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SiS formation via gas phase reactions between atomic silicon and sulphur-bearing species

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ABSTRACT

The potential energy surface for the Si + SH and Si + SH₂ reactions is explored using the highly accurate explicit correlation multireference configuration interaction method. For atomic silicon colliding with SH, SiS + H is predicted to be the main reaction channel with no activation energy. The reaction Si + SH₂ → SiS + H₂ is found to be largely thermodynamically favourable, but likely to be slow, due to its spin forbidden nature. Several details on possible mechanisms are evaluated, and implications for astrochemical models are discussed. Among other results, we show that SiS is stable towards collisions with H and H₂, and that the HSiS molecule will quickly be converted to SiS in collisions with atomic hydrogen.

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

1 INTRODUCTION

The SiS molecule was first detected in 1975 at CW Leonis (IRC+10216), a well-studied evolved carbon star, together with the SiO molecule (Morris et al. 1975). Dickinson & Kuiper (1981) also observed the two molecules together, and found SiS was less abundant than SiO (Dickinson & Kuiper 1981). Further studies detected the presence of SiS towards O-rich AGB stars, with abundances significantly lower than around C-rich AGB stars (Danilovich et al. 2018).

Apart from the envelopes of evolved stars, SiS was detected in a few star-forming regions associated with strong outflow activity, like Orion KL (Ziurys 1988, 1991; Tercero et al. 2011) and SgrB2 (Dickinson & Kuiper 1981).

Recently, a systematic search for SiS in low-mass star-forming regions was carried out in the framework of the IRAM Large Program ASAI (Lefloch et al. 2018). Emission from the SiS transitions $J_{\text{up}} = 4\text{--}15$ between 72 and 272 GHz was searched for in a sample of 10 regions at different stages of protostellar evolution, from pre-stellar to late Class I. SiS was detected towards the protostellar shock region, L1157-B1, only (Podio et al. 2017). The abundance was found very low ($\sim 10^{-8}$), about 2 orders of magnitude less than SiO. The results of this survey led the authors to conclude that SiS cannot be a simple product of gas phase chemistry in molecular clouds. Its formation requires specific conditions, which are best found in shocks.

The lack of SiS detection in such environments is quite surprising in regard of the frequent observations of SiO, another silicon-bearing species, which has become a probe of protostellar shocks.

Observational studies of Orion KL and SgrB2 show that the SiS and SiO line profiles are similar, pointing to a common shock origin. However, the recent study of SiS emission in the L1157-B1 shock region with the NOEMA interferometer by Podio et al. (2017) showed evidence for a strong gradient of [SiO/SiS] abundance ratio across the shock region, implying that SiS and SiO have different chemical pathways. The origin of SiO is relatively well constrained: atomic silicon is first released from the dust grain cores through sputtering in the shock, and subsequently reacts with OH and/or atomic O in the gas phase.

SiS chemistry has been relatively poorly studied until now and only recently significant progress has been made in the field. In circumstellar envelopes, it is well established that SiS is formed in the densest and hottest parts of the inner envelope, close to the stellar photosphere, where it is thought to form under thermochemical conditions (see e.g. Prieto et al. 2015; Schöier et al. 2007). Recent accurate theoretical calculations (Paiva, Lefloch & Galvão 2018; Zanchet et al. 2018) have shown that SiS is readily destroyed in the presence of atomic oxygen O, which naturally accounts for the lower abundance of SiS with respect to SiO, while implying that they have different origins.

The physical conditions in star-forming regions are obviously very different from those in circumstellar envelopes, so that both formation and destruction SiS pathways are a priori very different. It is therefore necessary to investigate other reactions which could play a role in SiS chemistry, taking into account possible other actors in the shocked gas. Zanchet et al. (2018) proposed that the main SiS formation reactions in outflows are Si + SO and Si + SO₂, while SiS is efficiently destroyed by reaction with atomic O. Further theoretical calculations showed that SiH + S and SiH + S₂ collisions (Rosi et al. 2018) are also potential candidates for SiS formation. Whereas most of silicon is stored in the core of dust grains,

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Gusdorf et al. (2008) concluded that about 1 per cent of silicon abundance is present in the form of SiO on to the grain mantles in L1157-B1, based on their analysis of the SiO line emission. At the surface of dust grains, atomic Si gets easily hydrogenated into SiH₄. Hence, a small fraction of silicon, in the form of silicon hydrides, could be present on to the grain mantles and easily released in the gas phase either through thermal evaporation or non-thermal (sputtering) processes (Mackay 1995) and subsequently converted into SiH by photodissociation in the gas phase. These studies are in line with Podio et al. (2017) who speculated that in the interstellar medium SiS could form through slow gas-phase processes involving a fraction of the released silicon (either in the form of Si or SiH_n) with simple sulphur bearing species S/S₂/HS, instead of being released from grain cores (Podio et al. 2017).

In this article, we explore another possibility, based on revised chemical models of S-chemistry, which predict that depending on the evolutionary stage of pre-stellar cores, HS and H₂S could be highly abundant at the surface of dust grains and constitute the main reservoirs of sulphur (Vidal et al. 2017). In a shock violent enough to erode the core of dust grains and release atomic Si in the gas phase, the molecules HS and H₂S which constitute part of the grain mantles, would be also rejected into the gas phase. Here, we explore the viability of gas phase reactions between HS and H₂S with atomic silicon as sources of SiS in the interstellar medium.

2 AB INITIO METHODS

The energies reported in this work were obtained by explicitly correlated multireference configuration interaction (MRCI-F12) calculations (Shiozaki, Knizia & Werner 2011; Shiozaki & Werner 2011, 2013), using the cc-pVQZ-F12 (VQZ-F12) basis set (Peterson, Adler & Werner 2008). This method is state-of-the-art for accurately describing bond breaking/formation (Trabelsi & Francisco 2018) and the results are close to the complete basis set limit. All energies were enhanced with the Davidson (+Q) correction, thus approximating up to quadruple excitations. (Werner & Knowles 1988a, b).

The reference wavefunction was obtained from complete-active-space-self-consistent-field (CASSCF) calculations (Knowles & Werner 1985; Werner & Knowles 1985), with 11 electrons in 9 orbitals for the Si + SH case, and 12 electrons in 10 orbitals for the Si + SH₂ one. For both reactions, several electronic states and different spin multiplicities were treated, in order to provide a complete description of both systems. Geometry optimizations, vibrational frequencies, and zero-point energy (ZPE) corrections are also at the CASSCF level.

The probabilities of singlet-triplet transitions are discussed in terms of the magnitude of the spin-orbit coupling (SOC). For this purpose, the full spin-orbit matrix was calculated with the Breit-Pauli operator (Berning et al. 2000) as implemented in MOLPRO (Werner et al. 2015). The spin-free electronic Hamiltonian eigenstates, labelled $|S\rangle$, $|T, 1\rangle$, $|T, 0\rangle$ and $|T, -1\rangle$, are used to build the total Hamiltonian matrix representation ($H_{el} + H_{SO}$). The singlet-triplet spin-orbit transition probabilities will depend on the magnitude of the V_{SO} term, which is defined as

$$V_{SO}^2 = \sum_{M_S=-1}^1 |\langle T, M_S | H_{SO} | S \rangle|^2. \quad (1)$$

We have employed the MOLPRO (Werner et al. 2015) package in all calculations.

3 RESULTS AND DISCUSSION

3.1 Formation of SiS through Si + HS collisions

To study the reaction between the mercapto radical (HS) with atomic silicon we started at the dissociated limit and gradually approached the reactants by 0.05 Å while relaxing all other degrees of freedom (valence angle and HS bond distance). The results are shown in Fig. 1, where it can be seen that the formation of SiS via Si + HS collisions is largely favourable from the thermodynamic point of view, with an exothermicity of approximately 241 kJ mol⁻¹. A potential well corresponding to a bound SiSH molecule is achieved in the process. No activation energy is involved in the reaction, and therefore it is likely to happen very fast. It also occurs adiabatically in a single electronic state, without crossings with excited ones. The other electronic states lead to an excited form of the SiS radical, and the reaction is endothermic in this case, therefore not contributing significantly to the overall rate.

Although not visible in the energy scale of Fig. 1, the inverse reaction ($H + SiS \rightarrow SiSH$) needs to overcome a small entrance barrier of 5.4 kJ mol⁻¹ (here named TS2) to achieve the potential well. In fact, this figure shows only a one-dimensional cut over the minimum energy path for the $Si + SH \rightarrow SiS + H$ abstraction route, but another isomer of the triatomic system also exists, and an isomerization mechanism is also possible. These two reaction paths are described together in the schematic representation of Fig. 2. The energies (including ZPE corrections) and vibrational frequencies of the main structures are shown in Table 1.

When studying the SiH + S reaction, Rosi et al. (2018, 2019) also explored the ground doublet state of the SiSH triatomic system, and achieved results similar to those given in Fig. 2. This work explored further excited electronic states, contributing to a better understanding of the reactive system. Furthermore, our calculations are based on multireference methods, and are more suitable in bond breaking regions. Indeed, the barrier for the $H + SiS$ reaction (TS2) calculated in this work is 44 per cent lower than formerly predicted.

Thus, we have two possible pathways for the formation of the SiS molecule: first, an attack of atomic silicon to the mercapto radical, followed by a direct HS bond break through a small exit barrier (TS2), and second, the formation of SiSH followed by isomerization to HSiS (TS1), with no exit barrier involved.

Finally, although a stable HSiS molecule has not been observed thus far, reactions between H and SiS in the surface of a grain could in principle yield this triatomic species. A more in depth discussion about this species will be given in Section 3.3.

3.2 Formation of SiS through Si + H₂S collisions

For the formation of SiS via hydrogen sulphide, the reaction paths are more complex and involve crossings between singlet and triplet electronic states of a bound SSiH₂ molecule. Since ground state atomic silicon has a triplet electronic configuration, and H₂S is a singlet species, the collision process can only happen adiabatically on the triplet state of the tetratomic system, and for this reason we start the discussion considering triplet states only.

3.2.1 Triplet state

The reaction paths in the triplet electronic state are summarized in Fig. 3. It is shown that the reaction between the silicon atom in its ground (³P) state and H₂S molecule can generate three well-defined isomers of the tetratomic system. First, the interaction leads

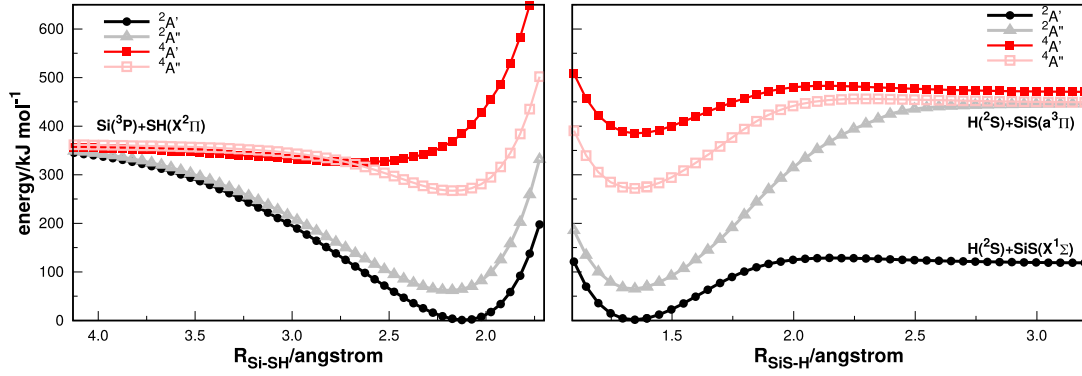


Figure 1. Dissociation of the SiSH molecule at the MRCI(Q)-F12/VQZ-F12 level. Each step is separated by 0.05 Å. The black and grey lines correspond to doublet states of A' and A'' symmetry, respectively, while the red and pink ones correspond to triplet states.

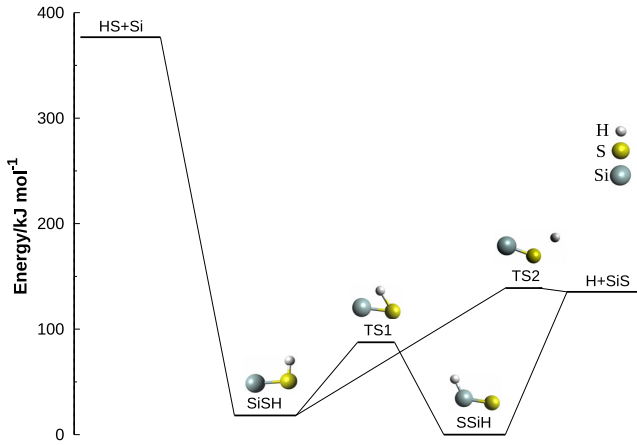


Figure 2. Schematic view of the potential energy surface for the SiS formation reaction through Si + HS. Energies are at the MRCI(Q)-F12/VQZ-F12 level without ZPE corrections.

Table 1. Properties of the stationary points of HS + Si PES.^a

	E	$E(\text{ZPE})$	ω_1	ω_2	ω_3
SiSH	18.2	18.4	496	614	2524
TS1	87.5	79.2	570	1206i	1638
TS2	138.9	123.6	348	680	1228i
SSiH	0.0	0.0	690	702	2200
Si + HS	376.7	370.8	2600	—	—
SiS + H	135.4	118.2	724	—	—

^aEnergies are given in kJ mol⁻¹ and frequencies (ω) in cm⁻¹.

barrierlessly to H₂SSi, which lies 53 kJ mol⁻¹ below reactants and shows a SiS bond distance of 2.56 Å. After a H atom migration transition state (TS1) is overcome, the SHSiH isomer is obtained, with a shorter SiS bond distance of 2.13 Å and a dihedral angle of 90 deg. Note that the energy of the transition state lies below reactants, and thus this isomerization is open for collision at whatever temperature. The deepest minimum in the triplet electronic state is however the SSiH₂ structure, which can only be obtained from the initial reactants through two subsequent isomerization steps. It is easily seen that the bonding of the two hydrogen atoms to silicon is much more energetically favourable than to sulphur, the energetic difference between H₂SSi and SSiH₂ being 94 kJ mol⁻¹.

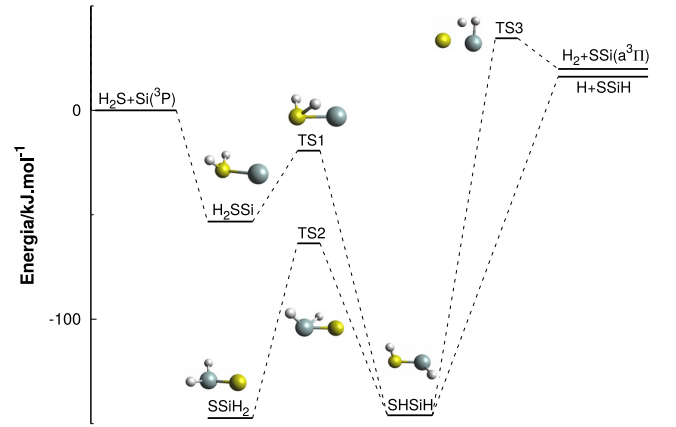


Figure 3. Reaction paths for H₂S + Si in the triplet state. Potential energy surface minima are represented as well as transition states (TS) between them. Energies are at the MRCI(Q)-F12/VQZ-F12 level.

In this figure, it is also seen that the SHSiH structure, shows also a very stable configuration, lying only 0.4 kJ mol⁻¹ above SiSH₂.

However, the desired product molecules (SiS and H₂) present singlet ground states and, as shown in Fig. 3, the Si(³P) + SH₂ collision can only lead adiabatically to H₂ + SiS($a^3\Pi$) and H + HSiS. These two product channels are endothermic, with the H + SSiH one lying 16.1 kJ mol⁻¹ above reactants, and thus these reactions are not likely to occur, except in extreme conditions. The formation of ground state SiS must therefore occur through a crossing with the singlet potential energy surface (PES), which is discussed below.

3.2.2 Singlet state

Fig. 4 shows the main stationary structures of the singlet PES together with the triplet ones discussed above. Three isomers also exist in the singlet (closed shell) PES, with their energy lying much lower than the triplet ones. The overall global minimum corresponds to the SSiH₂ molecule, lying even lower (19.2 kJ mol⁻¹) than the lowest dissociation limit H₂ + SiS. This structure shows a double SiS bond with a bond length of 1.94 Å. There are also trans and cis planar SHSiH structures, which are metastable with respect to H₂ + SiS dissociation and have SiS bond lengths of 2.13 and 2.15 Å, respectively. The isomerization barrier between SSiH₂ and the trans structure (TS5) is seen to be very high, making this structure quite

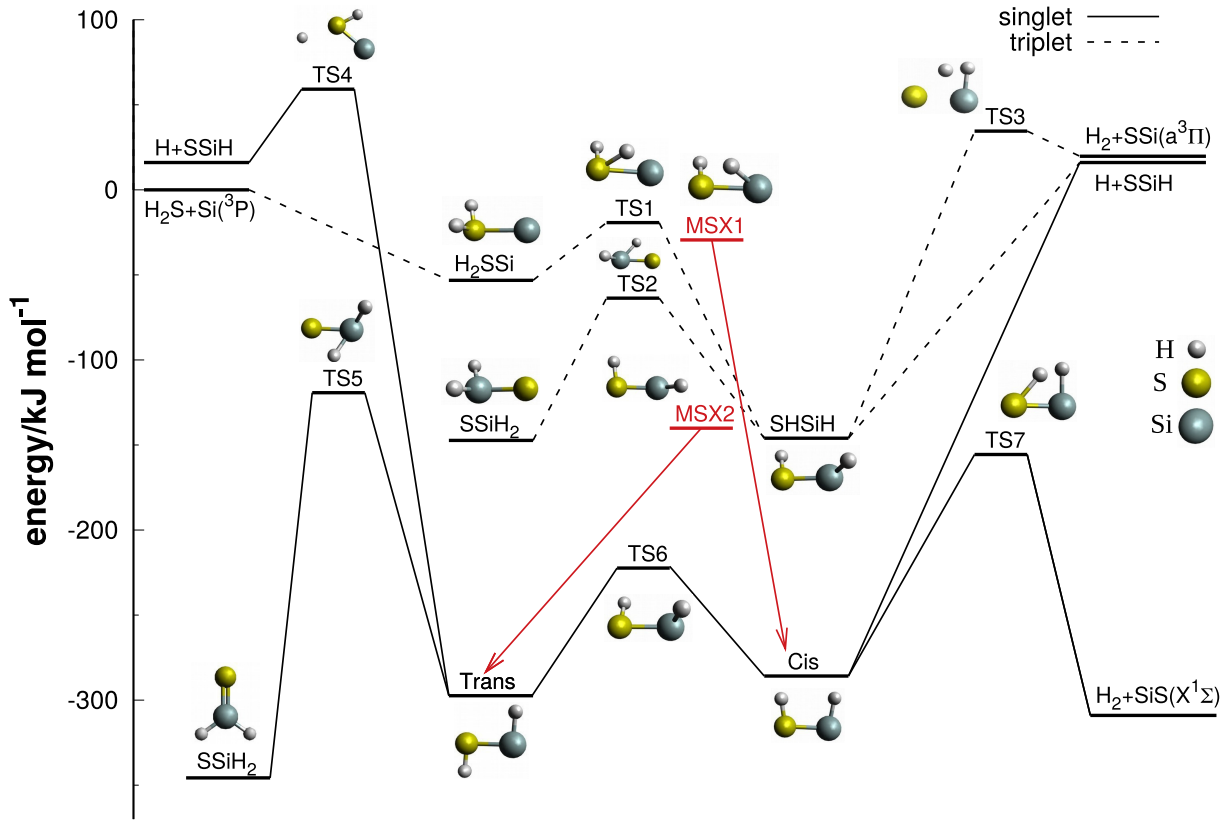


Figure 4. The proposed reaction path for $\text{H}_2\text{S} + \text{Si}$. Solid lines indicate the singlet states and dashed lines the triplet ones. The red bars indicate the energy of singlet/triplet crossings, and the red arrows give possible paths after a triplet to singlet transition occurs. Energies are at the MRCI(Q)-F12/VQZ-F12 level.

stable, if ever formed. The cis-trans isomerization barrier (TS6) lies 69 kJ mol^{-1} above the trans minimum.

The $\text{H}_2 + \text{SiS}$ reaction does not have the possibility of reaching any low lying dissociation limit, and for this reason SiS is stable with respect to collisions with H_2 in the gas phase. Therefore, we predict here that SiS will not be destroyed by neither atomic nor molecular hydrogen, which is relevant for understanding its abundance in the ISM.

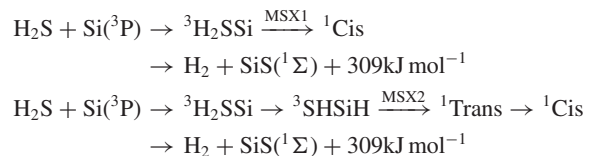
3.2.3 Intersystem crossings and the $\text{Si} + \text{H}_2\text{S} \rightarrow \text{SiS} + \text{H}_2$ reaction

As argued above, the title reaction can only happen via a triplet to singlet crossing, which makes the rate constant for such process likely to be much lower than the $\text{Si} + \text{HS} \rightarrow \text{SiS} + \text{H}$ case. Nevertheless, it occurs without a reaction barrier (and thus have zero activation energy in the Arrhenius equation). After surveying the whole singlet and triplet PES of the tetratomic complex, we are in a position to describe the overall mechanism.

Starting at the $\text{Si} + \text{H}_2\text{S}$ reactants on their ground state (triplet PES), the collisions will likely form the H_2SSi species, which may easily isomerize to the SHSiH (through TS1), all in the triplet PES. Within this reaction path, we have found a singlet-triplet crossing, at which point both states become degenerate and a transition among them is more likely to occur. This crossing is actually a seam on the potential energy hypersurface, and the minimum energy on the seam of crossing (MSX) has geometry and energies very close to that of TS1 (the structure is hereafter named MSX1). If a spin transition occurs at this point, the system will likely dissociate to

form the SiS molecule, as there are no other singlet dissociation channel below $\text{Si} + \text{H}_2\text{S}$ reactants. These product molecules would carry the excess energy as translational or rovibrational excitation of the diatomics.

Another crossing point was found at the same path, but with lower energy (MSX2). The geometry and energy of this crossing is very close to the triplet SHSiH minimum. The red arrows displayed in Fig. 4 show the path that a steepest descent on the singlet PES would leave, if the crossing occur exactly at MSX1 or MSX2. Although any given trajectory could dissociate directly right after the crossing process, two probable reaction mechanisms are:



The likelihood of such intersystem crossings will depend on the magnitude of the SO coupling. This was calculated at the MRCI/aug-cc-pVQZ level for both MSX1 and MSX2, with the results of 71 and 46 cm^{-1} , respectively. Therefore, the path described above going through MSX1 is the most likely, since it is more direct and easily reached, and also shows a larger SO coupling.

The energies (also including ZPE corrections) and vibrational frequencies for all stationary structures described above are given numerically in Table 2, including crossings points and asymptotic limits.

Table 2. Properties of the stationary points of singlet and triplet PESs.^a

	<i>E</i>	<i>E</i> (ZPE)	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6
Triplet structures								
SHSiH(³ X)	199.7	195.0	351	516	621	703	2292	2613
H ₂ SSi(³ X)	292.4	289.9	178	446	450	1179	2588	2606
SSiH ₂ (³ X)	198.4	195.4	519	539	768	970	2283	2300
TS1	326.4	313.1	345	526	754i	780	1438	2558
TS2	282.0	269.7	554	643	671	1349i	1690	2264
TS3	380.2	365.4	404	641	847	1554i	1634	1872
Singlet structures								
Cis	59.8	56.0	496	501	687	851	2159	2555
Trans	48.2	46.1	520	596	675	941	2161	2633
H ₂ SSi	321.9	317.0	234	441	584	1310	2140	2346
SSiH ₂	0.0	0.0	667	707	732	1093	2337	2343
TS4	404.9	381.2	314	341	526	549	1244i	2193
TS5	226.4	214.2	541	572	775	1640i	1760	2194
TS6	123.3	115.2	400	617	657i	683	2314	2505
TS7	190.1	178.1	588	974	999	1571	1601i	1737
Minima on the seam of singlet-triplet crossings								
MSX1	316.3	–	–	–	–	–	–	–
MSX2	205.5	–	–	–	–	–	–	–
Asymptotic limits								
H ₂ + SiS(¹ Σ)	36.7	19.2	724	4226	–	–	–	–
H ₂ + SiS(³ Π)	365.5	346.5	482	4226	–	–	–	–
H ₂ S + Si(³ P)	345.7	337.1	1182	2613	2637	–	–	–
H ₂ S + Si(¹ D)	416.8	408.2	1182	2613	2637	–	–	–
HSiS + H	361.9	336.6	690	702	2200	–	–	–

^aEnergies are given in kJ mol^{−1} relative to the global singlet minimum, and frequencies (ω) are in cm^{−1}.

3.3 HSiS in the ISM

The HSiS molecule has not been detected in the interstellar medium thus far, although its rotational transitions have been measured experimentally by Brown, Yamamoto & Saito (1997). As discussed in Section 3.1, reactions between H and SiS at the surface of a grain could in principle yield this chemical species, although not the reaction in gas phase.

However, it can also be inferred from Fig. 4 that if the HSiS species forms in the ISM, it will quickly react with H atoms to yield H₂ + SiS, which is largely energetically favoured and shows no activation energy. Hence, HSiS will disappear very quickly in shock regions, making its detection all the more difficult.

Combining the two informations given above, another possible source of the SiS molecule in the ISM that can be proposed from this work, is a two-step process: (i) collisions between Si + SH on the surface of grain-forming HSiS, followed by (ii) collision between HSiS + H leading to H₂ + SiS, which is predicted above to be fast.

3.4 Final remarks

The results presented here represent a first step in the study of SiS formation from atomic Si and mercapto radical SH. Our calculations show that the reaction between SH and atomic Si is effective in shocks and contributes to SiS formation in such environments. The importance of this contribution with respect to other formation pathways remains to be quantified, though a full modelling of SiS chemistry is beyond the scope of this article. The next step is the determination of the reaction rate coefficients to quantify the importance of this reaction under various physical and chemical conditions, relatively to other formation pathways like the reactions between atomic Si and SO/SO₂, as proposed by Zanchet et al. (2018) for protostellar outflows/shocks.

We note that the scenario considered here could also occur in diffuse molecular clouds, where atomic Si and SH are present in the gas phase (Sofia, Cardelli & Savage 1994; Neufeld et al. 2015).

In the envelopes of evolved stars, as recalled in the Introduction, SiS is observed to form close to the stellar photosphere and is then injected into the expanding envelope (Prieto et al. 2015). The SiS spatial distribution appears to be more compact than those of other Si-bearing species like SiO and SiC₂ (Massalkhi et al. 2019). Zanchet et al. (2018) proposed that this fact could result from the destruction of SiS with O atoms. In the expanding circumstellar envelope, molecules are no longer protected from the external UV radiation field and photodissociation becomes important, affecting species like CO or H₂O. This results into an increase of O abundance in the gas phase, which then rapidly reacts with SiS to produce SiO (Zanchet et al. 2018).

4 CONCLUSIONS

Using highly accurate multireference calculations, we have explored the energies involved in two SiS forming reactions in order to shed light on its formation in the interstellar medium. It is shown that the HS molecule is easily converted to SiS by collisions with atomic silicon in the gas phase. The reaction between Si and H₂S is also predicted to be possible despite its spin forbidden nature. The reaction pathway for several mechanisms are predicted and discussed. Among other results, we show that SiS is stable towards collisions with H₂ and H, and that the HSiS molecule will quickly be converted to SiS in collisions with atomic hydrogen.

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