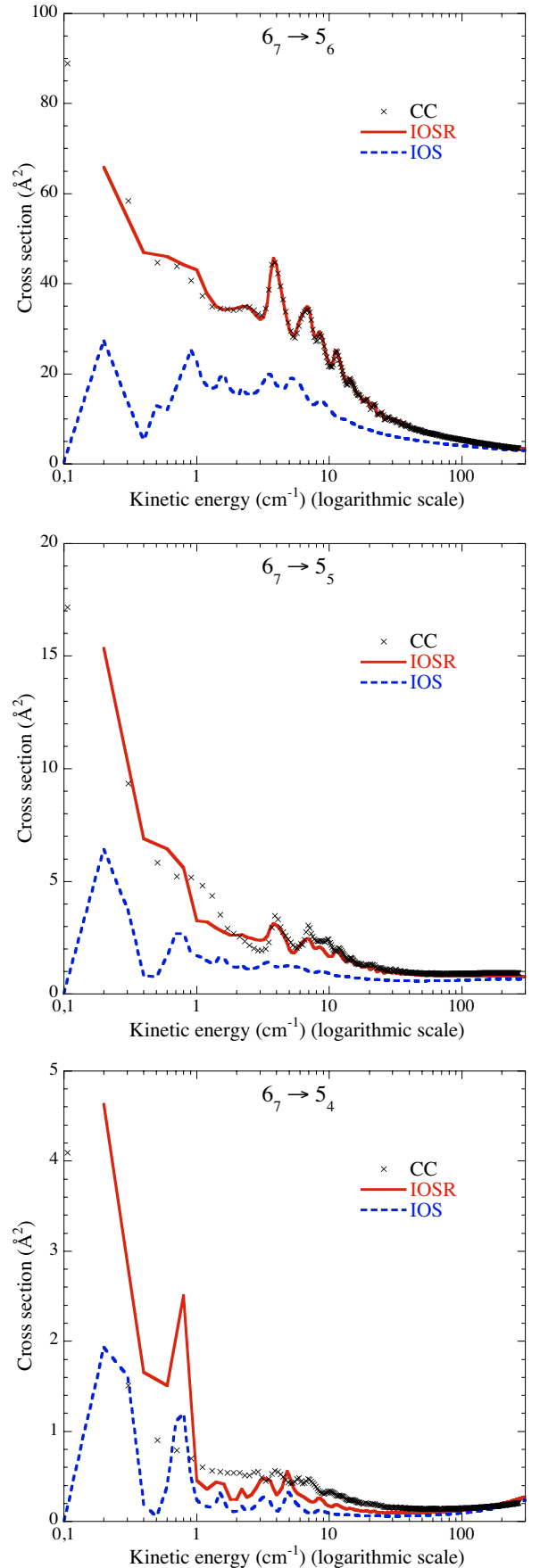


Fig. 2. Comparison between cross sections obtained with the CC, IOSR and IOS approaches.

Table 2. Downward rate coefficients of fine structure levels of SO in collision with He as a function of kinetic temperature (in units of $\text{cm}^3 \text{s}^{-1}$).

N_j	N'_j	100 K	200 K	300 K	N_j	N'_j	100 K	200 K	300 K
0 ₁	... 1 ₀	1.47e-12	1.05e-12	9.84e-13	4 ₅	... 1 ₀	1.74e-12	2.11e-12	2.21e-12
1 ₂	... 1 ₀	2.04e-12	2.02e-12	2.09e-12	4 ₅	... 0 ₁	1.43e-12	1.37e-12	1.53e-12
1 ₂	... 0 ₁	2.13e-11	2.09e-11	2.17e-11	4 ₅	... 1 ₂	1.70e-11	1.62e-11	1.60e-11
2 ₃	... 1 ₀	2.08e-12	1.85e-12	1.77e-12	4 ₅	... 2 ₃	2.57e-11	2.73e-11	2.91e-11
2 ₃	... 0 ₁	1.55e-11	1.64e-11	1.74e-11	4 ₅	... 1 ₁	7.62e-12	9.20e-12	9.65e-12
2 ₃	... 1 ₂	2.74e-11	2.84e-11	2.99e-11	4 ₅	... 2 ₁	3.98e-13	4.65e-13	6.16e-13
1 ₁	... 1 ₀	1.43e-13	5.76e-14	3.50e-14	4 ₅	... 3 ₄	3.74e-11	3.80e-11	3.99e-11
1 ₁	... 0 ₁	2.47e-11	2.60e-11	2.79e-11	4 ₅	... 2 ₂	1.44e-12	1.50e-12	1.82e-12
1 ₁	... 1 ₂	3.55e-11	3.88e-11	4.16e-11	4 ₅	... 3 ₂	3.90e-12	5.29e-12	6.01e-12
1 ₁	... 2 ₃	3.51e-11	3.15e-11	3.02e-11	3 ₃	... 1 ₀	2.67e-14	1.09e-14	6.52e-15
2 ₁	... 1 ₀	1.64e-11	1.71e-11	1.84e-11	3 ₃	... 0 ₁	1.75e-11	1.60e-11	1.54e-11
2 ₁	... 0 ₁	3.38e-12	3.43e-12	3.59e-12	3 ₃	... 1 ₂	1.35e-11	1.42e-11	1.51e-11
2 ₁	... 1 ₂	7.73e-12	6.95e-12	6.73e-12	3 ₃	... 2 ₃	2.71e-11	2.88e-11	2.94e-11
2 ₁	... 2 ₃	4.35e-12	4.44e-12	4.79e-12	3 ₃	... 1 ₁	1.41e-11	1.57e-11	1.70e-11
2 ₁	... 1 ₁	1.43e-12	1.30e-12	1.33e-12	3 ₃	... 2 ₁	8.97e-13	7.69e-13	7.27e-13
3 ₄	... 1 ₀	3.55e-13	3.12e-13	3.35e-13	3 ₃	... 3 ₄	9.38e-12	1.02e-11	1.13e-11
3 ₄	... 0 ₁	1.25e-11	1.19e-11	1.17e-11	3 ₃	... 2 ₂	3.04e-11	3.25e-11	3.42e-11
3 ₄	... 1 ₂	2.15e-11	2.30e-11	2.46e-11	3 ₃	... 3 ₂	1.65e-12	1.66e-12	1.75e-12
3 ₄	... 2 ₃	3.20e-11	3.26e-11	3.44e-11	3 ₃	... 4 ₅	2.03e-11	2.42e-11	2.60e-11
3 ₄	... 1 ₁	1.99e-12	1.80e-12	1.92e-12	4 ₃	... 1 ₀	1.03e-11	9.32e-12	8.98e-12
3 ₄	... 2 ₁	4.84e-12	5.58e-12	5.81e-12	4 ₃	... 0 ₁	1.02e-12	9.69e-13	1.02e-12
2 ₂	... 1 ₀	7.03e-14	2.72e-14	1.55e-14	4 ₃	... 1 ₂	5.87e-12	6.88e-12	7.14e-12
2 ₂	... 0 ₁	2.49e-11	2.68e-11	2.84e-11	4 ₃	... 2 ₃	7.98e-13	9.43e-13	1.25e-12
2 ₂	... 1 ₂	2.92e-11	2.76e-11	2.75e-11	4 ₃	... 1 ₁	2.97e-12	2.65e-12	2.53e-12
2 ₂	... 2 ₃	1.68e-11	1.80e-11	1.93e-11	4 ₃	... 2 ₁	2.18e-11	2.33e-11	2.49e-11
2 ₂	... 1 ₁	2.28e-11	2.30e-11	2.40e-11	4 ₃	... 3 ₄	5.95e-12	8.27e-12	9.50e-12
2 ₂	... 2 ₁	1.23e-12	1.24e-12	1.30e-12	4 ₃	... 2 ₂	2.47e-12	2.56e-12	2.73e-12
2 ₂	... 3 ₄	2.96e-11	3.20e-11	3.27e-11	4 ₃	... 3 ₂	4.54e-11	4.68e-11	4.84e-11
3 ₂	... 1 ₀	1.66e-11	1.72e-11	1.80e-11	4 ₃	... 4 ₅	2.09e-12	2.60e-12	2.96e-12
3 ₂	... 0 ₁	3.43e-12	3.02e-12	2.89e-12	4 ₃	... 3 ₃	5.33e-12	5.61e-12	5.71e-12
3 ₂	... 1 ₂	1.66e-12	1.58e-12	1.70e-12	4 ₄	... 1 ₀	1.21e-14	4.87e-15	2.86e-15
3 ₂	... 2 ₃	9.91e-12	1.15e-11	1.19e-11	4 ₄	... 0 ₁	2.06e-12	2.08e-12	2.32e-12
3 ₂	... 1 ₁	2.56e-12	2.75e-12	2.93e-12	4 ₄	... 1 ₂	1.96e-11	2.08e-11	2.11e-11
3 ₂	... 2 ₁	3.74e-11	3.67e-11	3.76e-11	4 ₄	... 2 ₃	7.92e-12	8.48e-12	9.35e-12
3 ₂	... 3 ₄	2.02e-12	2.33e-12	2.83e-12	4 ₄	... 1 ₁	1.48e-11	1.49e-11	1.49e-11
3 ₂	... 2 ₂	3.60e-12	3.30e-12	3.25e-12	4 ₄	... 2 ₁	1.37e-13	1.11e-13	1.14e-13

For the next levels ($5 < N \leq 15$), the downward cross sections were calculated using the exact CC method for total energies up to 300 cm^{-1} , the IOSR approximation (Eq. (3)) was used for energies between 300 and 700 cm^{-1} and the pure IOS approach (Eq. (2)) for energies up to 2000 cm^{-1} . For the highest levels ($15 < N \leq 30$), the downward cross sections were calculated using the IOSR approach for total energies up to 700 cm^{-1} and the pure IOS for energies up to 2000 cm^{-1} . With this method, we have described all the threshold energy ranges with a CC or a IOSR approach.

From this “hybrid treatment”, we can evaluate the accuracy of the corresponding results. The first source of error comes from the PES. Recent investigations by Valiron (2005) permitted evaluation of the influence of the PES errors on the inelastic rates: accurate PES with few cm^{-1} accuracy such as the PES used in this work should lead to a 5–10% accuracy in the rates. However, the main source of uncertainties comes from the scattering calculations. For all the levels with $N > 5$, as explained above, it is clear that systematic errors result from the use of IOSR and IOS approximation instead of a full CC treatment.

The difference between IOSR and IOS for total energies larger than 700 cm^{-1} is very small and the errors are mainly due to the use of IOSR for total energies larger than 300 cm^{-1} . For levels with $5 < N \leq 15$, the difference between IOSR and CC cross sections at 300 cm^{-1} is smaller than 10% for $\Delta j = \Delta N$ transitions and smaller than 30–40% for $\Delta j \neq \Delta N$ transitions. For the highest levels ($15 < N \leq 30$), the errors can be greater at low energies (up to a factor of 2) since the thresholds are not described correctly, but the difference decreases with increasing energies and is of the same order of magnitude as that found for the lowest levels at high energies. After a Boltzmann average, we can expect a reasonable error compared to a full CC calculations for all rate coefficients between levels with $5 < N \leq 15$: less than 5% for $\Delta j = \Delta N$ transitions, less than 20–30% for the small rate coefficients involving $\Delta j \neq \Delta N$ transitions. For the highest levels, the error can be up to 50% for low temperatures (50–100 K) but becomes similar to that of the lowest levels for higher temperatures.

The rate coefficients between the first N levels are displayed in Tables 2 and 3 for temperatures equal to 100, 200 and 300 K.

Table 3. Downward rate coefficients of fine structure levels of SO in collision with He as a function of kinetic temperature (in units of $\text{cm}^3 \text{s}^{-1}$).

N_j	N'_j	100 K	200 K	300 K	N_j	N'_j	100 K	200 K	300 K				
4 ₄	...	3 ₄	...	2.03e-11	2.33e-11	2.48e-11	5 ₄	...	2 ₁	...	2.23e-11	2.24e-11	2.23e-11
4 ₄	...	2 ₂	...	1.99e-11	2.18e-11	2.37e-11	5 ₄	...	3 ₄	...	1.33e-12	1.64e-12	1.85e-12
4 ₄	...	3 ₂	...	2.31e-12	2.43e-12	2.46e-12	5 ₄	...	2 ₂	...	4.65e-12	4.91e-12	4.97e-12
4 ₄	...	4 ₅	...	6.63e-12	7.44e-12	8.29e-12	5 ₄	...	3 ₂	...	2.57e-11	2.74e-11	2.94e-11
4 ₄	...	3 ₃	...	3.19e-11	3.39e-11	3.63e-11	5 ₄	...	4 ₅	...	3.06e-12	5.12e-12	6.47e-12
4 ₄	...	4 ₃	...	1.59e-12	1.64e-12	1.80e-12	5 ₄	...	3 ₃	...	2.12e-12	2.22e-12	2.42e-12
5 ₆	...	1 ₀	...	7.00e-14	1.11e-13	1.77e-13	5 ₄	...	4 ₃	...	4.63e-11	4.88e-11	5.13e-11
5 ₆	...	0 ₁	...	6.23e-12	7.54e-12	8.04e-12	5 ₄	...	4 ₄	...	5.43e-12	6.21e-12	6.60e-12
5 ₆	...	1 ₂	...	2.21e-12	2.33e-12	2.74e-12	5 ₄	...	5 ₆	...	1.67e-12	2.81e-12	3.63e-12
5 ₆	...	2 ₃	...	2.18e-11	2.12e-11	2.12e-11	5 ₅	...	1 ₀	...	4.30e-15	1.81e-15	1.09e-15
5 ₆	...	1 ₁	...	2.68e-13	4.36e-13	7.02e-13	5 ₅	...	0 ₁	...	1.07e-11	1.26e-11	1.30e-11
5 ₆	...	2 ₁	...	2.53e-12	3.54e-12	4.06e-12	5 ₅	...	1 ₂	...	1.53e-12	1.75e-12	2.20e-12
5 ₆	...	3 ₄	...	2.82e-11	3.05e-11	3.35e-11	5 ₅	...	2 ₃	...	1.57e-11	1.80e-11	1.90e-11
5 ₆	...	2 ₂	...	6.84e-12	9.02e-12	1.00e-11	5 ₅	...	1 ₁	...	1.31e-12	1.45e-12	1.75e-12
5 ₆	...	3 ₂	...	8.21e-13	1.05e-12	1.24e-12	5 ₅	...	2 ₁	...	4.85e-13	5.69e-13	5.92e-13
5 ₆	...	4 ₅	...	4.15e-11	4.23e-11	4.41e-11	5 ₅	...	3 ₄	...	5.85e-12	6.46e-12	7.16e-12
5 ₆	...	3 ₃	...	1.60e-12	1.91e-12	2.35e-12	5 ₅	...	2 ₂	...	1.73e-11	1.73e-11	1.76e-11
5 ₆	...	4 ₃	...	2.39e-12	3.80e-12	4.73e-12	5 ₅	...	3 ₂	...	2.22e-13	2.18e-13	2.62e-13
5 ₆	...	4 ₄	...	9.65e-12	1.24e-11	1.38e-11	5 ₅	...	4 ₅	...	1.46e-11	1.78e-11	1.95e-11
5 ₄	...	1 ₀	...	1.14e-12	1.13e-12	1.26e-12	5 ₅	...	3 ₃	...	2.49e-11	2.69e-11	2.89e-11
5 ₄	...	0 ₁	...	3.14e-12	3.54e-12	3.65e-12	5 ₅	...	4 ₃	...	2.98e-12	3.45e-12	3.66e-12
5 ₄	...	1 ₂	...	6.46e-13	7.61e-13	9.57e-13	5 ₅	...	4 ₄	...	3.50e-11	3.66e-11	3.92e-11
5 ₄	...	2 ₃	...	3.76e-12	5.39e-12	6.24e-12	5 ₅	...	5 ₆	...	5.11e-12	6.31e-12	7.42e-12
5 ₄	...	1 ₁	...	5.21e-13	4.89e-13	5.28e-13	5 ₅	...	5 ₄	...	1.57e-12	1.70e-12	1.88e-12

One observes a very slow variation of the coefficients with temperature. The results presented in this paper, the excitation rate coefficients for other temperatures and other transitions will be made available on our web site (Basecol).

4.2. Comparison with previous work

We compare our results to those of Green (1994), by transforming the SO-H₂ rates into SO-He rates through the relation (Schöier et al. 2005):

$$k_{\text{SO-He}} = k_{\text{SO-H}_2} \left(\frac{\mu_{\text{SO-H}_2}}{\mu_{\text{SO-He}}} \right)^{\frac{1}{2}}. \quad (7)$$

Figure 3 compares rate coefficients for a number of transitions frequently observed at millimeter wavelengths. The difference is not a function of the temperature and does not change significantly when temperature increases. Large differences exist for the $0_1 \rightarrow 1_0$ transition. They are due to the incorrect description of the energy levels in the approach of Green (1994) where fine structure is not taken into account. More generally, all downward transitions with $\Delta N > 0$ should be described by a method that takes into account the exact fine structure splitting of the energy levels. For the other transitions with $\Delta j = \Delta N$, the differences are not so large and decrease when N increases. However, a difference of a factor of 2–3 is observed for the $6_5 \rightarrow 5_4$ transition (Fig. 3) and more generally for all transitions described with the IOSR approach. We checked the accuracy of those rate coefficients against CC calculations; the difference is partially due to the use by Green (1994) of the PES calculated for the CS-He system with an electron gas model, modified at long range to smoothly join the asymptotic

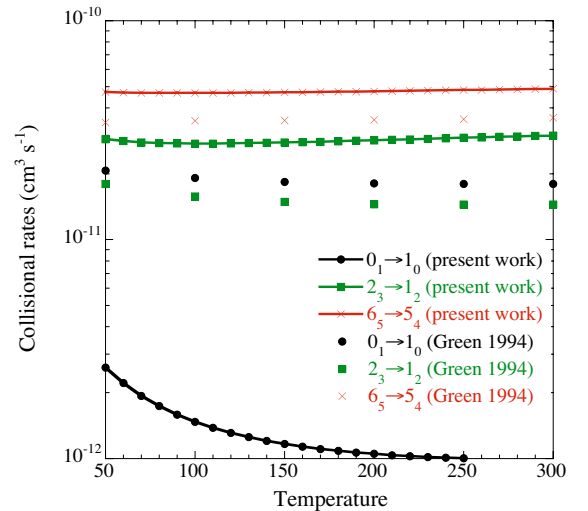


Fig. 3. Comparison between our rate coefficients (line + symbols) from 50 to 300 K with the results of Green (1994) (symbols).

interaction of CS with H₂. As mentioned by Thomas et al. (1980), the electron gas model may lead to rates with error of up to a factor of 2–3, and Green pointed out that one might expect as much as a factor of 2–3 error for his calculated individual rate coefficients. The scaling factor given by Eq. (7) assumes that the cross section for SO-He and SO-H₂ collisions are the same. Other than the differences in the PES, the difference in the reduced masses of the two colliding systems may contribute to different values of the cross sections. This will be tested in future work.

5. Conclusion

We have extended into high temperature (50–300 K) our previous calculations obtained in the CC approach for low temperatures (Paper I). As a full CC cannot be used for high energies involving a very large number of open channels, we have defined a hybrid procedure combining the accurate CC approach to correctly define the first rotational levels with two approximate methods (IOS and IOS scaling relationship from spin-free cross sections). The final accuracy of the calculated rate coefficients is expected to be 5% for $\Delta j = \Delta N$ transitions and less than 20–30% for $\Delta j \neq \Delta N$ transitions compared to full CC calculations. A comparison with previous work by Green (1994) shows large differences, particularly for the first rotational levels. The consequences for astrophysical modeling are under study.

Acknowledgements. All the scattering calculations were performed at the IDRIS-CNRS center (Institut de Développement et des Ressources en Informatique Scientifique du Centre National de la Recherche Scientifique) under project 050883 and at the SIO of the observatory of Meudon.

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