Rotational de-excitation of tricarbon monosulfide (C_3S) in collision with (He): potential energy surface and rates

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Received: 9 August 2020 / Accepted: 9 November 2020 / Published online: 7 December 2020
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Abstract Despite that the tricarbon monosulfide (C_3S) is among the first sulfur-containing carbon-chain molecules to be detected in the interstellar medium, no studies focused on the determination of its collisional rates. These rate coefficients are essential to estimate the abundance of C_3S in the interstellar medium. Computations of the $C_3S(^1\Sigma^+)$ downward rate coefficients, induced by collision with He, are performed by averaging the integral cross sections at low temperature (below 25 K). Calculations of the cross sections in the close-coupling quantum time independent formalism for $E_c \leq 110 \text{ cm}^{-1}$ and $J \leq 10$ are based on a new 2-D potential energy surface. This PES is obtained from the explicit correlated coupled cluster with a single, double and perturbative triple excitation [ccsd(t)-f12] ab initio approach and the aug-cc-pVTZ basis sets. The PES have a global minimum of -55.69 cm^{-1} located at $R = 6.25 \text{ bohr}$ and $\theta = 94^\circ$, and a second minimum of -36.95 cm^{-1} at $R = 9.35 \text{ bohr}$ and $\theta = 0^\circ$. A comparison of C_3S rates with those of the iso-electronic molecule C_3O was made. The results indicate a great temperature dependence of the rates for transitions of $\Delta J > 2$. We expect that the new collisional data will allow for accurate determination of the C_3S abundance in several interstellar regions.

Keywords ISM molecules · Molecular data · Scattering · Rate coefficient · Cross section coefficient

1 Introduction

The sulfur-containing carbon-chain compounds play an important role in chemical formation of several interstellar regions and sources. The first interstellar detection of the C_3S molecule was in the Taurus Molecular Cloud-1 (TMC1) by Kaifu et al. (1987). The C_3S molecule was identified, by laboratory microwave spectroscopy, by Yamamoto et al. (1987), who confirmed the presence of this molecule in the interstellar medium (ISM). These authors have used the three strong unidentified lines detected by Kaifu et al. (1987) in their survey of the cold dark clouds of TMC1. This study gives the rotational constants and the dipole moment used by some authors (Cernicharo et al. 1987; Bell et al. 1993) to estimate the column densities of C_3S . More than the $4 \rightarrow 3$, $7 \rightarrow 6$ and $8 \rightarrow 7$ transitions, two other new lines ($2 \rightarrow 1$ and $3 \rightarrow 2$) were detected later by Kaifu et al. (2004) in the same source (TMC1) including a new detection of the $C_3^{34}S$ isotopomer. For another, similar source, namely IRC+10216, Cernicharo et al. (1987) reported the detection of 11 lines. Later, Bell et al. (1993) had observed C_3S in the envelopes of C-rich AGB stars.

Another detection has been also reported by Iino et al. (2014) for the $59 \rightarrow 58$ observed transition in Neptune's stratosphere. Earlier, Tercero et al. (2010) made a comparison with the chemical composition of the nearest high-mass star-forming Orion KL, conducted with a view on deficient sulfur-bearing species. For such species, higher rotational temperatures ($15 < T < 26 \text{ K}$) are shown, meaning that the sulfur-bearing molecules preferentially reside in a warmer and denser part. It was the first detection of C_3S in warm clouds.

Recently, spectral line survey observations conducted on the high-mass protostar candidate NGC 2264 CMM3 led to the identification of several molecular species such as C_3S

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(Watanabe et al. 2015). For this molecule, the column density was estimated with fixed excitation temperature. Despite that NGC 2264 CMM3 and Orion KL are both high-mass protostars, there are significant chemical differences and different excitation conditions. Indeed, the molecular rotational temperatures are much higher in Orion KL than in NGC 2264 CMM3. In addition, the intensities of carbon-chain molecules such as C_3S , are found to be stronger in NGC 2264 CMM3. The abundance of C_3S relative to $C^{34}S$ are also found to be higher by an order of magnitude in NGC 2264 CMM3 than in Orion KL.

More recently, Vastel et al. (2018) carried out a highly sensitive, unbiased spectral survey of the molecular emission of the L1544 pre-stellar core with a high spectral resolution. These authors reported the detection of C_3S among other sulphur bearing species. They used a radiative transfer modeling to determine the observed column densities.

Many models have been established to predict the formation processes, densities and astrochemistry of sulfur-bearing carbon chains such as the C_3S molecule in different media ((Millar and Herbst 1990) in TMC1 and SgrB2, (Hirahara et al. 1992; Sakai et al. 2007; Gratier et al. 2016; Vidal et al. 2017) in TMC1, (Millar et al. 2001; Howe and Millar 1990) in IRC+10216).

To understand the differences of the C_3S critical density, depending on its location in the ISM, we have to precisely determine the rotational excitation/de-excitation rates. In fact, these rates are essential for the de-excitation conditions of the region studied. That is why we perform in this paper a rotational excitation/de-excitation rates calculation of C_3S induced by collision with helium. In Sect. 2, we give the calculated Potential Energy Surface (PES), describing the interaction of the rigid C_3S with He, which was adapted for the dynamical computations. We present in Sect. 3, the rotational excitation/de-excitation cross sections generated by quantum dynamical calculations in a fully converged coupled-channel formalism. These cross sections are then averaged over thermal distribution of velocities, giving the intended de-excitation rate coefficients. Finally, we present in Sect. 4, a discussion of those rates with a conclusion as regards their astrophysical relevance and a comparison with the isoelectronic C_3O molecule (Khadri and Hammami 2019).

2 Potential energy surface calculation

2.1 Geometry and methods

The C_3S molecule is considered as a rigid rotator, where the internuclear bond distances were frozen to their experimental equilibrium values with a linear geometry. This approximation is sufficient to compute the interaction energy

Fig. 1 Jacobian coordinates system for the C_3S –He collisional system

of the C_3S molecule with He and leads to the following linear structure adopted (lengths in Ångstrom): $r(C1 - C2) = 1.2724$; $r(C2 - C3) = 1.3028$; $r(C3 - S) = 1.5323$. The axis connecting the C_3S atoms was taken as the principal axis of inertia. In addition, the center of the reference frame is taken as the center of mass of this target molecule. Thus, owing to the recommended values of bond lengths for the neutral $^1\Sigma^+$ ground state (Ohshima and Endo 1992), this center of mass is between the ($C3$) and (S) atoms, too close to the carbon. We notice that the rotational de-excitation sections are greater than the vibrational ones for low temperatures ($T < 100$ K), as in our case, and the first vibrational excitation energy for C_3S is at $\omega = 151\text{ cm}^{-1}$ (Garand et al. 2009).

Figure 1 shows the geometries used to compute the C_3S –He PES, where the two Jacobi coordinates R and θ were in use. R is the distance from the helium atom to the C_3S center of mass, and θ is the angle between the R vector and the C_3S principal inertia axis. The $\theta = 0^\circ$ orientation corresponds to the He located towards the sulfur atom.

The Molpro (2010) package code was used for the $C_3S(^1\Sigma^+)$ –He van der Waals complex to carry out the electronic *ab initio* calculations. These computations were done at the explicitly correlated closed-shell coupled cluster approach with the single, double and perturbative triple excitation [CCSD(T)-F12a] (Adler et al. 2007) method and the aug-cc-pVTZ basis sets using a grid of 46 values for the molecule–atom separation and 19 values of the θ angle. Indeed, we varied the R distance from 4 to 40 bohr in steps of 0.25 from 4 to 10 bohr, 0.5 from 10 to 15 bohr, 1 from 15 to 20 bohr, 2 from 20 to 30 bohr and two geometries at 40 and 100 bohr and we varied the θ angle between 0° and 180° in steps of 10° . All these configurations lead to 893 electronic energies, examined in the C_s symmetry point group.

Fig. 2 Bi-dimensional cut of the interaction potential in cm^{-1} , of $\text{C}_3\text{S-He}$ as a function of R and θ . Negative values in red, positive values in blue. Zero energy is set at infinite R

The interaction potential V_{int} defined below is used as a correction for the *ab initio* energies by means of the usual counterpoise procedure of Boys and Bernardi (1970):

$$V_{\text{int}}(R, \theta) = E_{\text{C}_3\text{S-He}}(R, \theta) - E_{\text{C}_3\text{S}}(R, \theta) - E_{\text{He}}(R, \theta) \quad (1)$$

where $E_{\text{C}_3\text{S-He}}$ is the global electronic energy of the $\text{C}_3\text{S-He}$ complex, $E_{\text{C}_3\text{S}}$ is the energy of the C_3S molecule and E_{He} is the energy of the helium atom. All these energies are performed using the full basis set of the total system.

The residual interaction energy value at large distance ($R = 100$ Bohr) for each θ angle was subtracted to remedy the size-consistent deficiency of the ccsd(t)-f12 method. In particular, near the minimum of interaction for $\theta = 90^\circ$, the residual interaction value is $\sim 0.2 \text{ cm}^{-1}$. The accuracy of the basis set and method used in these calculations is similar to earlier studies (Ben Khalifa et al. 2019; Khadri and Hammami 2019).

2.2 PES analysis

A cut of the PES of $\text{C}_3\text{S-He}$ as a function of R and θ , displayed in Fig. 2, shows two minimums with a strong anisotropy. The approach of taking He perpendicular to the molecular axis toward C_3 atom leads to the appearance of a global minimum at the position of $R = 6.25$ bohr and $\theta = 94^\circ$ with a well depth of -55.69 cm^{-1} . The second minimum is found at the position of $R = 9.35$ bohr and $\theta = 0^\circ$ with a well depth of -36.95 cm^{-1} , corresponding to the approach of taking He collinear to the molecular axis toward (S) atom. For a better understanding of the PES shape we analyzed the charge repartition in the C_3S molecule using a Natural Bond Orbital (NBO) calculation with the MRCI method and the aug-cc-pVQZ basis set. This gave a charge

distribution as follows: (+0.22361) for (C1), (-0.51585) for (C2), (+0.00009) for (C3) and (+0.29215) for (S).

The appearance of the minimum towards $\theta = 94^\circ$ is essentially due to the high interaction between the positive charge distribution with the helium electronic cloud. Indeed, the lower electron density near the positive carbon (C3) reduces the Pauli exchange repulsion, and the interaction becomes stronger. That is why the He atom attacks the carbon side (C3); the negative charge is on the side of the carbon (C2) (-0.51585), while the sulfur charge is positive (+0.29215). The same behavior already explains the effect of the charges on (C1C2) (-0.29224) and (C3S) (+0.29224) leading to the appearance of the second minimum towards $\theta = 0^\circ$ and to an increase of the repulsion of both moieties. This repulsion explains the shape of the potential towards $\theta \sim 0^\circ$ and $\theta \sim 180^\circ$.

2.3 Fit of the PES

The 2D-PES was fitted with an analytical representation (Phillips et al. 1995) in order to perform dynamical computations. For this purpose, we used an expansion of the *ab initio* potential in terms of spherical harmonics:

$$V(R, \theta) = \sum_{\lambda=0}^{\lambda_{\text{max}}} V_{\lambda}(R) P_{\lambda}(\cos \theta), \quad (2)$$

where the $P_{\lambda}(\cos \theta)$ are the Legendre polynomials and the radial functions $V_{\lambda}(R)$ were calculated by adjusting the λ coefficients for each value of R . This was done by projections using quadrature. Terms with λ up to $\lambda_{\text{max}} = 72$ (Wernli et al. 2007) were considered to take account of the big anisotropy of the interacting potential. During the procedure of the scattering calculation, an extrapolation and interpolation of the $V_{\lambda}(R)$ coefficients was performed using the POTENL routine of the MOLSCAT code (Hutson and Green 1994). This procedure was done to obtain the values of the interaction at each R separation. The first $V_{\lambda}(R)$ components were plotted and presented in Fig. 3.

3 Dynamical calculation

3.1 Cross sections

The MOLSCAT package (Hutson and Green 1994) was used to compute the cross sections $\sigma_{J' \leftarrow J}(E_c)$ using the close-coupling approach (CC). By taking into account a sufficient number of closed energy channels, we have considered the scattering calculations with $J \leq 10$ as optimal rotational level. In order to have converging cross sections, several tests were carried out where, for all collisional energies

Fig. 3 Dependence on R of the first $V_\lambda(R)$ components for $0 \leq \lambda \leq 10$

$E_c \leq 110 \text{ cm}^{-1}$, the rotational basis was optimized and fixed at $J_{\text{max}} = 21$. The rotational levels were calculated for the $B_0 = 0.09641347 \text{ cm}^{-1}$ and $D_0 = 69.58 \times 10^{-7} \text{ cm}^{-1}$ rotational constants (Yamamoto et al. 1987) and the reduced mass $\mu = 3.7803982$. Cross sections are calculated over a grid of total energy by steps of $\Delta E_c = 0.1 \text{ cm}^{-1}$ for $0.1 \leq E_c \leq 50 \text{ cm}^{-1}$, $\Delta E_c = 0.2 \text{ cm}^{-1}$ for $50 < E_c \leq 100 \text{ cm}^{-1}$ and $\Delta E_c = 0.5 \text{ cm}^{-1}$ for $100 < E_c \leq 110 \text{ cm}^{-1}$.

For collision energies, in the same order of magnitude or lower than the value of the PES global minimum well depth ($E_c \leq 50 \text{ cm}^{-1}$), the step size energy is small enough to allow for a good description of resonances. In Fig. 4, we present the kinetic energy variation of the cross sections $\sigma_{J' \leftarrow J}(E_c)$ of C_3S in collision with the He atom, for transitions from the ground state to J (panel a) with $1 \leq J \leq 10$ and from J to $J + 1$ (panel b) with $0 \leq J \leq 3$. These shape resonances indicate the possibility of the He atom to be trapped, for a short time, into the potential well, leading to the formation of a quasi-bound state. These resonances disappear, for all cross sections, with a smooth behavior for energies greater than 20 cm^{-1} .

We notice in panel a of Fig. 4, the shape of cross sections for the two first transitions, which decrease continuously whereas for the other ones they decrease; then increase. For large values of ΔJ we notice less visible resonances. Panel b shows that the $0 \rightarrow 1$ transition is the greatest in magnitude and resonances. In the range between 2 and 8 cm^{-1} all the transitions overlap enormously with weaker resonances. The observations seen in the shape of the cross sections will undoubtedly have an influence on the values of the collision rates.

Fig. 4 Kinetic energy dependence of the rotational cross sections of C_3S in collision with He for transitions from the ground state to J (panel a) and from J to $J + 1$ (panel b)

3.2 Rate coefficients

After the dynamical calculation, the relevant state to state cross sections $\sigma(E_c)$ were integrated over a Maxwell–Boltzmann distribution of kinetic energies to obtain the collision rate coefficients $k(T)$ between two rotational levels $J' \leftarrow J$. The grid of total energies used to compute the cross sections are sufficient to perform calculations, for the first 11 rotational levels, collision rates for $T \leq 25 \text{ K}$. The results are displayed in Fig. 5 where the rotational de-excitation rate coefficients of the C_3S –He system are plotted as a function of the kinetic temperature for transitions corresponding to J to 0 (panel a) and J to $J - 1$ (panel b) with $1 \leq J \leq 10$. For average values of ΔJ , we see a monotonic behavior of $k(T)$

Fig. 5 Temperature dependence of rate coefficients of C₃S in collision with He for transitions corresponding to: J to 0 (panel a) and J to $J - 1$ (panel b)

in a way very similar to C₃O (Khadri and Hammami 2019), not like the usual increase seen for average and larger ΔJ .

For kinetic temperatures below 8 K, some de-excitation transitions from J to $J - 1$ levels (panel b) have rates that increase, while they decrease for transitions between the lowest levels ($1 \rightarrow 0$, $2 \rightarrow 1$ and $3 \rightarrow 2$). This behavior has been observed for other systems (Bop et al. 2017). From panel b of Fig. 5, it clearly appears that the rate coefficients for transitions with $\Delta J = 1$ increase with the initial level J with smaller and smaller differences for large J . This behavior is also observed for the cross sections for relatively large energies. This can be due to the low value of the rotational constant of C₃S (~ 0.1). So the kinetic energy dominates and the statistical approach may be valid. For larger temperatures, the C₃S rates show the same trend as found for C₃O. This leads us to think that, for very low temperatures,

Fig. 6 Comparison of de-excitation rates (in $\text{cm}^3 \text{s}^{-1}$) at 10 K (red dots) and 20 K (blue marks) for the C₃S–He collision, this work vs. C₃O–He (Khadri and Hammami 2019). A black continuous line shows the 1 : 1 ratio

it is the large rotational levels that are more solicited, in a different way from the generally known trend.

4 Discussion and conclusion

In the literature no collision coefficients are available for the C₃S molecule. This necessitated the authors to use the detected C₃S lines to calculate the rotational level populations and so they derived with some accuracy the column density by assuming the molecule's dipole moment (Cernicharo et al. 1987; Bell et al. 1993). The disadvantage of the given column density values is that they depend heavily on the source size and shape as well as on the single rotation temperature assumption. Thus, the determined values are uncertain in a way that can reach a factor of 2 or more. The lack of data concerning collision rates for C₃S led us to make a comparison of the values determined in this work with those recently obtained for the similar and isoelectronic valence molecule C₃O (Khadri and Hammami 2019). In Fig. 6, we present a de-excitation rates comparison of C₃S/C₃O with He computed at 10 K and 20 K.

For the C₃O (Khadri and Hammami 2019) rates previously published, we used the same calculation approach as used in the present work. We see in Fig. 6 that the expected concordance on the rotational rates is not obtained. According to this figure, we notice that the more the temperature increases, the more the ratio $k(\text{C}_3\text{O-He})/k(\text{C}_3\text{S-He})$ approaches the unit (the black continuous line). In addition, the two molecules have almost the same rates for the range between 5×10^{-11} and $10^{-10} \text{ cm}^3 \text{s}^{-1}$, corresponding to the values of the $\Delta J = 1, 2$ transitions. Outside of this range,

the rates' ratio goes in favor of C_3S . This difference may be due to two features, either to the interaction with the collision partner (He) or to the rotational structure of the target molecule C_3S/C_3O . In our case, the two PESs of the C_3S –He and C_3O –He systems are very similar, so that the potential wells are of the same order, $\sim 55\text{ cm}^{-1}$ for C_3S –He and $\sim 53\text{ cm}^{-1}$ for C_3O –He, as also the anisotropy is the same for both systems. Meanwhile, the rotational constant of C_3S ($\sim 0.096\text{ cm}^{-1}$) is almost half that of C_3O ($\sim 0.16\text{ cm}^{-1}$). This makes the rotational levels of C_3S tighter than those of C_3O and their velocity coefficients larger. However, the new rate values are required for the determination of the C_3S abundance in the ISM, since those of C_3O are not appropriate.

The high relevance of the C_3S molecule led us to perform computations of the rotational de-excitation rates with He. In this paper, we have determined a precise 2-D Potential Energy Surface for the C_3S –He system. The two PES minima show moderate well depths of about -55.69 cm^{-1} (global minimum) and -36.95 cm^{-1} . This state-of-the-art PES allowed us to perform high quality rotational dynamic computations for collision energies up to 110 cm^{-1} . The cross sections were then averaged over the collision energy, for temperatures up to 25 K, to get the rotational de-excitation rates. We expect great changes in the abundance of the C_3S outer Local Thermodynamic Equilibrium (LTE) conditions.

Data availability Tables of de-excitation rates may be obtained from the authors by request.

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