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Recent updates of gas-phase chemical reactions and molecular lines of SiS in CLOUDY

Gargi Shaw [1], Gary Ferland [2] and M. Chatzikos [2]

[1] *Department of Astronomy and Astrophysics*
Tata Institute of Fundamental Research
Mumbai 400005, India
[2] *Department of Physics and Astronomy*
University of Kentucky
Lexington, KY 40506, USA

ABSTRACT

Here we present our current update of CLOUDY on gas-phase chemical reactions for the formation and destruction of the SiS molecule, its energy levels, and collisional rate coefficients with H_2, H, and He over a wide range of temperatures. As a result, henceforth the spectral synthesis code CLOUDY predicts SiS line intensities and column densities for various astrophysical environments.

Keywords: ISM: molecules, ISM: abundances

INTRODUCTION

The spectroscopic simulation code CLOUDY simulates physical conditions in NLTE astrophysical plasma over a wide range of physical parameters (temperature, density, radiation field etc.) using *ab initio* microphysics, and predicts the resulting column density and spectra over the entire electromagnetic range. Details about CLOUDY can be found in Ferland et al. (2013, 2017); Gay et al. (2012); Shaw et al. (2005, 2017, 2020, 2022)[1].

Silicon sulfide (SiS) has been observed in massive star formation regions (Ziurys 1988) and circumstellar envelopes around evolved stars (Bieging & Tafalla 1993). Its rich rotational spectrum can be observed using ALMA. Motivated by this, we recently updated the spectral synthesis code CLOUDY to predict the column density and rotational line intensities of SiS in various astrophysical environments. This work is basically an extension of our previous work (Shaw et al. 2022) which aimed to predict more molecular lines with better accuracy.

With our git repository management, GitLab hosting infrastructure and continuous autonomous testing, we aim to move the Cloudy project to a more rapid release schedule, something like the Ubuntu project. As part of this development cycle, we aim to announce improved physics in various publications. The advance in the chemistry described here gives Cloudy greater power to interpret molecular line observations.

CALCULATIONS AND RESULTS

All numerical calculations presented here are performed using the development version of the spectral simulation code CLOUDY, last described by Ferland et al. (2017); Shaw et al. (2022).

The density and line intensity of SiS lines depend on the chemical reaction rates and the internal structure, together with Einstein's radiation coefficients and collisional rate coefficients. We include energy levels, Einstein's radiation coefficients and collisional rate coefficients with H_2 for the SiS using LAMDA database (Schöier et al. 2005). It includes energy levels up to J=40. There are 40 radiative and 820 collisional transitions covering a temperature range of 10 to 2000 K. Anusuri (2019) quantum dynamically calculated rotational excitations of SiS with H. It also includes 11 transitions over the temperature range of 5 to 300 K. However, CLOUDY uses collisional data in the LAMDA format, which uses deexcitation rate coefficients. Hence, we calculate the deexcitation rate coefficients from the excitation rate

Corresponding author: Gargi Shaw
gargishaw@gmail.com

[1] https://nublado.org

coefficients following the formula, $\Gamma_{ul} = \Gamma_{lu} \times (g_l/g_u) \times \exp(h\nu/kT)$. For the given temperature range, H-collisional rate coefficients are larger than the H_2-collisional rate coefficients. However, collisions with H_2 are more important than the collisions with H because of its larger abundance where SiS is present. Further, we include collisional rate coefficients with He following Vincent et al. (2007); Toboła et al. (2008) for the lowest four rotational levels for a temperature range of 40-1400 K. This range of temperature is set by the calculations of Vincent et al. (2007); Toboła et al. (2008).

We include 32 formation and 10 destruction reactions for SiS from the UMIST Database for Astrochemistry, UDfA (RATE12; Millar et al. 1997; McElroy et al. 2013). In addition, we include four more reactions, SiH + S → SiS + H, SiH + S_2 → SiS + SH, Si + SO_2 → SiO + SO, and Si + SO_2 → SiS + O_2 from Zanchet et al. (2018). All four of these reactions have a constant rate coefficient, $1{\times}10^{-10}$ cm^3s^{-1}. Reactions, Si + HS→ SiS + H, S + SiN → SiS + N, S + SiH_2 → SiS+ H + H, S + HCSi → SiS + CH, Si + S_2 → SiS + S are taken from Willacy & Cherchneff (1998). Whereas, Si + H_2S → SiS + H_2 , H_2 + SiS^+ → $HSiS^+$ + H, and S+ SiH_2^+ → $HSiS^+$ + H are taken from Doddipatla et al. (2021) and the Kinetic Database for Astrochemistry, respectively[2]. We found that among these reactions, Si + HS → SiS + H plays a very significant role in the formation of SiS.

As a test, we first model a generic H II region and a PDR calculation to study the abundances of SiS for similar environments. Our model is described by Shaw et al. (2022), and the input script of this model, "h2_orion_hii_pdr.in", is publicly available with the CLOUDY download under the directory `tsuite`. In a nutshell, the H II region starts at a distance of $10^{17.45}$ cm away from the ionizing star and extends into the PDR and dense molecular region up to A_V = 1000 mag. The hydrogen density at the ionized face is 10^4 cm^{-3} with the gas-phase abundances similar to the average gas-phase abundances in the Orion Nebula. Panel 1 of Figure 1 shows the variation of density of SiS, S, Si, S^+, and Si^+ across the cloud as a function of Av. The red, blue, and black solid lines represent the abundances of SiS, Si, and S. Similarly, blue and black dashed lines represent the abundances of Si^+ and S^+. Panel 2 of Figure 1 shows the temperature across the same cloud. Panel 3 shows the predicted intensities of various rotational lines of SiS that can be observed by ALMA. It is clear from the plot that SiS forms deep in the cloud (Av > 10) where the temperature is lower (25 to 35 K). Our model predicted column density of SiS is $10^{15.76}$ cm^{-2}. These advances will be part of the 2023 release of CLOUDY.

In future, we will include higher vibrational energy levels and rovibrational transitions of SiS to CLOUDY to make it applicable to JWST observations.

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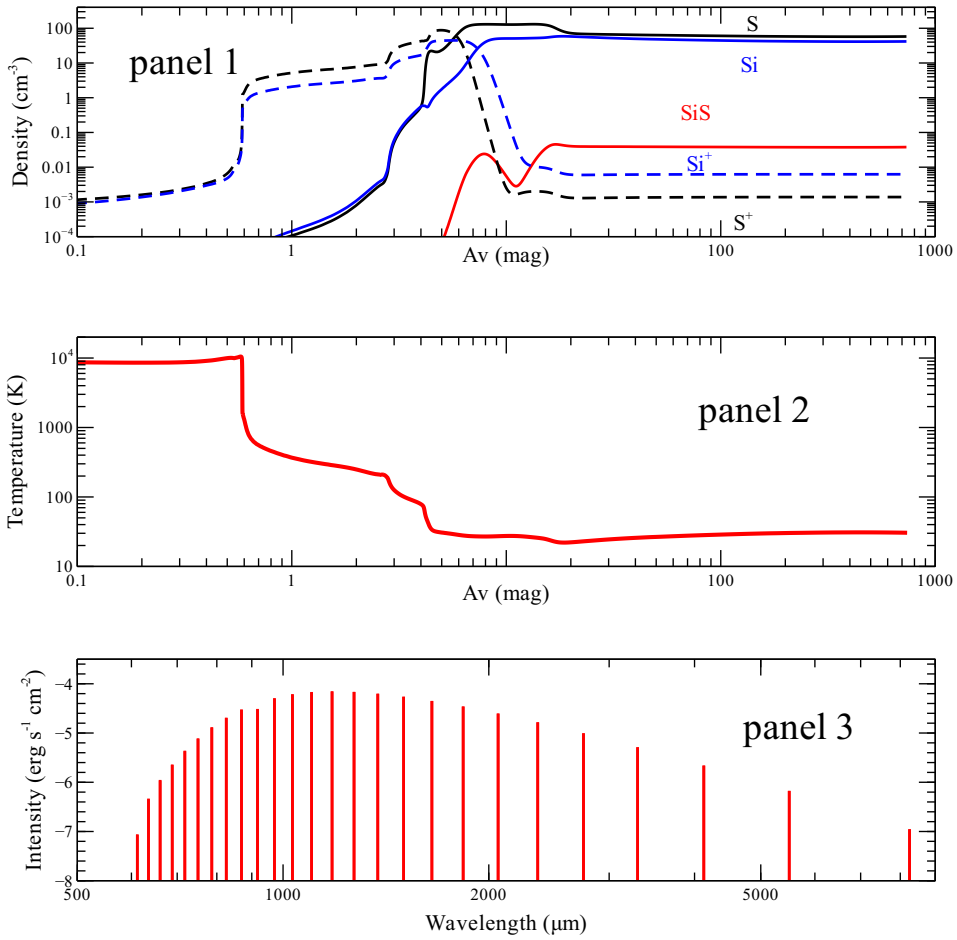

Figure 1. Panel 1: Variation of SiS density as a function of A_V for an H II and PDR model ("h2_orion_hii_pdr.in" from the CLOUDY download under the directory `tsuite`.) Panel 2: Variation of temperature across the cloud. Panel 3: Model predicted intensities of various SiS rotational lines.

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