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# Chemical Richness of protoplanetary Disks and related physical Properties

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**Abstract.** There are now several observational proofs that protoplanetary disks orbiting around T Tauri stars are planet forming sites. Studying planet formations in disks requests both high sensitivity and high angular resolution (at Taurus distance, 0.1'' means 15 au or 3 times the distance of Jupiter to the Sun). Moreover, H<sub>2</sub>, the main gas component remains difficult to observe, its mid-IR transitions only trace warm gas near the disk surface. Our knowledge on gas disk relies on trace molecules (CO, CN, CS, HCN, HCO<sup>+</sup> ...) observed by powerful large interferometers such as NOEMA and ALMA. I present here some recent results from ALMA and NOEMA showing that we start to quantitatively unveil the physical and chemical properties of planet forming disks.

## 1 Introduction

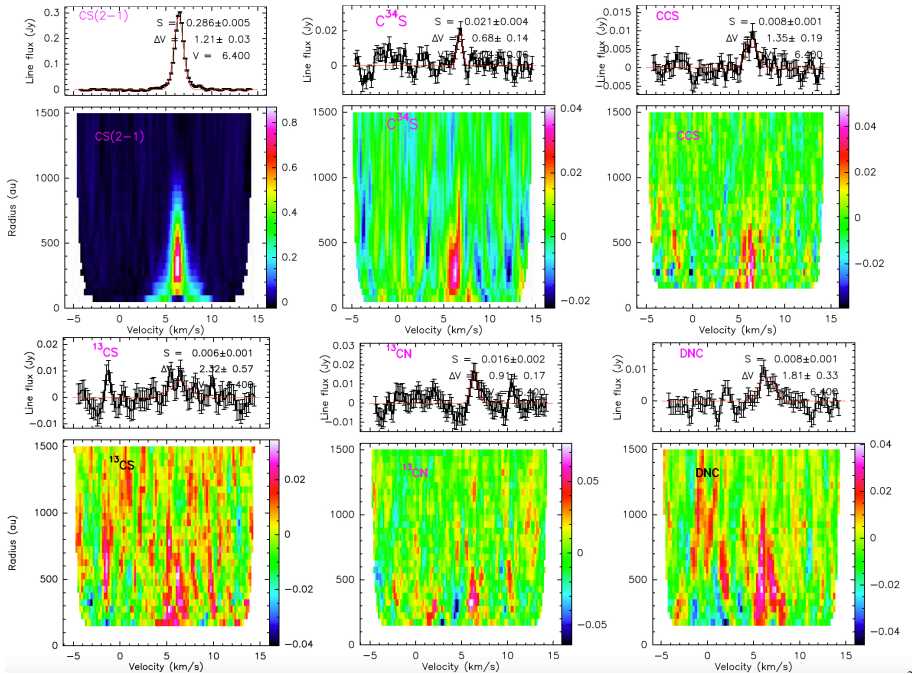
In the early 2000's, the input of many ground-based and spatial facilities provided the first constraints on radial and vertical structures of gas and dust disks orbiting low mass T Tauri stars. It is now established that dust disks contain grains which have already grown up to sizes of the order of at least 1 mm, these large grains being settled onto the mid-plane. The upper layer of the disk still harbors small grains, dynamically coupled to the gas, which absorb the stellar and interstellar radiations. They create a warm layer at intermediate altitude, while the interior of the shielded disk is colder with temperatures as low as 10 K in the dense mid-plane at radii > 50-100 au. With the exception of the upper disk surface, the gas temperature is essentially controlled by the dust temperature. At the disk upper surface, the incident UV flux from the central object photo-dissociates molecules making a (dense) PDR. On the contrary, the outer mid-plane corresponds to a region where most molecules stick onto dust grains and are severely depleted in the gas phase by combined effects of low temperatures, high densities and high extinction limiting photo-desorption. Typically, the CO snowline (~17-25 K, e.g. [1]) in a T Tauri disk is expected at a radius of ~ 20-40 au. Closer to the star, the mid-plane is warm enough, molecules are in the gas phase as above the cold mid-plane where the temperature remains high enough (T > 17-25 K) and thermal (and photo) desorption creates a molecular rich layer from which most mm/submm molecular emission originates. Many recent observations support such a layered molecular disk structure. One of the most famous example being given by the ALMA observations of CO in HD163296 by [2]. They directly image the CO layers above and below the mid-plane, confirming at the same time, the existence of the molecular layer and the vertical temperature gradient. Such a

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peculiar structure makes the retrieval of disk properties from observations not straightforward, often requiring the support of a detailed modeling of dust and gas, including chemical models and all their complexity. Moreover, observations need to have sufficient spatial (better than 40-50 au) and spectral (0.15-0.05 km/s) resolutions to properly constrain the altitude and the kinematics of the observed molecular layer.

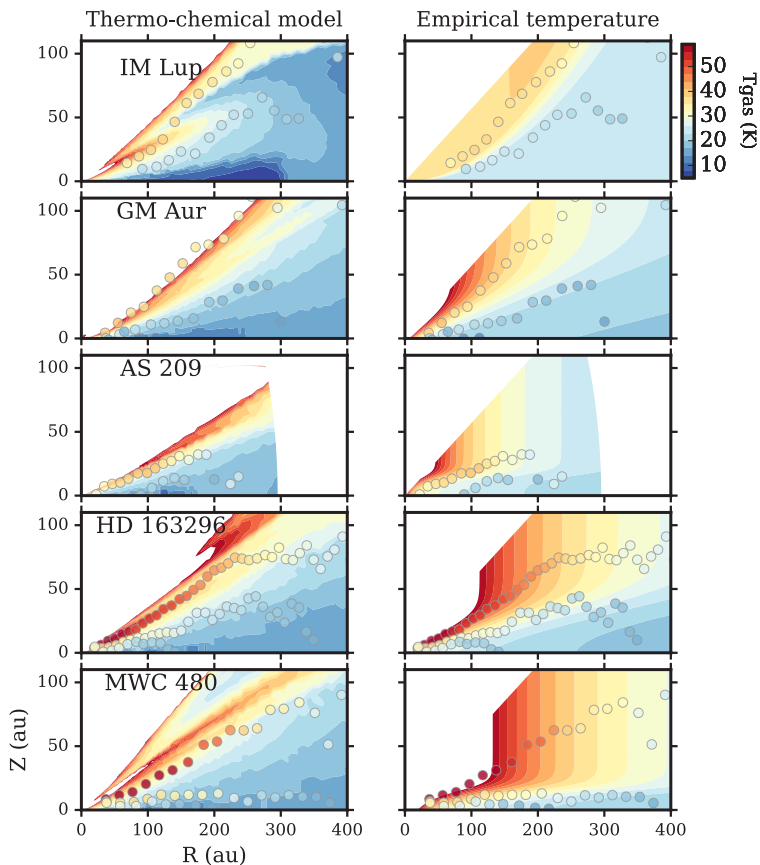
## 2 Molecular Complexity in Disks



**Figure 1.** Adapted from Phuong et al., 2021 [10]. Velocity-Radius plots of several molecule detected at 3mm with NOEMA and PolyFix in the GG Tau A disk (first detection of CCS in a disk). The data have been locally corrected from the value of the Keplerian speed (the mass of the central stars being known, the Keplerian speed can be properly calculated everywhere in the disk), de-projected from the disk inclination and each radius has been then azimuthally averaged.

A compilation of molecular detection in disks by [9] reveal that there are about 45 molecules (including isotopologues) detected in low-mass (TTauri) and intermediate mass (HAe) disks. Most detections arise from the warm molecular layer. A few species, such as H<sub>2</sub>O, are detected in warm inner disks. Only two species with 6 atoms (CH<sub>3</sub>OH and CH<sub>3</sub>CN) have been detected, most of the species have two or three atoms.

ALMA images at moderate angular resolution (typically 0.3'') of abundant molecules such as CS, C<sub>2</sub>H, HCN or CN reveal the presence of rings (e.g. [14]). These rings likely originate from a mix of local variations in density, column density and temperature together with changes in the UV penetration and grains properties. Detailed chemical analyses of the observations also tend to favor in TTauri disks a C/O ratio around  $\sim 1$ , larger than in the interstellar medium, at least in a significant area in the disks in which it has been measured ([14, 15]).



**Figure 2.** Adapted from Zhang et al., 2021 [6]: comparison between the ALMA (MAPS) observations of CO lines and a thermo-chemical modeling (left) and a simple parametric model for the disk structure (right). Surface brightness temperature measurements for CO,  $^{13}\text{CO}$ , and  $\text{C}^{18}\text{O}$  2-1 lines are given by circles (highest circles correspond to CO 2-1).

## 2.1 An example of a molecular Survey: the GG Tau dense Ring

Using NOEMA and thanks to the flexibility of PolyFix, Phuong et al. 2021, [10] have recently reported the first deep survey done in a proto-planetary disk in the 3mm range (from 2.6 to 4.2mm) that contains many fundamental transitions of simple molecules. They observed the Keplerian outer disk around the triple star GG Tau A located in Taurus ([3]). Thanks to its high mass ( $0.15 M_{\odot}$ ) and large size (outer radius 800 au), it is a good laboratory to study the "cold chemistry" occurring in T Tauri disks.

Among the thirty-eight molecules which were observed, only seventeen were detected, including CCS seen for the first time in a T Tauri disk (there is also a marginal detection of OCS). Fig.1 presents Sulfur and Nitrogen bearing species (DNC,  $^{13}\text{CN}$ , CS,  $\text{C}^{34}\text{N}$ ,  $^{13}\text{CS}$  and CCS). With the exception of CS, most them where detected at low SNR (of the order of 6-8). Very interestingly and despite a low angular resolution, most sulfur-bearing species seem to originate from the dense ring (180-260 au from the stars) while deuterated species are observed in the outer, colder, less dense disk (radius beyond 260 au and up to 800 au) as expected from chemical models.

## 3 High angular and spectral Resolution Imaging of bright Lines

### 3.1 Gas structure from resolved CO maps

Mapping several lines from CO isotopologues appears as a powerful method to retrieve the gas disk structure, in particular its temperature. In T Tauri disks, the first rotational levels of CO are thermalized and optically thick, typically sampling surfaces at 3 scale-heights. Optically thinner lines from  $^{13}\text{CO}$  and  $\text{C}^{18}\text{O}$  2-1 reach an opacity around 1 closer to the disk plane. This opacity difference was used for the first derivation of the vertical kinetic temperature profile ([4] and [5]).

Thanks to the ALMA resolving power and sensitivity, imaging CO lines in a few T Tauri and Herbig Ae disks in the context of the MAPS large program, Law et al., 2021 [7] were recently able to directly compare the altitude of the observed CO layers with a simple parametric model for the gas temperature ([4]), as it is shown right side of Fig.2. Zhang et al., 2021 [6] used a thermo-chemical model to derive the whole disk structures by comparing with these observations (Fig.2). They conclude that the observational method and the thermo-chemical modeling agree within a temperature range of 15-40 K that corresponds to the typical temperature of the molecular layer of T Tauri disks.

### 3.2 Gas Mass

Going one step further, Schwarz et al., 2021 [8] studied the disk orbiting the T Tauri GM Aur by using all the CO lines observed by ALMA on this object (1-0, 2-1, 3-2 and 6-5 lines of several CO isotopologues) and the HD 1-0 line observed by the Herschel Satellite. They found that the disk is more massive than originally thought with a gas mass of about  $0.2 M_{\odot}$ . In this specific case, the mass derivation was obtained using a thermo-chemical code to model the HD and CO lines. This impressive study, using in total eleven CO lines, shows that deriving accurate disk masses remains a complex task and suggests that at least a fraction of disks might be massive enough to be gravitationally unstable.

### 3.3 Deriving the Turbulence

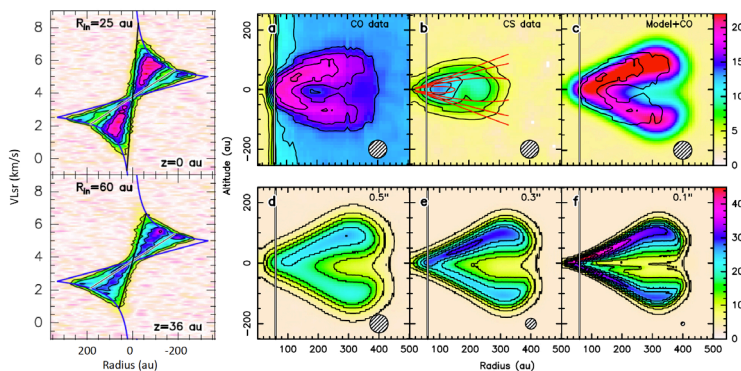
Dartois et al., 2003 and Pietu et al., 2007 [4, 5] have shown that the local turbulence  $\delta v_{turb}$  in a disk can be derived from the local line-width provided the thermal component is accurately known. Using the PdBI, Guilloteau et al., 2011 [16] used the "heavy" molecule CS to minimize the impact of the thermal component and found subsonic turbulence in the DM Tau disk. With the advent of ALMA, several studies show that disks have a low turbulence. Teague et al., 2016 [17] demonstrated that absolute calibration errors limit the method accuracy to Mach numbers above about 0.1. Using several molecular tracers such as CO,  $\text{DCO}^+$  and CS, Flaherty et al., 2017, 2020 [18, 19] found low turbulence in the disks surrounding HD163296, MWC480, and V4046 Sgr, DM Tau remaining the only firm detection (Mach  $\sim 0.3$ ).

## 4 Edge-on Disks

Contrary to an inclined disk, an edge-on disk directly probes the vertical structure. In the Position-Velocity (PV) diagram of a Keplerian disk, there is a direct link between position and velocity. All radial lines correspond to constant disk radii and averaging along them directly gives the average molecular brightness at each specific radius. Cuts at various altitudes provides a direct, model-independent, tomography of the 2-D gas structure (Fig.3).

### 4.1 The Flying Saucer

Fig.3 shows the reconstruction of the CO and CS brightness distributions  $T_B(r,z)$  for the Flying Saucer (a T Tauri disk located in  $\rho$  Oph and inclined by  $87^\circ$  along the line of sight) obtained by Dutrey et al., 2017 [11] using ALMA data at  $0.5''$  (70 au at the source distance). Thermalized, optically thick lines as CO J=2-1 give directly access to the kinetic temperature of the gas, provided the angular resolution is high enough to reduce the beam dilution effect. The observed kinetic temperature from CO 2-1 by [11] is in good agreement with that reported by [6, 7] in similar T Tauri disks. In the Flying Saucer [11] also observed a clear depression around the mid-plane, where CO is expected to freeze onto grains. However, the limited angular resolution precludes any accurate determination of the temperature in this area.

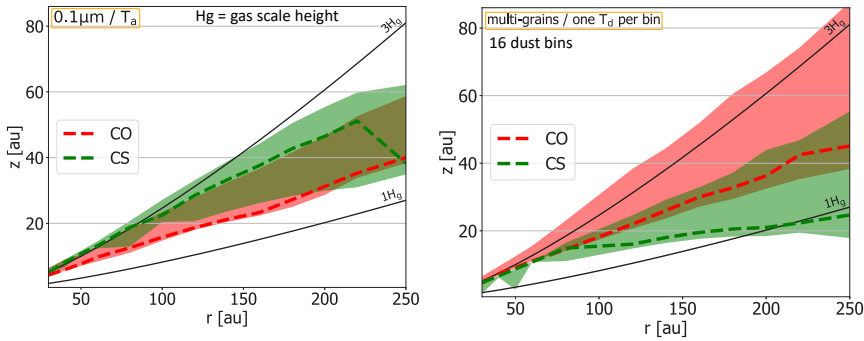


**Figure 3.** Adapted from Dutrey et al., 2021 [11], ALMA observations (CO 2-1 and CS 5-4) of the Flying Saucer edge-on disk. Left: two PV diagrams for CO at altitude  $z=0$  and 36 au. Right - Top panel CO, CS observations and the best model for CO with observations in black contours - Bottom panel: impact of the angular resolution, the north-south dissymetry is due to the  $3^\circ$  departure from edge-on.

### 4.2 Chemical Stratification and Models

The molecular stratification is directly visible in an edge-on disk. Fig.3 shows that the density tracer CS arises from a lower layer (about one scale-height), while CO, which characterizes the overall extent of the molecular gas, extends up to four scale heights. Such distributions can be unambiguously compared to model predictions. The models in Fig.4 are a first attempt of this, using two different chemical approaches. On the left, Gavino et al., 2021 [12] did a simple model using a single grain size ( $0.1 \mu\text{m}$ ). On the right, the disk physical model is similar (same  $\text{H}_2$  distribution and mass) but includes grain growth, dust settling and the proper dependence of dust temperature with grain sizes. By comparing with Fig.3, the differences on the CS and CO distributions are obvious. The simple model does not reproduce the observations, contrary to the second one. Edge-on disks can also be useful tools to directly calibrate thermo-chemical models.

The above examples illustrate the increasing accuracy of mm/submm studies of disks. These studies will allow in the forthcoming years a real understanding of planet forming disks, provided the integration time of the observations will be high enough to sample the molecular complexity and/or produce images of high quality.



**Figure 4.** Derived from Gavino et al., 2021 [12]: two chemical models for the edge-on disk of the Flying Saucer. The CO (red) and CS (green) distributions are shown. Dust temperatures are derived from a Monte-Carlo radiative transfer code. Left: a chemical model with a single grain size (0.1  $\mu\text{m}$ ). Right: model for the same disk ( $\text{H}_2$  distribution and mass) with dust growth, settling and a grain temperature depending on grain sizes.

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