Investigating Sulfur Chemistry in the HD163296 Disk (Postprint)

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Abstract

Sulfur chemistry in the formation process of low-mass stars and planets remains poorly understood. The protoplanetary disks are the birthplace of planets and its distinctive environment provides an intriguing platform for investigating models of sulfur chemistry. We analyzed the Atacama Large Millimeter/submillimeter Array observations of CS 7–6 transitions in the HD 163296 disk and performed astrochemical modeling to explore its sulfur chemistry. We simulated the distribution of sulfur-containing molecules and compared it with observationally deduced fractional column densities. We have found that the simulated column density of CS is consistent with the observationally deduced fractional column densities, while the simulated column density of C2S is lower than the observationally deduced upper limits on column densities. This results indicate that we have a good understanding of the chemical properties of CS and C2S in the disk. We also investigated the influence of the C/O ratio on sulfur-containing molecules and found that the column densities of SO, SO2, and H2S near the central star are dependent on the C/O ratio. Additionally, we found that the N[CS]/N[SO] ratio can serve as a promising indicator of the disk's C/O ratio in HD 163296. Overall, the disk of HD 163296 provides a favorable environment for the detection of sulfur-containing molecules.

Full Text

Investigating Sulfur Chemistry in the HD163296 Disk

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Abstract

Sulfur chemistry in the formation process of low-mass stars and planets remains poorly understood. Protoplanetary disks, as the birthplaces of planets, provide a distinctive environment for investigating sulfur chemistry models. We analyzed Atacama Large Millimeter/submillimeter Array (ALMA) observations of CS 7–6 transitions in the HD 163296 disk and performed astrochemical modeling to explore its sulfur chemistry. We simulated the distribution of sulfur-containing molecules and compared them with observationally deduced fractional column densities. We found that the simulated column density of CS is consistent with the observationally deduced fractional column densities, while the simulated column density of C_2S is lower than the observationally deduced upper limits. These results indicate that we have a good understanding of the chemical properties of CS and C_2S in the disk. We also investigated the influence of the C/O ratio on sulfur-containing molecules and found that the column densities of SO, SO_2, and H_2S near the central star are dependent on the C/O ratio. Additionally, we found that the N[CS]/N[SO] ratio can serve as a promising indicator of the disk's C/O ratio in HD 163296. Overall, the disk of HD 163296 provides a favorable environment for the detection of sulfur-containing molecules.

Key words: Protoplanetary Disks – Astrochemistry – Molecular Processes

1. Introduction

A protoplanetary disk (PPD) is a crucial intermediate stage in the evolution from an interstellar molecular cloud to a planetary system \cite{Le_{{{Gal}}*{{2021}}}}. PPDs serve both as conduits that inherit interstellar and protostellar organic chemistry and deliver it to planets and planetesimals, and as active producers of new organic molecules using the disk's inorganic and organic carbon reservoirs \cite{Oberg*{2023}}. Along with the well-studied carbon, nitrogen, and oxygen chemistry, sulfur-containing molecules have also been observed in PPDs (e.g., \cite{Guilloteau_{2013}, Cleeves_{2015}, Bergner_{2018}, Bergner_{2019}, Czekala_{2021}}). Sulfur is one of the most abundant elements in the interstellar medium and protoplanetary disks \cite{Asplund_{2009}} and plays crucial roles in prebiotic chemistry \cite{Chen_{2015}} and planetary habitability \cite{Ranjan_{2018}}. However, sulfur chemistry remains poorly understood in the formation processes of low-mass stars and planets.

Protoplanetary disks present an interesting experimental ground for investigating sulfur chemistry models because each disk exhibits a wide range of unique environments. The study of S-containing species has proven invaluable in reconstructing the chemical history and kinetics of the studied objects \cite{Keyte_{2023}}. So far, the main sulfur reservoirs have not yet been determined, and there remains substantial theoretical work to identify the chemical pathways that produce the observed distribution of sulfur species \cite{Le_{{{Gal}}_{{2019}}}}.

To date, six sulfur-containing molecules have been detected in protoplanetary disks \cite{Le_{{{Gal}}*{{2021}}}}: CS, H_2CS, H_2S, C_2S, SO, and SO_2, with CS being the most easily detected \cite{Dutrey*{1997}, Dutrey_{2011}, Teague_{2018}, Le_{{{Gal}}*{{2019}}}, Le*{{{Gal}}*{{2021}}}}. Hydrogen sulfide (H_2S) has long been considered a significant sulfur reservoir but was only recently detected in disks \cite{Phuong*{2018}}. The H_2S/CS gas-phase column density ratio is typically around 1/20 \cite{Phuong_{2018}}. In the MWC 480 disk, H_2CS was detected with a column density ratio N[H_2CS]/N[CS] = 2/3, suggesting that a substantial portion of the sulfur reservoir in disks exists in organic form \cite{Le_{{{Gal}}*{{2021}}}}. The oxygen-sulfur compounds detected in disks are SO and SO_2, which have only been detected in very few sources \cite{Booth*{2021}, Le_{{{Gal}}*{{2021}}}, Booth*{2023}}. Current observations and theoretical studies of disks indicate that the gas-phase C/O ratio may vary with radial position in the disk, and CS/SO serves as a probe to determine the elemental carbon-to-oxygen ratio \cite{Le_{{{Gal}}*{{2021}}}, Keyte*{2023}}.

The HD 163296 (MWC 275) system provides an ideal experimental platform to investigate chemical processes within a protoplanetary disk. It is a solitary Herbig Ae pre-main sequence (PMS) star with a spectral type of A1 and an age of approximately 6 million years \cite{Fairlamb_{2015}}. The star is encircled by a vast and luminous protoplanetary disk with an inclination of 46.7° and a position angle of 133° \cite{Huang_{2018a}}. Only CS 2–1 has been previously observed in HD 163296 \cite{Le_{{{Gal}}*{{2021}}}}. The observations by \cite{Le*{{{Gal}}_{{2021}}}} also covered transitions of C_2S and SO in HD 163296, but only upper limits were obtained.

In this paper, we present the detection of CS 7–6 toward HD 163296 using ALMA data and illustrate our astrochemical modeling of HD 163296 to study the formation and distribution of sulfur-containing species. We discuss the CS 7–6 line detection toward HD 163296 in Section 2. In Section 3, we showcase grids of disk chemistry models tailored to the HD 163296 disk and present the modeling results in Section 4. A detailed discussion is provided in Section 5, followed by a summary of our conclusions in Section 6.

2.1. Observational Details

The molecular line CS 7–6 data were extracted from the ALMA archive (project code 2016.1.01086.S; PI: Isella). The total on-source integration time was 28 minutes. Forty-two antennas were used during the observations, with baseline lengths ranging from 21.0 m to 3.6 km. For calibration, J1733-1304 was used as the flux calibrator, J1751-1950 as the phase calibrator, and J1924-2914 as the bandpass calibrator.

The data were calibrated using ALMA-supplied pipeline scripts and then imaged using the Common Astronomy Software Application package (CASA, version 4.7.2, \cite{McMullin_{2007}}). The continuum was subtracted in the UV data. The line-only UV data were cleaned using tclean with the multiscale algorithm (deconvolver="multiscale") and a Briggs robustness parameter of 0.5, resulting in a spatial resolution of 0.066 .

During imaging, a Keplerian mask[1] was used. The Keplerian mask was built based on the HD 163296 disk and star parameters from \cite{Czekala_{2021}}. For the spectral window containing CS 7–6, the bandwidth is 1.875 GHz, resulting in 976 channels with a channel width of 562 kHz, corresponding to a velocity width of 0.85 km s^{-1} at 342.883 GHz. The noise level of the line cube is 1.9 mJy $beam^{-1}$ per channel. The maximum recoverable scale of the observations is 0.953 .

[1] https://github.com/richteague/keplerian_{mask}

2.2. Observational Results

Figure 1 [Figure 1: see original paper] displays the integrated intensity (zeroth-moment) maps of the spatially resolved observations of the CS 7–6 rotational transition toward HD 163296. To construct these maps, we used the Python package bettermoments \cite{Teague_{Foreman}-Mackey_{2018}} with a hybrid mask combining a Keplerian mask and a 1σ clip to mask any pixels below this threshold. Figure 1 also shows the radial profile of the shifted and stacked spectra using the radial profile function in GoFish \cite{Teague_{2019}}. The disk physical parameters (i.e., disk inclination, disk position angle, mass of the central star, and distance) used are listed in Table 1 .

Based on the radial intensity profiles of CS 7–6 emission in HD 163296, we discovered the presence of a central hole, similar to the CS 2–1 emission reported by \cite{Le_{{{Gal}}{{2021}}}}. Following the method proposed by \cite{Huang{2018b}}, we modeled the radial profile of CS 7–6 as a sum of one or more Gaussian components using the Levenberg–Marquardt minimization implementation in LMFIT \cite{Newville_{2023}}. We found that CS 7–6 emission has two bright rings with centers ranging from 26 to 49 au, with a gap visible at 41 au. By comparing the radial intensity distributions of the CS 2–1 emission and the CS 7–6 emission (see Figure 2 [Figure 2: see original paper]), we observe that the location of one of the CS 7–6 rings (B49) is very close to the location of the CS 2–1 ring (B53, as described in \cite{Law_{2021a}}). However, the CS 7–6 emission shows a protruding ring within the central hole region of the CS 2–1 emission. Additionally, we can observe different morphology in the CS 7–6 radial intensity profile compared to the 1.25 mm dust continuum profile.

The CS 7–6 spectra are also depicted in Figure 1 for the HD 163296 disk, showing a typical double-peaked profile indicative of Keplerian rotation. The detection is made at a 24σ confidence level, with a peak flux of 104 mJy $beam^{-1}$ and an rms of 4.3 mJy beam^{-1} km s^{-1}, as measured from the emission-free regions of the integrated intensity map. The disk-integrated flux densities, S Δv, derived from this work and spectral line information for CS 7–6 are listed in Table 2 .

3.1. Chemical Models

In this study, we use the Nautilus three-phase model \cite{Wakelam_{2016}}, which includes the gas phase, dust surface (the top two layers of ice mantles), and inner ice mantles. The chemical network used in our study is derived from \cite{Vidal_{2017}}, which improves the understanding and representation of the sulfur chemical network. The chemical network contains 962 species and 10,913 reactions, including 7,040 gas-phase reactions and 3,873 surface reactions. The network includes various processes such as cosmic-ray desorption, photodissociation, photoionization, and adsorption/desorption between gas-phase and ice mantle species. We also utilized a constant universal photodesorption yield for all molecules.

To understand the chemistry of the disk during planetary formation, we started from the molecular cloud stage and ran dense cloud chemistry models for 1 million years. The physical conditions we considered included a grain and gas temperature of 10 K, a gas density of n_H = 2×10^4 cm^{-3}, a visual extinction of 15 mag, and a cosmic-ray ionization rate of 1.3×10^{-17} s^{-1}. The initial abundances are listed in Table 3 . The composition of the molecular cloud at the end of this stage was taken as the initial condition for the disk.

3.2. Disk Physical Models

We assume that the disk model is axisymmetric and includes gas, small dust, and large dust components. There is spatial coupling between the gas and small dust populations. The mass surface distribution of gas and small dust follows a self-similar viscous disk model, as described by \cite{Lynden-Bell_{{{Pringle}}*{{1974}}}} and \cite{Andrews*{2011}}. The disk structure is fully parameterized, with a surface density that follows the standard form of a power law with an exponential taper:

Σ = Σ_c (R/R_c)^γ exp[-(R/R_c)^(2-γ)]

where R_c is the characteristic scaling radius, Σ_c is the surface density at the characteristic radius, and γ is the gas surface density exponent. The vertical density structure is assumed to be a Gaussian function characterized by a scale height H(R) that is a power-law function of radius:

H(R) = H_{100} (R/100 au)^

The scale height is then given by H_{100} where f_i is the mass fraction of each mass component, H_{100} is the scale height at 100 au, and is a parameter that characterizes the radial dependence of the scale height. Here we fix =

1 for the gas and the small-grain population and = 0.2 for the large grain population \cite{Andrews_{2011}}.

Both dust populations follow a Mathis-Rumpl-Nordsieck grain distribution n(a) $a^{-3 \cdot 5}$ \cite{Mathis_{1977}}. The description of the dust grain population used in this study is adopted from \cite{Zhang_{2021}}. For a given dust density structure, we calculate the dust temperature structure using the Monte Carlo radiative transfer code RADMC3D \cite{Dullemond_{2012}}.

For the gas temperature, we used a two-layer model similar to the one proposed by \cite{Dartois_{2003}}, but later modified by \cite{Law_{2021b}} with different connection terms. Assuming that the midplane temperature T_{mid} and atmospheric temperature T_{atm} have power-law distributions with slopes q_{mid} and q_{atm}, respectively:

T_{mid} = T_{mid},100 (R/100 au)^q_{mid} T_{atm} = T_{atm},100 (R/100 au)^q_{atm}

Between the midplane and atmosphere, the temperature is smoothly connected using a hyperbolic tangent function:

T(r,z) = T_{mid} + (T_{atm} - T_{mid}) × tanh[(z/z_0)(R/100 au)^β]^α

We note that the parameter α determines the height at which the transition in the vertical temperature profile takes place, while β represents the variation of transition height across the radius. The physical disk parameters used in our model are given in Tables 1 and 4. Disk density and temperature profiles for HD 163296 are shown in Figure 3 [Figure 3: see original paper].

4. Modeling Results

In this section, we present the calculated abundance distribution of S-bearing molecules in the HD 163296 disk model in Figures 4 and 5, and discuss the sources and formation pathways of these molecules. In the following, J is added before the molecular formula to represent molecules on the ice surface.

CS and JCS: From Figure 4 [Figure 4: see original paper], we find that CS mainly exists in the gas phase between z/r 0.1 and z/r 0.3. In this region, the gas-phase abundance of CS can reach 10^{-7}. In the area near the midplane ($z/r < 0.1$), the abundance of CS is relatively low. As the distance from the central star increases, the abundance of CS increases from 10^{-25} to 10^{-9} in the region near the midplane. CS is produced through the bimolecular reaction $H + HCS \rightarrow CS + H_2$ and through electron recombination of HCS^+ and H_3CS^+ in the region of the disk where $z/r > 0.1$ and $z/r < 0.3$. HCS^+ and H_3CS^+ are generated through rapid ion-neutral reactions between S^+ and small hydrocarbons like CH_4. Subsequently, H_3CS^+ recombines with electrons to form neutral sulfur-bearing species such as CS and HCS. In the midplane of the disk, CS freezes out onto grain surfaces. The main destruction pathways for CS are reactions with

H_3^+, HCO^+, and OH. JCS storage is concentrated in an area near the midplane of the disk, with an abundance of 10^{-15}–10^{-13}.

H_2CS and JH_2CS: The abundance distribution of H_2CS shows a trend similar to CS and is mainly found at intermediate heights ($0.1 < z/r < 0.25$) in the HD 163296 disk. The abundance of H_2CS can reach 10^{-25}–10^{-9} at these intermediate heights. H_2CS is primarily formed through gas-phase reactions between S atoms and CH_3, as well as through electron dissociative recombination of H_3CS^+. Near the midplane, H_2CS is formed by chemical desorption in the gas phase through surface reactions $JS + JCH_3 \rightarrow H_2CS + H$ and $JH + JHCS \rightarrow H_2CS$. H_2CS is mainly destroyed by reactions with protonated ions (H^+, H_3^+, HCO^+) and freezes onto grain surfaces near the midplane. The JH_2CS abundance is 10^{-15}–10^{-13} in most regions with $z/r < 0.2$, similar to JCS.

C_2S and JC_2S: The distribution of C_2S is similar to that of CS and H_2CS, but the gas-phase abundance only reaches 10^{-25}–10^{-9} within a narrow middle height range ($0.15 < z/r < 0.25$). C_2S is formed partly through gas-phase neutral reactions between S atoms and C_2H, and partly through electron dissociative recombination of H_3CS^+ and H_2CS^+. The destruction reactions for C_2S are identical to those of H_2CS, which explains the similarity in their distributions. JC_2S exhibits lower abundance compared to JH_2CS and JCS due to its involvement in hydrogenation reactions that produce longer S-containing compounds (JHCCS).

H_2S and JH_2S: The abundance of H_2S in a localized area with radial distance $r > 150$ au and height z/r   0.2 is 10^{-7}. Part of the H_2S in the gas phase is generated through electron recombination of H_3CS^+, while another part is generated on dust particles and released into the gas phase through photodesorption by UV photons and cosmic-ray evaporation. We found that JH_2S mainly exists in ice near the midplane ($z/r < 0.1$), where the abundance of H_2S can reach 10^{-9}–10^{-7}. H_2S freezes onto grain surfaces in this area. JH_2S is produced through the reaction $JH + JHS \rightarrow JH_2S$.

SO and JSO: The abundance of SO is 10^{-11}–10^{-9} between z/r   0.1 and z/r   0.3. In the midplane, for r below 100 au, the abundance of SO is less than 10^{-17}. However, as the radius increases, the abundance progressively rises, eventually reaching 10^{-11}. SO is generated in the gas phase through the reaction S + OH at $0.1 < z/r < 0.3$. The destruction mechanism for SO resembles that of H_2CS, with SO being destroyed by H_3^+ and HCO^+. In the region near the midplane, SO freezes onto dust particles, an effect that is especially prominent for r below 200 au. In this zone, the abundance of JSO can reach 10^{-7}.

SO_2 and JSO_2: In localized regions (150 au $< r <$ 250 au) with z/r ranging from 0.1 to 0.2, the abundance of SO_2 is 10^{-11}–10^{-9}. Its formation in the HD 163296 disk occurs through the reaction: $SO + OH \rightarrow SO_2 + H$. JSO_2 exhibits a distribution similar to JSO since it is formed via surface reactions between JSO and JO.

OCS and JOCS: The abundance of OCS can reach 10^{-7} near $r > 200$ au and z/r 0.2. OCS is frozen onto ice in regions close to the midplane. We found that OCS is formed through reactions of S with CO, as well as reactions of CS with OH in the gas phase. The abundance of JOCS can reach 10^{-9} near the midplane, where JOCS can be formed through reactions of JS with JCO.

5.1. Comparison of Model-simulated Column Densities and Observationally Deduced Fractional Column Densities

This section presents the column densities of the species investigated using our model, as depicted in Figure 6. We compared the model results against existing observationally deduced fractional column densities and summarized the similarities and discrepancies. \cite{Le_{{{Gal}}*{{2021}}}} derived the disk-integrated column density of CS in the HD 163296 disk by observing the CS 2–1 transition. This estimation was made assuming optically thin lines and local thermal equilibrium (LTE), with excitation temperatures in the range of 10–30 K. \cite{Le*{{{Gal}}_{{2021}}}} also covered transitions of C_2S and SO in their study and estimated the upper limits of the SO and C_2S column densities. These results are depicted as shaded regions in Figure 6. In this section, our main focus is on simulating the column densities at a carbon-to-oxygen ratio of 0.7.

In Figure 6, we observe that the vertical column density of CS in our simulated HD 163296 disk increases with distance from the star. When $r > 100$ au, the column density of CS gradually becomes flat, reaching 10^{13} cm^{-2}. Our model results are consistent with the observationally deduced fractional CS column density (within an order of magnitude). In addition, we found a protruding ring in the CS 7–6 radial profile (B26), while the chemical modeling results show a protrusion in the radial column density of CS at 26–32 au (using different C/O ratio models). However, it should be noted that the column density obtained by \cite{Le_{{{Gal}}*{{2021}}}} does not represent radial variation. To achieve a more accurate comparison, additional CS lines must be observed. The vertical column density of C_2S increases with radius, reaching 10^{12} cm^{-2} in the outer disk region. Comparison with the observationally deduced upper limits on C_2S column densities from \cite{Le*{{{Gal}}_{{2021}}}} shows that our simulated C_2S vertical column density is lower. For the vertical column density of SO, we simulated its decrease from 10^{14} to 10^{12} cm^{-2} as it moves away from the central star. The simulated vertical column density of SO falls below the observationally deduced upper limits when r exceeds 180 au.

5.2. Impact of the C/O Ratio

With improving telescope resolution, there is a growing trend in the observational and theoretical study of molecules within protoplanetary disks. Specifically, there is increasing interest in understanding how the gaseous C/O ratio varies with radial position and between different disks. To simulate the impact of the C/O ratio on the column density of sulfur-containing molecules, we varied the C/O ratio from 0.5 to 1.5 (with C abundance fixed). Figure 6 illustrates the influence of the gas-phase C/O ratio on the column densities of CS, H_2CS, SO, SO_2, C_2S, and H_2S in the HD 163296 disk.

For CS, H_2CS, and C_2S, we found that a higher C/O ratio leads to higher column densities. This is because CS, H_2CS, and C_2S are produced through reactions of S with small hydrocarbons (CH_2 and CH_3), resulting in the formation of carbonated sulfur ions (HC_2S^+ and HC_3S^+), which subsequently undergo electron recombination to form neutral sulfur-bearing species (see Section 4 for more details). As the C/O ratio increases, the abundance of hydrocarbons also increases, leading to higher column densities of CS, H_2CS, and C_2S.

For SO and SO_2, their column densities are highly sensitive to the C/O ratio. When the C/O ratio changes from 0.5 to 1.5, the largest change in column density for SO and SO_2 is a decrease of four orders of magnitude. This occurs because when oxygen is scarce, the abundance of the precursor OH for SO decreases, resulting in low column densities of SO and SO_2. Additionally, we found that when the C/O ratio is less than 1.1, the overall trend of column density for SO and SO_2 decreases with increasing radius. When the C/O ratio is greater than 1.1, the column density of SO and SO_2 initially increases and then decreases with increasing radius. Due to observational limitations, we cannot determine the best-fitting model for the C/O ratio in the HD 163296 disk. However, when $C/O > 1.1$, the column densities of SO in more regions are lower than the observational upper limit of SO. Therefore, we speculate that the C/O ratio in the HD 163296 disk may be greater than 1.1.

The column density of H_2S is sensitive to the C/O ratio in the region close to the central star ($r < 100$ au). When the C/O ratio is 1.5, the column density of H_2S is highest. This is because a high C/O ratio increases the abundance of H_3CS^+, which subsequently reacts with electrons to generate H_2S in the gas phase.

We found that when $r < 50$ au, the column density of OCS increases with a higher C/O ratio. This is because in this region, CO exists in the gas phase, and OCS is primarily formed through reactions of S with CO. A higher C/O ratio leads to a higher abundance of CO, resulting in a larger column density of OCS. However, when $r < 70$ au, a higher C/O ratio leads to a lower column density of OCS. In this case, CO is frozen onto icy surfaces, and OCS formation depends on the abundance of OH. A higher C/O ratio leads to a lower abundance of OH, resulting in a lower column density of OCS.

5.3. C/O Ratio Probe in HD 163296

As shown in Figure 7 [Figure 7: see original paper], our modeling results indicate that the column density ratio N[CS]/N[SO] changes by more than one order of magnitude when the C/O ratio varies from 0.5 to 1.5. This suggests that the N[CS]/N[SO] ratio is a promising probe for the disk C/O ratio in HD 163296.

\cite{Bosman_{2021}} constrained the C/O ratio in HD 163296 by interpreting high-resolution C_2H observations. They found that a C/O ratio greater than 2 was required to match the high column density ($>10^{13}$ cm^{-2}) of C_2H in the HD 163296 disk, though it is not obvious what causes the radial structures in the C_2H column density. As the exoplanet community endeavors to measure the C/O ratio in planetary atmospheres, observational and theoretical studies of disks are increasingly focused on understanding how gas-phase C/O varies with radial position and between disks \cite{Keyte_{2023}}. Our modeling results show that N[CS]/N[SO] varies significantly as the C/O ratio changes in HD 163296. This may indicate that N[CS]/N[SO] is an ideal probe of the variation of gas-phase C/O with radial position in the HD 163296 disk.

On the other hand, the column density ratios of N[H_2CS]/N[CS], N[C_2S]/N[CS], and N[OCS]/N[CS] remain largely unchanged with variations in the C/O ratio, even though OCS contains oxygen. Of particular interest is the N[H_2S]/N[CS] column density ratio, which, as observed in Figure 7, exhibits significant changes with the C/O ratio when $r < 100$ au. This may imply that N[H_2S]/N[CS] can potentially trace the C/O ratio in the inner disk. However, further validation of these model results is required through more observations of diverse samples.

5.4. Investigating the Column Density Ratios of Sulfur-containing Molecules in HD 163296

Our simulation results show that N[H_2CS]/N[CS] falls within the range of 0.1 to 2/3 in HD 163296. Previous observations of H_2CS in protoplanetary disks have been limited, with only a few disks detected thus far \cite{Codella_{2020}, Le_{{{Gal}}*{{2021}}}}. \cite{Le*{{{Gal}}_{{2021}}}} detected H_2CS in the MWC 480 disk, and their findings indicate a column density ratio of approximately 2/3 for N[H_2CS]/N[CS], suggesting that a significant portion of the sulfur reservoir in disks exists in organic form (i.e., C H S_z). Our calculations show that N[H_2CS]/N[CS] reaches a value of 2/3 for $r > 300$ au, similar to the observations in the MWC 480 disk. This suggests the possibility of detecting H_2CS in the HD 163296 disk.

H_2S has been observed in several PPDs \cite{Riviere-Marichalar_{2021}, Riviere-Marichalar_{2022}}. \cite{Riviere-Marichalar_{2021}} detected H_2S in several young stellar objects located in Taurus and indicated that the displayed value range for the N[H_2S]/N[CS] ratio was 0.12–0.38. Our model shows that the N[H_2S]/N[CS] ratio is greater than 0.1 in most regions, suggesting that the disk of HD 163296 is a favorable environment for detecting H_2S. The N[C_2S]/N[CS] ratio is mainly around 0.1 in most regions, similar to the ratio in molecular clouds \cite{Vastel_{2018}}. The N[OCS]/N[CS] ratio is generally below 0.1 after r exceeds 20 au, indicating that OCS is difficult to detect in the HD 163296 disk.

6. Conclusions

We have analyzed ALMA observations of CS 7–6 toward the HD 163296 disk and conducted astrochemical modeling to explore its sulfur chemistry. The main results of our study can be summarized as follows:

1. The CS 7–6 rotational transition was detected toward the HD 163296 disk.
2. We conducted astrochemical modeling of HD 163296 and compared the two-dimensional disk astrochemical model with observationally deduced fractional column densities of CS, C_2S, and SO in the HD 163296 disk. We found that the CS and C_2S chemistry appears to be well understood, with the simulated CS column density showing good agreement with the observed column density calculated under LTE. The simulated C_2S column density falls below the observational upper limits.
3. We investigated the influence of the C/O ratio on sulfur-containing molecules. We found that the column densities of SO and SO_2 are highly sensitive to the C/O ratio, and the column density of H_2S is particularly sensitive to the C/O ratio in the vicinity of the central star ($r < 100$ au).
4. Using the astrochemical disk model, we discovered that the N[CS]/N[SO] ratio serves as a promising indicator of the C/O ratio in the HD 163296 disk. Furthermore, the ratios of N[H_2CS]/N[CS], N[C_2S]/N[CS], and N[OCS]/N[CS] exhibit minimal variations with changes in the C/O ratio. Notably, N[H_2S]/N[CS] shows potential for tracking the C/O ratio in inner disks.
5. Our modeling results suggest that the disk of HD 163296 is a promising environment for detecting sulfur-bearing molecules such as H_2CS and H_2S.

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