H$_2$S Formation in Dark Clouds.


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Abstract

Sulfur is of fundamental importance in a wide variety of phenomena such as life on Earth. This element is one of the most abundant elements in space \( \text{S/H} \sim 1.3 \times 10^{-5} \), but sulfurated molecules are not as abundant as expected, thus a better understanding of sulfur chemistry is needed. We study and model the abundance of \( \text{H}_2\text{S} \) in two prototypical dark clouds, TMC1 and Barnard 1, to shed light on the physical and chemical processes involved in \( \text{H}_2\text{S} \) creation and destruction. Our observations are consistent with a PDR model in which \( \text{H}_2\text{S} \) is formed in grain mantles and released to gas phase via photodesorption. We cannot discard the contribution of other desorption processes, such as chemical desorption and/or grain-grain collisions, to enhance the \( \text{H}_2\text{S} \) abundance.

1 Introduction

Astrochemistry is an important tool to characterize the evolution of molecular gas from diffuse clouds to dense cores. In this dynamical evolution, gas cooling and gas ionization degree regulate cloud collapse. Sulfur plays an important role in this collapse since it is one of the most abundant elements in the universe, with a relative abundance of \( \text{S/H} \sim 1.3 \times 10^{-5} \) [1], and it is the main donor of electrons in the 3.7 - 7 magnitude range. Despite its high relative abundance, sulfurated compounds are not as abundant as expected in molecular clouds. Sulfur is thought to be depleted by a factor of \( 10^3 \) inside dark clouds compared to its cosmic abundance. The missing sulfur might be locked into grain mantles (e.g. [18]), which would form \( \text{H}_2\text{S} \) preferentially due to the high hydrogen abundance and mobility in the ice matrix. Therefore, studying the abundance of the \( \text{H}_2\text{S} \) molecule, which cannot be explained solely by gas-phase chemical reactions [24], may shed light into the physical and chemical processes responsible for sulfur depletion. We investigate the \( \text{H}_2\text{S} \) gas-phase abundance in two prototypical dark clouds: TMC1 and Barnard 1.

2 TMC1 and Barnard 1

TMC1, part of the Taurus molecular cloud (TMC), is one prototypical filamentary dark cloud cold core with quiescent star forming regions, at 140 pc. One of the largest Planck Galactic Cold Clumps (PGCC) groups in TMC is the Heiles Cloud 2 [13][20][22]. Malinen et al [17] identified two long filaments in HCL 2 at the eastern edge of the Taurus Molecular Ring, based on near-IR (NIR) extinction and Herschel data; one of these filaments was TMC-1. There are three visual extinction peaks along the TMC-1 filament, the well-known positions TMC1-CP, TMC1-C2 and TMC1-NH3 (see Fig. 1).

Barnard 1, embedded in the western sector of the 30pc wide molecular cloud complex Perseus, is a close (230pc) and young, intermediate-mass star forming cloud. It is known to host class 0 protostars [11][12], providing a bridge between the low-mass star formation of Taurus, and the massive star forming regions such as the Orion molecular cloud. This core
hosts two candidates for a first hydrostatic core \cite{8}, B1b-N and B1b-S, proving its young star formation. We observed through a cut associated with the extinction peak in B1b (see white marks in Fig. \ref{fig:maps}), which is the most prominent core in B1.

3 IRAM 30m and Yebes 40m telescopes

This work is based on data from the GEMS IRAM 30m Large Program (Gas phase Elemental abundances in Molecular CloudS, PI: A. Fuente) and complementary observations carried out with the Yebes 40m telescope. Using the wide bandwidth of the IRAM 30m receivers, we can observe the most intense 3mm and 2mm lines of these species with only 4 receiver setups. As backends we used the Fast Fourier Transform spectrometers (FFTS) correlators, which provide a frequency resolution of $\sim 49$ kHz, enough to resolve the narrow lines expected in this dark cloud. The Yebes 40m telescope is equipped with HEMT receivers for the 2.2-50 GHz range, and a SIS receiver for the 85-116 GHz range. Single-dish observations in K-band (21-25 GHz) and Q-band (41-50 GHz) can be performed simultaneously. The intensity scale is $T_{MB}$ and calibration errors are $\sim 20\%$.

4 $\text{H}_2\text{S}$ abundances

The analysis of the $J = 1 \rightarrow 0$, $J = 2 \rightarrow 1$ and $J = 3 \rightarrow 2$ lines of CS and its isotopologues allows us to derive reliable values of line opacities and hydrogen densities towards the considered regions. We use Markov Chain Montecarlo sampling methods \cite{5} as described in \cite{7}, and the radiative transfer code RADEX \cite{23} to estimate the physical conditions of the gas.
the ortho-H$_2$S abundances we have used the code RADEX and the collisional coefficients for ortho-H$_2$O [4], assuming thermal ortho-para ratio for H$_2$ and scaled to ortho-H$_2$S. We hence fit the line intensities of the o-H$_2$S $J = 1_{1,0} \rightarrow 1_{0,1}$ line assuming the physical conditions derived from CS observations. The H$_2$S abundance is calculated assuming an ortho-to-para ratio of 3. Fig. 2 shows the H$_2$S abundances as a function of the visual extinction in TMC 1 and Barnard 1b. The H$_2$S gas-phase abundance reaches its maximum value, $X$(H$_2$S) $\sim 1 - 3 \times 10^{-8}$, at the edges of the clouds. For visual extinctions larger than $\sim 10$ mag, the abundance steeply decreases until values of $\sim$ a few $10^{-10}$ at $A_V \sim 20$ mag. For dust grain temperatures below the H$_2$S evaporation temperature, $\sim 50$ K [16], the H$_2$S molecules are expected to stick on grains in every collision and the depletion time scale is given by

$$X(H_2S) \propto t_{st} \equiv \frac{1}{n_{gr} \sigma_{gr} v_0} \propto \frac{1}{n\sqrt{T}}.$$  

(1)

Fig. 2 shows the derived H$_2$S abundances abundances as a function of the gas kinetic temperature and the parameter, $n\sqrt{T}$. Towards both sources, the H$_2$S abundance decreases as $\sim \frac{1}{n\sqrt{T}}$, which corresponds to the slope of -1 seen in Fig. 2, as expected when molecular freeze-out on grain surfaces is the main destruction mechanism. The scattering in the estimated values of the H$_2$S abundances is, however, large. Besides, the H$_2$S abundances estimated towards Barnard 1-b seems to be systematically higher than those towards TMC 1 by a factor of $\sim 3$.

5 Chemical model

One interesting issue is to compare the sulfur and oxygen chemistry. Similarly to H$_2$O, H$_2$S cannot be efficiently formed in gas phase in dark clouds. The observed abundances of H$_2$S should be the consequence of the desorption of H$_2$S molecules from the grain surfaces. The physical conditions in dark clouds greatly constrain the possible desorption mechanisms: thermal desorption is only feasible for grain temperatures greater than 50 K [16], and sputtering is important in fast shocks ($v_s > 5$ km s$^{-1}$), requiring our line profiles to be much wider. In a first approximation, we can consider that photodesorption by UV field and secondary photons are the main desorption agents. We have adapted the analytical model proposed for H$_2$O by
When the visual magnitude increases, the abundance relative to water found in comets is of the order of 2% [2], thus we take the saturation value as $f_{S,H_2S} = 0.02$. In the low visual magnitude and density regime, both gas-phase H$_2$S formation and destruction processes are proportional to $G_0$. As a consequence, the gas-phase H$_2$S abundance should reach an equal value, independently of $G_0$.

Equations (3) and (4) determine the H$_2$S abundance for given values of $A_v$ and $n$. Now, we discuss the general properties of the model before going into detail on the selected sources. When the visual magnitude increases, $f_{S,H_2S}$ in Eq. (4) increases as well, reaching a saturation value. The abundance relative to water found in comets is of the order of 2% [2], thus we take the saturation value as $f_{S,H_2S,max} = 0.02$. In the low visual magnitude and density regime, both gas-phase H$_2$S formation and destruction processes are proportional to $G_0$. As a consequence, the gas-phase H$_2$S abundance should reach an equal value, independently of $G_0$. 

Figure 3: Fits of the dust temperature vs $A_V$ for the three cuts in TMC 1 and the one in Barnard-1b, according to [14] parameterization. The best fit value of the incident UV field is $\chi_{UV} \sim 6.5$ for TMC 1 and $\chi_{UV} \sim 24$ for Barnard-1b, in units of the Draine field.
Once saturation occurs, $X(\text{H}_2\text{S})$ in Eq. 3 starts dropping due to the increasing density, and therefore depletion onto grains. In the shielded regime, the flux of secondary photons, $\Phi_{SP}$ and the gas density determine the $\text{H}_2\text{S}$ abundance. Values of $\Phi_{SP}$ between 750 and a few $10^4$ photon cm$^{-2}$ s$^{-1}$ have been reported in the literature [10][21]. We let $\Phi_{SP}$ to vary within this range.

6 Comparison with observations

In order to compare our model with the TMC 1 and Barnard 1b observations, the incident radiation field needs to be quantified. This is done using the parametric expression that relates dust temperature, visual magnitude, and Draine field reported by [14]. We obtain the best fit with incident UV field of $\chi_{UV} \sim 6.5$ for TMC 1 and $\chi_{UV} \sim 24$ for Barnard-1b, in units of the Draine field (see Fig. 3). We have introduced these numbers in equations (3) and (4) to fit the $\text{H}_2\text{S}$ abundances and obtain a reasonable fitting of the observed $\text{H}_2\text{S}$ abundances with $\Phi_{SP} = 2 \times 10^4$ photons cm$^{-2}$ s$^{-1}$ in TMC 1 and $\Phi_{SP} = 4 \times 10^4$ photons cm$^{-2}$ s$^{-1}$ in Barnard 1b (see Fig. 4). Within this scenario, the difference between the measured $\text{H}_2\text{S}$ abundance between TMC 1 and Barnard 1b is due to a different cosmic ray ionization rate. A more detailed and complete chemical modeling of the two targets is required to confirm this hypothesis. First of all, we need to take into account the 3D physical structure of the cores in order to derive a precise $\text{H}_2\text{S}$ abundance profile. Recent laboratory work suggests that chemical desorption might be important for $\text{H}_2\text{S}$ [19]. To introduce chemical desorption in the model would allow to explain the $\text{H}_2\text{S}$ abundance in the shielded cloud with a lower secondary photons flux. Our simple model considers adsorption and desorption processes but does not account for surface chemistry and thus neglects the influence that the grain temperature is expected to have in the $\text{H}_2\text{S}$ formation rate. Moreover, although fast shocks are not occurring in these dense clouds, [23] suggests that sputtering by grain-grain collisions could be efficient to desorb molecules at low velocities, hence increasing the $\text{H}_2\text{S}$ abundance.
7 Conclusions

Single-dish observations of two nearby dark clouds, TMC1 (140 pc) and Barnard 1 (235 pc) are used to investigate the chemistry of H$_2$S in starless cores. We have found that the H$_2$S abundance presents its maximum abundance at the cloud edge, X(H$_2$S) $\sim 1 - 3 \times 10^{-8}$ and decrease with density towards the visual extinction peaks. To explain this behavior we propose a simple chemical model which assumes that H$_2$S is formed on grain mantles, and released into gas via photodesorption. Even though this model is quite simple, we find a general agreement with the observations which supports that hydrogenation of S atoms on the grain surfaces is the main formation path for H$_2$S.

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