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Multi-line Diagnostics of the Interstellar Medium

Gas phase Elemental abundances in Molecular cloudS (GEMS)

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Abstract. Gas phase Elemental abundances in Molecular CloudS (GEMS) is an IRAM 30m Large Program aimed at determining the elemental abundances of carbon (C), oxygen (O), nitrogen (N), and sulphur (S) in a selected set of prototypical star forming filaments. Elemental abundances have a key role in the star formation process by driving the gas cooling rate and the gas ionization degree. Defining elemental abundance as the amount of a given atom in volatiles, the elemental abundances of C, O, and N in the interstellar medium are currently known within a factor of a few. However, the elemental abundance of S remains uncertain by several orders of magnitude, and its determination is one of the most challenging goals of this program. This is a review of the observational, theoretical, and modeling effort that GEMS team is doing to improve our knowledge of the sulphur chemistry. Our results suggest that the sulphur elemental abundance depends on the local physical conditions and the star formation activity in the environment.

1 Introduction

In recent years, space telescopes such as Spitzer and Herschel have revolutionized our view of star-forming regions. Now, we know that interstellar filaments are almost everywhere in the Milky Way and are the preferred site for star formation. Herschel FIR continuum maps probed the dust to visual extinctions of $A_V \sim 1$ mag, thus establishing the physical conditions of pre-stellar cores and those of the diffuse clouds out of which they are formed. These maps provide an unprecedented observational database allowing for the first time to have a good description of the different phases of collapsing molecular clouds. However, we need additional ingredients to complete our understanding of the star formation process, in particular we need to include chemistry. Gas chemistry regulates fundamental processes to form a star, such as the gas temperature and the coupling of the gas with the magnetic field. Molecular filaments can fragment to form pre-stellar cores to a large extent because molecules cool the gas, thus diminishing the thermal support relative to self-gravity. Gas chemistry is also regulating the abundance of electrons in the gas. The ionization fraction controls the coupling of magnetic fields with the gas, driving the dissipation of turbulence and angular momentum transfer, and therefore it plays a crucial role in the cloud collapse and the dynamics of accretion discs. The gas ionization fraction as well as the molecular abundances depend on the elemental depletion factors [2]. In particular, Carbon (C) is the main donor of electrons in the cloud surface ($A_v < 4$ mag) and, because of its lower ionization potential, Sulfur (S) might

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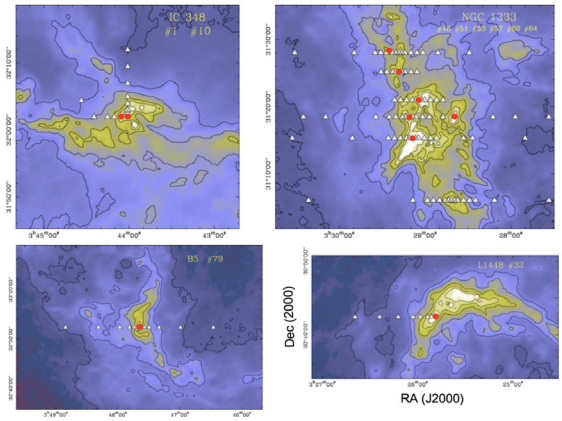

Table 1.- Molecular tracers

	A_V < 10 mag	A_V > 10 mag
X(e^-)	^{13}CO, HCO$^+$, H^{13}CO$^+$	C^{18}O, HC^{18}O$^+$, N_2H^+
n(H_2)	CS, C^{34}S	C^{34}S, ^{13}CS, SO
C/H	^{13}CO, HCN, CS	C^{18}O, H^{13}CN
O/H	^{13}CO, SO	C^{18}O, SO, ^{34}SO
N/H	HCN	H^{13}CN, N_2H^+
S/H	CS, C^{34}S, SO, HCS$^+$	C^{34}S, ^{13}CS, SO, ^{34}SO

Figure 1. Maps of the dust opacity at 850 μm towards IC 348, NGC 1333, B5, and L1448 [13]. Positions observed with the IRAM 30 m telescope are indicated with triangles. Red circles indicate the positions of the starless cores. Table 1 shows the species used as tracers of the physical and chemical conditions in the different cloud layers.

be the main donor in the ∼3.7−7 magnitudes range that encompasses a large fraction of the molecular cloud mass. Depletions of C and O determine the cooling gas rate since CO and CII are main coolants in molecular clouds. The determination of the elemental abundances at different depths into prototypical molecular clouds is the goal of the "Gas phase Elemental abundances in Molecular CloudS" (GEMS) IRAM 30m Large program.

2 Observational Database

GEMS methodology consists of deriving the elemental abundances and the gas ionization fraction by fitting the fractional abundances of a set of selected molecules using a state-of-the-art chemical model. These species were selected for being well-known tracers of the gas density and for being the most abundant compounds containing a given element that can be observed in the (sub-)mm range (see Table 1). The observations were carried out with the IRAM 30m telescope from July, 2017 to December 2019, and the details of the observational strategy were described by [6]. These observations are now public and can be downloaded from IRAM Data Archive.

The GEMS sample is composed of 29 starless cores located in Taurus, Perseus and Orion. In each cloud, we observed sets of typically ∼9-20 positions, separated by uniform steps of visual extinction, and aligned forming a cut intersecting the filament at the location of a visual extinction peak. Examples of these cuts in different regions of Perseus are shown in Fig. 1. This strategy allows us to probe the different layers of the cloud in the vicinity of the selected starless cores. The cuts were selected to avoid protostars and molecular outflows that could affect the chemical composition of the molecular cloud, hindering the study of molecular depletion. In total, we observed 12 cuts (99 positions) in Taurus, 14 cuts (153 positions) in Perseus, and 3 cuts (53 positions) in Orion.

Our sample includes cuts in regions with different physical conditions and star formation activity. The Taurus molecular cloud is considered as the prototype of isolated formation of low mass stars. In contrast to Taurus, the molecular clouds in Perseus are known to be forming star clusters. The group of cores in IC348 and NGC 1333 are close to the optical

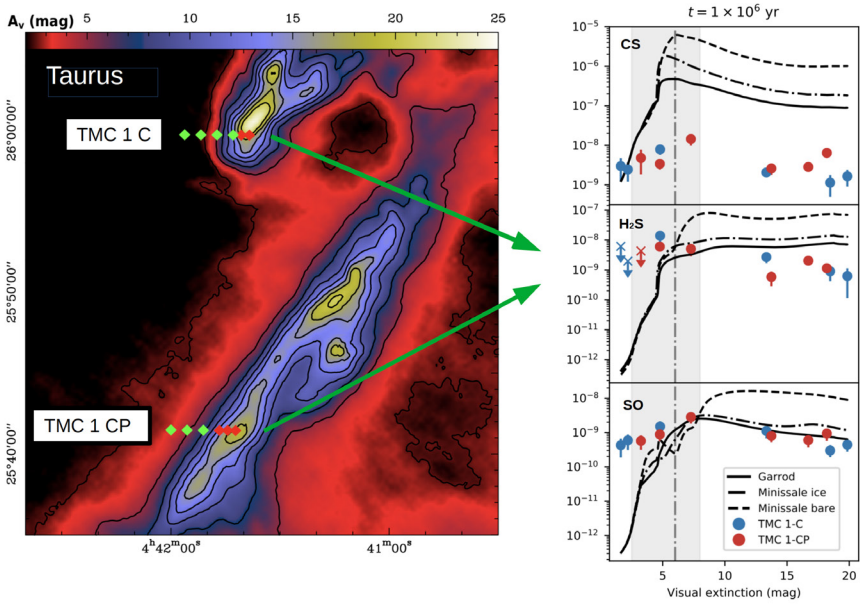

Figure 2. *left* Visual extinction map of the filament TMC 1. The positions observed are indicated with diamonds. The cuts labeled TMC 1 C and TMC 1 CP are modeled assuming that the associated cores are are well described with the physical structure of a Bonnor-Ebert sphere. Furthermore, we use the chemical model Nautilus [11] to predict the N(CS), N(H_2S), and N(SO) column densities at different impact parameters. In the *right* panel, the obtained values normalized with N_H are compared with model predictions with [S/H] = 1.5×10^{-5}. It should be noticed that while the results of H_2S and SO are well described by the model, the column density of CS is over-predicted by more than an order of magnitude (see [7]).

clusters and might be the future generation of clustered stars. However, Barnard 1 and L1448 are located in a more quiescent region. Orion is the closest massive star formation region and the only one in which this kind of study can be done with single-dish telescopes. A detailed description of the sample was reported by [10].

We were able to detect several lines of CS to derive molecular hydrogen densities, only in 244 positions out of the 305 positions observed. Using these densities, we calculated the chemical abundances of 14 species: ^{13}CO, C^{18}O, HCO$^+$, H^{13}CO$^+$, HC^{18}O$^+$, HCN, H^{13}CN, HNC, HCS$^+$, CS, SO, ^{34}SO, H_2S, and OCS [10]. These abundances constitute the GEMS molecular database that is used here to derive the sulphur elemental abundance. In addition to these species, a few complex compounds such as CH_3OH and H_2CS were detected towards the visual extinction peaks. The chemistry of CH_3OH and H_2CS has been studied by [12] and [3].

3 Testing chemical models: TMC1 and Barnard 1b

Chemical models are a key stone for deriving elemental abundances. In practice, we estimated the elemental abundances through chemical modeling of the 14 species included in the GEMS molecular database. Unfortunately, the sulphur chemistry was poorly known, which introduces large uncertainties in the estimate of the sulphur elemental abundance ([S/H]). For this reason, the GEMS team have carried out a large experimental and theoretical effort to

improve the sulphur chemical network. In particular we focused on the chemistry of SO, H_2S, and CS, which are ubiquitous species in the interstellar medium.

The reaction rates of the main formation and destruction paths for SO were estimated using *ab initio* calculations by [4] and [6]. It is well-known that H_2S is formed on the grain surfaces under the physical conditions prevailing in dark clouds. Then, the molecules detected in gas phase should have been ejected from the grain surfaces through thermal and non-thermal desorption processes. In the cold and dense gas, only non-thermal desorption processes are efficient. [5] estimated the photo-desorption yield of H_2S. Photo-desorption is an efficient desorption mechanism in the cloud border where UV photons are not attenuated. [7] investigated the efficiency of the reactive chemical desorption of H_2S as a function of the optical depth into the cloud. They concluded that the efficiency of chemical desorption decreases when the grains are covered with a thick ice mantle. [1] estimated the reaction rate of CS + O → CO + S that was proposed to be an important destruction mechanism of CS.

The updated sulphur chemical network was used by [7] to fit the observations of CS, SO, and H_2S, in TMC1 and Barnard 1b. They concluded that it was not possible to accurately fit the three molecules using the same value of [S/H]. While the abundances of H_2S were better fitted assuming the solar value ([S/H]=1.5×10^{-5}), the abundance of CS could only be fitted assuming a sulphur depletion of >10 [1, 8]. This problem remains even including the new CS + O → CO + S reaction rate as calculated by [1].

4 Sulphur elemental abundance

Our goal is to determine the sulphur elemental abundance, i.e., the amount of sulphur atoms in volatiles ([S/H]). Our large molecular database allows us to carry out a statistic study to explore possible trends of [S/H] with the local physical parameters (n, T_g) and environment ($\zeta(H_2)$, χ_{UV}). We predicted the chemical abundance using Nautilus 1.1 [11], which is a three-phase model that takes into account gas, ice surface, and ice mantle chemistries. The chemical network updated by [7] was adopted for these calculations. We run the three grids of models shown in Table 2 in order to fit the abundances of CO, HCO^+, HCN, HNC, CS, HCS^+, H_2S, SO, OCS towards the 244 positions of the molecular database. In order to avoid degeneracies, we imposed some restrictions to the values of A_V, n(H_2) and T_g: i) the visual extinction is assumed to be in the range $A_V \times 0.5$ and $A_V \times 0.5 + 2$, where A_V is the value obtained from Herschel data, and the factor 0.5 accounts for the fact the the cloud is expected to be illuminated from the back and the front; ii) the density is assumed to be in the range $0.5\times$n(H_2) and $5 \times$ n(H_2) where n(H_2) is the value derived from the fitting of CS lines [10]; and iii) the gas kinetic temperature is allowed to vary between T_d and T_d+ 5 K, where T_d is the dust temperature obtained from Herschel data. During the fitting process, [S/H], $\zeta(H_2)$ and *Age* are allowed to vary among the values: *Age* = 0.1,1,10 Myr, [S/H] = 8×10^{-8}, 1.5×10^{-6}, 1.5×10^{-5}, $\zeta(H_2)$ = (1, 5, 10, 50) $\times$ 10^{-17} s^{-1}. In order to find the *best-fit* model, we minimize the parameter D_{iff} that is defined by,

$$D_{iff} = 1/n_{obs} \times \Sigma_i [log_{10}(X^i_{mod}) - log_{10}(X^i_{obs})]^2 \quad (1)$$

where n_{obs} is the number of species detected at each position, X^i_{mod} is the predicted abundance for the species i, and (X^i_{obs}) is the abundance of the species i derived from GEMS observations. The results are used to construct the histograms shown in Fig. 3. We detect clear differences between the studied molecular cloud complexes. The majority of the positions in Taurus and Perseus are best fitted with *Age*=0.1 Myr, while the majority of the positions in Orion are fitted with *Age* > 1 Myr. Regarding [S/H] which is the most interesting parameter for us, most of the positions in Taurus and Perseus are fitted with [S/H] =

Table 2. Chemical models parameters.

Taurus	
n_H	3.16×10^3 cm^{-3} to 3.16×10^6 cm^{-3} in steps of $\times$ 3.16
A_V	1.5 mag to 11.5 mag in steps of 2 mag
T_g	10 K to 45 K in steps of 5 K
CRIR	(1.0, 5.0, 10, 50) x 10^{-17} s^{-1}
χ_{UV} (Draine)	5.0
$[S/H]$	(1.5, 0.15, 0.008) $\times10^{-5}$
Perseus	
n_H	3.16×10^3 cm^{-3} to 3.16×10^6 cm^{-3} in steps of $\times$ 3.16
A_V	1.5 mag to 13.5 mag in steps of 2 mag
T_g	10 K to 45 K in steps of 5 K
CRIR	(1.0, 5.0, 10, 50) x 10^{-17} s^{-1}
χ_{UV} (Draine)	25.0
$[S/H]$	(1.5, 0.15, 0.008) $\times10^{-5}$
Orion	
n_H	3.16×10^3 cm^{-3} to 3.16×10^6 cm^{-3} in steps of $\times$ 3.16
A_V	1.5 mag to 11.5 mag in steps of 2 mag ,15.5 mag, 20 mag
T_g	10 K to 45 K in steps of 5 K
CRIR	(1.0, 5.0, 10, 50) x 10^{-17} s^{-1}
χ_{UV} (Draine)	50
$[S/H]$	(1.5, 0.15, 0.008) $\times10^{-5}$

1.5×10^{-6}. On the contrary, a large fraction of the positions in Orion are better fitted with [S/H]= 1.5×10^{-5}. This suggests that environment changes the sulphur elemental abundance, the harsh environment of Orion giving rise to the lowest sulphur depletion. It is also interesting to explore possible trends with visual extinction and density. There is no clear trend with visual extinction in our cuts. However, sulphur depletion seems to depend on density. The positions with lower densities are more likely associated with [S/H] = 1.5×10^{-6}, while the positions with higher densities are usually associated with [S/H] = 8×10^{-8}. In addition to the environment, the value of [S/H] depends on the local density, with sulphur depletion increasing with density. A word of caution should be put in this latter conclusion. Since only 53 out of the 244 positions belong to Orion, these histograms are dominated by the positions in Taurus and Perseus, and the extrapolation of this conclusion to Orion is risky. Additional observations are needed to have a statistically significant number of positions in Orion.

5 Summary

We present the molecular database and first results of the GEMS project. This program is focused on the observation of 29 starless cores located in proto-typical filaments of the nearby star-forming regions Taurus, Perseus, and Orion. These regions have different degrees of star formation activity, and therefore different physical conditions, providing a possibility to explore the effect of the environment on gas chemistry. The project includes observations towards 305 positions distributed in 29 cuts that have been selected to avoid recently formed stars and their associated bipolar outflows. The gas chemistry in these positions is therefore not affected by the shocks produced by these energetic phenomena and/or the UV radiation coming from internal sources. We have used chemical modeling with an updated sulphur network to determine the sulphur elemental abundance in the three studied regions. Our results suggest that environment is determining the sulphur elemental abundance, with the

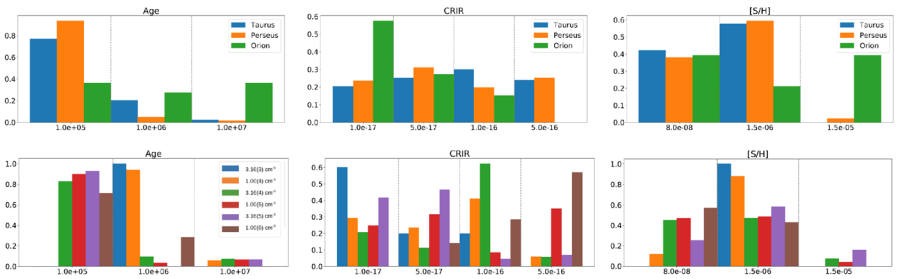

Figure 3. The panels show the statistics of the results of our fitting to the GEMS molecular database. The points are segregated in bins according with their localization (Taurus, Perseus, or Orion molecular cloud complexes) in the upper row, and in bins of density in the bottom row.

sulphur depletions decreasing in regions with higher star formation activity. In Taurus and Perseus, there is a trend with density that suggests that sulphur depletion increases towards the densest regions of the cloud. We would like to comment that the large number of positions observed in GEMS provides an unprecedented opportunity to investigate the chemistry of dark clouds.

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