

Sulfur chemistry in early star-forming cores: a non-LTE analysis of SO₂ and SO

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ABSTRACT

The chemical behavior of sulfur in the interstellar medium (ISM), particularly in the dense regions where stars form, is still far from being well understood. Questions such as which is the main sulfur reservoir in the ISM remain unanswered. Studying interstellar sulfur-bearing molecules contributes to understanding the chemical behavior of this element in the ISM. Star-forming regions in their most early phases, when complex interstellar chemistry begins to activate, are favorable sites to carry out this type of research. We present results which are complementary to recent, extensive work which made use of data from the Atacama Large Millimeter Array. We focus on the emission of SO₂ and SO obtained towards 37 dense molecular cores embedded in cold clumps. Through an analysis of non-local thermodynamic equilibrium (non-LTE), the abundances of these molecular species were estimated. In general a good agreement was obtained with the LTE results previously presented.

Keywords: ISM: molecules – ISM: abundances — ISM: clouds — Stars: formation

INTRODUCTION

Our understanding of the sulfur behavior in interstellar environments is still incomplete. One of the main problems is that it is seen to be more highly depleted in dense regions compared to diffuse ones (Laas & Caselli 2019; Rivière-Marichalar et al. 2019). If the abundance of sulfur in the gas-phase is measured through the emission of molecular lines in such dense regions, a few percent of the cosmic value will be obtained (Woods et al. 2015; Fontani et al. 2023). Hence, the question is where is the missed sulfur. Despite the big efforts done to ask this question, the primary carrier of sulfur is still unknown in both gas and solid-phase (Artur de la Villarmois et al. 2023).

Recently, in Martinez et al. (2024) we presented an extensive study of the ³⁴SO, SO₂, NS, SO, SO⁺, and H₂CS in a sample of 37 cores at early star-forming stages. This study was based on the analysis of these molecular species under local thermodynamic equilibrium (LTE) assumptions. Based on our results we proposed that the chemistry involved in the formation of each of the mentioned sulfur-bearing species may similarly depend on the temperature in the range 20-100 K. This temperature dependence supports the hypothesis suggesting that sulfur may be frozen in the dust grains in dense and cold interstellar regions as proposed in previous works (e.g. Laas & Caselli 2019), and hence, as the temperature rises, the abundance of sulfur-containing molecules also increases.

The abundance ratio X(SO)/X(SO₂) is of particular interest as it was proposed as a chemical clock, useful in determining the evolutionary stage of a molecular core (Wakelam et al. 2004, 2011). In our previous study (Martinez et al. 2024) we found some results supporting that, however, given that it was done under the LTE assumptions, and due to its importance, we decided to carry on a non-LTE study of the behavior of these molecules in the same sample of cores. Non-LTE models are generally necessary to obtain more accurate results and a deep understanding of molecules in the ISM.

DATA, SOURCE SAMPLE, AND PROCEDURE

* Colaborator in the citizen science project Ciencia Popular developed by S.P. and M.O. at IAFE

Using the same data set as in [Martinez et al. \(2024\)](#), we focus on the SO₂ $v=0$ 8(2,6)–7(1,7) and SO $v=0$ $^3\Sigma$ 9(8)–8(7) lines at 334.673 and 346.528 GHz. The Atacama Large Millimeter Array (ALMA) project from which data were retrieved (2017.1.00914; PI: Csengeri) consists of observations towards 37 massive infrared quiet clumps in the inner Galaxy from the APEX Telescope Large Area Survey of the Galaxy (ATLASGAL).

The cores embedded in each ATLASGAL source were identified from the continuum emission at 0.87 mm, and molecular spectra were extracted from a beam area at the peaks (for details see our previous work; [Martinez et al. 2024](#)).

RADEX code ([van der Tak et al. 2007](#)) was used to obtain the SO and SO₂ column densities ($N(\text{SO})$ and $N(\text{SO}_2)$). The used inputs are: the line peak intensity (T_p), the FWHM line width (Δv), the kinetic temperatures (T_K), and the volume density of the regions ($n(\text{H}_2)$). T_p and Δv were obtained from Gaussian fits to each line, T_K was derived from rotational diagrams of the CH₃OH 7(1,7)–6(1,6)++ and 12(1,11)–12(0,12)+ lines at 335.582 and 336.865 GHz. Details regarding these parameters can be found in our previous study and in Zenodo¹. Given the kind of the analyzed sources, we assume a typical density $n(\text{H}_2)$ of 10^6 cm^{-3} uniformly for all the cores.

RESULTS

From RADEX we obtained SO and SO₂ column densities ($N(\text{SO})$ and $N(\text{SO}_2)$) for each core. Then, using the molecular hydrogen column density ($N(\text{H}_2)$) obtained in [Martinez et al. \(2024\)](#), the molecular abundances ($X = N(\text{molecule})/N(\text{H}_2)$) was derived.

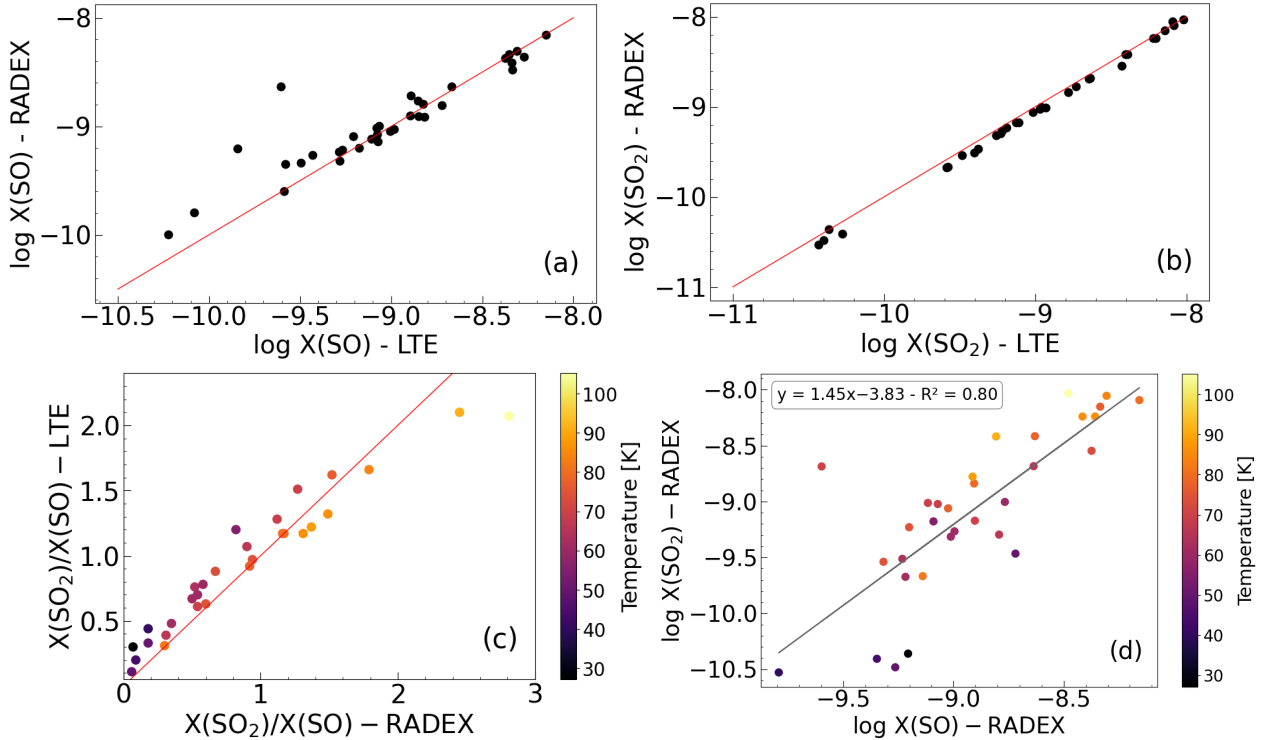


Figure 1. Comparisons of the SO and SO₂ abundances obtained from RADEX and LTE (Panels a and b). Comparison between the abundance ratios obtained from both methods (Panel c). Red lines represent the $y = x$ locus. Panel d shows $X(\text{SO})$ vs $X(\text{SO}_2)$ obtained from RADEX with a linear interpolation. In the last two panels the point colors correspond to the kinetic temperature measured in the cores, and the scale is presented in the bar at the right.

Figure 1 (Panels a and b) shows the comparisons between the SO and SO₂ abundances obtained from RADEX (this work) and by assuming LTE (from [Martinez et al. 2024](#)). Panel c displays the same but comparing the abundance

¹ <https://doi.org/10.5281/zenodo.14036845>

ratios adding a color code representing the core temperatures. Finally, Panel d shows the relation between both abundances obtained from RADEX with the same color code.

DISCUSSION

Panels a and b in Fig. 1 show that the obtained SO and SO₂ abundances from non-LTE and LTE methods are quite similar. Such a similarity is closer in X(SO₂). In the case of X(SO) there are some outlier points indicating that the corresponding abundances derived from RADEX are larger than those obtained by assuming LTE. It will be interesting to identify the corresponding sources and analyze possible reasons of this issue.

The comparison between the abundance ratios (Panel c in Fig. 1) derived from both methods, in general, shows that the LTE assumption yields X(SO₂)/X(SO) ratios larger than those derived from RADEX, and interestingly, it seems to occur mostly in colder cores.

Finally it is important to remark that the relation X(SO₂) vs. X(SO) obtained from RADEX (see linear interpolation in Panel d) is similar to that obtained from LTE (see [Martinez et al. 2024](#)). While these results present some more dispersion than in the LTE case, it is also observed a clear increase in the abundances correlating with the increasing gas temperature, supporting that these sulfur-bearing species may be used as chemical clocks.

CONCLUDING REMARK

We conclude that the LTE and non-LTE analysis of the SO₂ $v=0$ 8(2,6)–7(1,7) and SO $v=0$ ³Σ 9(8)–8(7) lines produce similar results in early star-forming cores with temperatures between 20 and 100 K. This is an important point to take into account in future sulfur-bearing molecules studies.

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