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Unveiling the third dimension: vertical structure as a probe of planet formation conditions

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Citation

Paneque Carreño, T. (2024, September 13). *Unveiling the third dimension: vertical structure as a probe of planet formation conditions*. Retrieved from <https://hdl.handle.net/1887/4083418>

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Unveiling the third dimension: vertical structure as a probe of planet formation conditions

Proefschrift

ter verkrijging van
de graad van doctor aan de Universiteit Leiden,
op gezag van rector magnificus prof. dr. ir. H. Bijl,
volgens besluit van het college voor promoties
te verdedigen op vrijdag 13 september 2024
klokke 10:00 uur
door

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geboren te Madrid, España
in 1997

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ISBN:

Cover design: Juan Carlos Cortés

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Chapter 1

Introduction

In the north of Chile, due to its natural conditions and isolation, the Atacama desert is a unique window to observe the universe. For many centuries the local native indigenous groups, called in their language *Lickan Antay* and in current spanish *Atacameños*, looked up at the universe and focused not only on the bright stars, but on the dark areas that contrasted against the glow. What western cultures decided to name the Milky Way was known as the River of Life, River of Stars or River Above to the *Lickan Antay*. Within this River of Stars, which we now know is the projection of our galaxy seen in the sky, the *Lickan Antay* observed the dark regions to mark their constellations. In these obscure zones they drew a number of creatures seen in the Andes such as a llama and her baby, a fox, a snake and a toad. This interpretation of the sky was related to their cosmovision, where they proposed that all the beings and experiences they had on earth should have a representation in the stars.

Thousands of years later, many astronomers remain interested in those dark regions and, from the same Atacama desert, point the largest telescopes in the world to observe them. It is now known that they are dark because small dust grains absorb the starlight at optical frequencies, leading to high visual extinctions (Bergin & Tafalla 2007). Most importantly, these dark clouds are associated with star-forming regions (Bok 1948) and, while our eyes are not able to see past the dust, instruments such as the Atacama Large Millimeter/submillimeter Array (ALMA¹) can reveal their secrets. ALMA is built on the Chajnantor plateau, a sacred place for the *Lickan Antay* that means “place of departure” in the Kunza language. Located at an altitude of 5000 meters one of the main science goals of ALMA is to look into these dark and cold regions to understand the processes that lead to star and planet formation.

¹ALMA is a partnership of ESO (representing its member states), NSF (USA) and NINS (Japan), together with NRC (Canada), NSTC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ

Such fundamental questions regarding the origin of our planet must be answered through global participation and, indeed, ALMA is a testimony to scientific and international collaboration. The observatory is composed of 66 antennas that work simultaneously while they are spread over nearly 16 kilometers in the Chajnantor plateau. Groups of antennas and their technology are provided by consortiums from more than 20 countries across North America, Europe and East Asia, including Chile as host country and collaborator.

The analysis and results presented in this thesis have been possible due to the capabilities of ALMA, that since the start of its operations in 2013 has revolutionized the view of planet formation (see for example the iconic first high-resolution image of a protoplanetary disk around HL Tau, ALMA Partnership et al. 2015). Through observations and theoretical understanding of the cold universe, as traced at (sub-)millimeter wavelengths we have the unique opportunity to look back towards our origins. How did the earth form? May other planetary systems have similar conditions? What are the key processes that govern the initial epochs? As the *Lickan Antay* did centuries ago - and are still doing to this day - we observe the conditions in our surroundings and look for them in the skies, only going a bit further. In practice, we measure abundances and take data from the Solar System, predict possible scenarios for earth's formation and search the dark clouds for clues as to whether we may or may not be correct.

1.1 Star and planet formation

The process of planet formation is intrinsically linked to stellar formation. Stars form from the collapsing material of dark and cold molecular clouds with characteristic densities $>10^2 n_{\text{Hcm}}^{-3}$ (hydrogen nuclei per cubic centimeter, Öberg & Bergin 2021a). The initial cloud composition is expected to be mostly gas, with one percent of sub-micron dust particles formed of silicates and carbonaceous material (Bohlin et al. 1978; Henning 2010). Through their high densities, molecular clouds shield themselves against external radiation and achieve low temperatures (10-20 K) in their centers, where denser structures, known as pre-stellar cores, can assemble (Bergin & Tafalla 2007). Pre-stellar cores slowly rotate while they reach densities of $\sim 10^6$, temperatures of ~ 10 K and sizes of order ~ 0.1 pc (Terebey et al. 1984; Myers & Benson 1983; Bergin & Tafalla 2007). Cores that are dense enough to overcome turbulence, thermal and magnetic pressure, gravitationally collapse inwards conserving angular momentum to form one or multiple protostars (Shu 1977; Galli & Shu 1993).

Going from a pre-stellar core to a planetary system, young stellar objects (YSOs) are classified into Classes (0, I, II or III) through the analysis of the slope of their spectral energy distribution (SED) between 2-25 μm (Lada 1987, see also Figure 1.1). In the earliest Class 0/I stage, a protostar will be actively accreting material from its surrounding cloud core or protostellar envelope while angular momentum conservation acts by spreading out the accreting material to form a rotating disk-like structure (Cassen & Moosman 1981). This deeply embedded Class 0/I phase is hard to observe at millimeter wavelengths, as the envelope material

blocks the emission from the protostar and disk (Williams & Cieza 2011; Tobin et al. 2015; Ohashi et al. 2023).

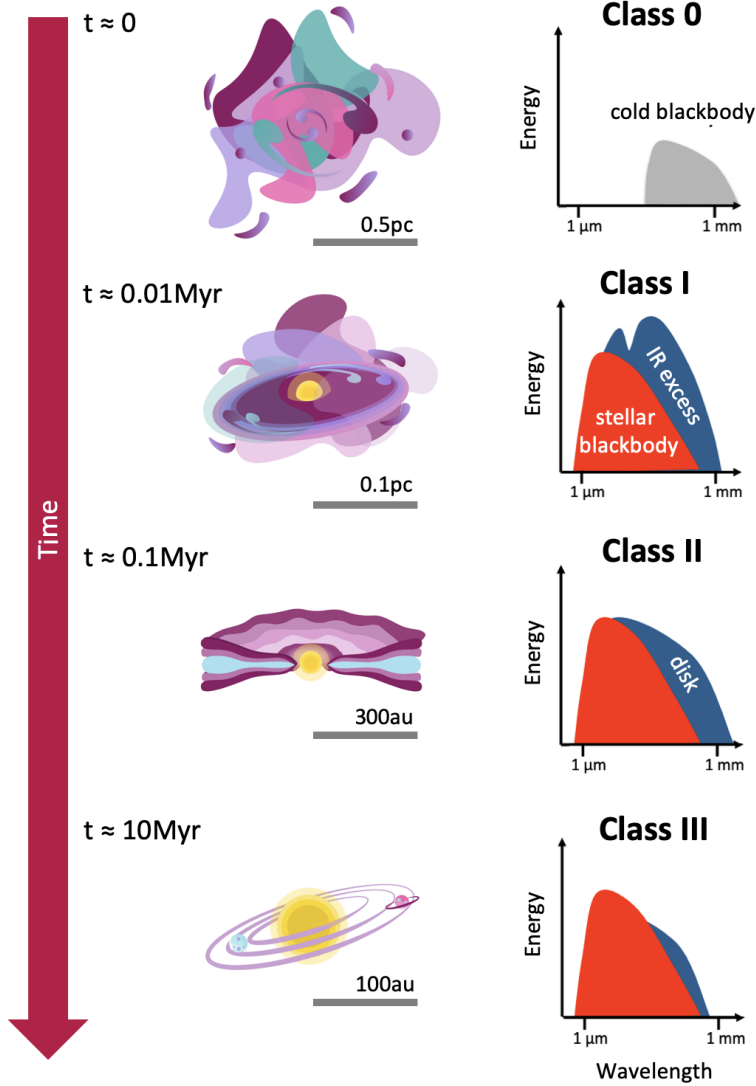


Figure 1.1: Schematic of star and planet formation timeline. Left: evolutionary stages from pre-stellar core to planetary system. Right: typical SEDs and respective classification, corresponding to each stage. SEDs adapted from A. Miotello’s PhD thesis.

As time passes, in $\sim 0.5\text{--}1$ Myr, the protostellar envelope is dispersed via molecular outflows and accretion, revealing a pre-main sequence star and a Keplerian disk (Williams & Cieza 2011; Öberg & Bergin 2021a). These circumstellar ac-

cretion disks are named protoplanetary or planet-forming disks, as they are the birthplaces and host the material reservoir of planetary systems. The Class II protoplanetary disk stage may last $\sim 1\text{--}10$ Myr (Mamajek 2009) and ends when most of the disk material has either accreted onto the star, formed planets, or has been dispersed through photoevaporative winds and other processes (Alexander et al. 2006a,b; Pascucci et al. 2023). Finally, a planetary system is produced, which may continue evolving through collisions or interactions between its components (e.g., Wyatt 2018).

This thesis focuses on the protoplanetary disk phase, where the primordial planet-forming material can be readily observed and characterized at (sub-)millimeter wavelengths at high spatial and spectral resolution (e.g., Andrews et al. 2018; Öberg et al. 2021b). By tracing the material composition and distribution at mm wavelengths, it is possible to probe the ongoing processes and understand the planet-forming environment.

1.2 Protoplanetary disks

1.2.1 Composition and mass

1.2.1.1 Dust

Like their parent clouds, protoplanetary disks are gas-rich structures with solid particles accounting for only a few percent of their mass. Studying the dust component of disks is crucial for understanding planetesimal core and rocky-planet formation (Testi et al. 2014). The amount of solid particles will inform on how much material remains to form planetary cores, to obtain this number one must have an estimate of the total dust surface density or total dust mass. It is also relevant to estimate the size of these particles, as it can be used to predict their aerodynamic behavior when interacting with the gas reservoir (Whipple 1972; Weidenschilling 1977).

Assuming optically thin dust continuum emission, the total flux of the disk (F_ν) can be related to the total dust mass (M_{dust}) following,

$$F_\nu = \frac{B_\nu(T_d)\kappa}{d^2} M_{\text{dust}} \quad (1.1)$$

where d is the distance to the source, B_ν the Planck spectrum at the assumed dust temperature T_d and κ the dust opacity. This relationship was first proposed by Hildebrand (1983). In most studies, T_d and κ are disk-averaged values calculated from the stellar properties and an assumed grain porosity. From the estimated dust mass, typically an ISM-like gas-to-dust ratio of 100 is considered to calculate the total disk (e.g., Andrews et al. 2013; Ansdell et al. 2016; Barenfeld et al. 2016; Pascucci et al. 2016; Ansdell et al. 2017; Cazzoletti et al. 2019; Stapper et al. 2022). Overall, estimates of the disk mass extracted from the continuum flux can be uncertain, given the number of assumptions used to estimate the physical parameters (temperature, porosity, gas-to-dust ratio), however this approach to

extract dust masses has been largely used in the literature and may give a first-order approach to measuring the disk material (for further discussion see Miotello et al. 2023).

The initial dust reservoir consists of μm -sized grains, however as these solids grow, the presence of large dust grains will alter the dust opacity of the emission, which in the (sub-)millimeter regime is related to the frequency of the observations such that $\kappa \propto \nu^\beta$. For grains of millimeter or larger sizes, β becomes smaller. In the Rayleigh-Jeans regime ($h\nu \ll kT$), the intensity of optically thin emission relates to the frequency as $I_\nu \propto \nu^\alpha$, where $\alpha = \beta + 2$ (Draine 2006; Testi et al. 2014). Studies of the opacity spectral index β confirm dust growth in protoplanetary disks, as they find dust aggregates larger than millimeter sizes (e.g., Tazzari et al. 2021a,b). Including more realistic processes affecting dust emission, such as scattering (e.g., Sierra et al. 2021; Carrasco-González et al. 2019) or polarization effects (e.g., Kataoka et al. 2016) can vary these values. The presence and distribution of large and small dust grains will have a direct effect on the protoplanetary disk heating processes, as μm -sized dust will couple to the gas and effectively shield disk regions from energetic radiation, while larger particles will settle towards the midplane and affect the chemical reservoir by sequestering volatiles in their ice mantles or creating dust over-densities (D’Alessio et al. 2005; Henning 2010; Andrews 2020).

1.2.1.2 Gas

The bulk of the gaseous disk material is molecular hydrogen (H_2), however due to the lack of permanent dipole moment, its emission is extremely faint at the typical temperatures (20–30 K) and conditions of the outer ($>20\text{ au}$) disk (Field et al. 1966). A less abundant isotopologue, hydrogen deuteride (HD), can be detected at protoplanetary disk conditions in its fundamental rotational transition ($J = 1 - 0$), however, there are some caveats to interpreting HD emission (e.g., Trapman et al. 2017; Calahan et al. 2021) and there are no current facilities that may observe it at $112\ \mu\text{m}$ (Kamp et al. 2021). Realistically, the best alternative for probing the gas reservoir is carbon monoxide (CO). CO is the second most abundant molecule after H_2 and its chemistry has been deeply studied in many astrochemical contexts, as it is the most abundant gas-phase carrier of interstellar carbon (van Dishoeck & Black 1988; Miotello et al. 2023).

CO is readily detected at (sub-)millimeter wavelengths in protoplanetary disks, particularly in its main isotopologue $^{12}\text{C}^{16}\text{O}$ (Dutrey et al. 1997; Ansdell et al. 2016; Pascucci et al. 2016; Eisner et al. 2016; Cieza et al. 2019; Long et al. 2018; Ansdell et al. 2017; Cazzoletti et al. 2019). The survival of CO in gas phase is regulated by its photodissociation due to UV photons and CO freeze-out onto dust grains at low ($\leq 20\text{ K}$) temperatures. CO manages to achieve column densities sufficient to self-shield from UV photons and survive at high abundance throughout the disk (Aikawa et al. 2002; van Dishoeck & Black 1988). Its characteristics have made it the most used molecular probe of disk conditions and it is used to trace the disk extent (Ansdell et al. 2016; Law et al. 2022), hunt for kinematical signatures (Teague et al. 2018a; Pinte et al. 2018b; Izquierdo et al. 2022, 2023),

as a temperature probe (Law et al. 2021b) and disk mass tracer (Miotello et al. 2014, 2016; Stapper et al. 2024).

Beyond CO and its isotopologues, molecules that have been frequently detected in protoplanetary disks environments include; CN, HCN, H₂CO, CS, HCO⁺, N₂H⁺, H₂O, C₂H, among others (e.g., Dutrey et al. 1997; Thi et al. 2004; Dutrey et al. 2007; Hogerheijde et al. 2011; Öberg et al. 2021a,b; Booth et al. 2023). Precursors of complex organic molecules such as methanol (Walsh et al. 2016; Booth et al. 2021) and dimethyl ether (Brunken et al. 2022) are less frequently observed, but exemplify the rich chemistry that may be occurring in these epochs (see also Booth et al. 2024). It is still an open question whether the chemical composition of the disk gas is directly inherited from the interstellar medium and molecular cloud or if significant reprocessing occurs during/before this phase. Indeed, for the most studied case of CO, multiple studies support that CO abundance considerably reduces (between one or two orders of magnitude) throughout the early stages of planet and stellar formation passing from an abundance of $\sim 10^{-4}$ (with respect to H₂) to $10^{-5} - 10^{-6}$ (e.g., Zhang et al. 2019, 2020; Schwarz et al. 2016; Bergin et al. 2014; Bosman et al. 2018).

1.2.2 Disk evolution

Above all, protoplanetary disks are accretion disks and their main physical process is to funnel material onto the central stellar object (Hartmann et al. 2016; Manara et al. 2023). Accretion is a fundamental problem in astrophysics, as it requires a mechanism through which particles lose angular momentum in order to move closer and accrete onto the central object (for dedicated reviews see Hartmann et al. 2016; Lesur et al. 2023). In protoplanetary disks there are two main scenarios proposed to enable this process; (1) viscosity inside the disk that transports angular momentum to the outer disk (Shakura & Sunyaev 1973) or (2) magnetically-driven disk winds that disperse mass from the upper layers, thus taking angular momentum away (Blandford & Payne 1982).

Viscous evolution has traditionally been the preferred theory for driving protoplanetary disk evolution due to its simplicity (i.e., it can be expressed analytically), but the exact physical origin of the viscosity is still not clear. Considering the disk as a viscous fluid, the first cause of viscosity would be the random collisions between gas particles, creating a molecular viscosity. However, protoplanetary disks are not viscous like honey or other thick fluids, in fact, the viscosity of a gas can be estimated as $\nu \sim v_{th}\lambda$ where v_{th} is the thermal speed of the molecules and λ the mean-free path. We can estimate these parameters based on reasonable assumptions of disk conditions and calculate $\lambda \sim 1/n\sigma$, where n is the molecular number density and σ the collision cross-section. Overall, estimates of molecular viscosity yield $\nu \sim 10^5 \text{ cm}^2 \text{ s}^{-1}$ (Armitage 2015). For a disk with characteristic size r , the viscously-driven evolution timescale (t_v) follows,

$$t_v = \frac{r^2}{\nu} \quad (1.2)$$

Therefore, on its own, the estimated molecular viscosity would drive disk evo-

lution within a timescale of $\sim 10^{13}$ yr, much larger than the protoplanetary disk lifetime, which survives roughly for a few Myr (Williams & Cieza 2011; Mamajek 2009). This large viscous timescale proves that molecular viscosity alone cannot be responsible for disk evolution. Shakura & Sunyaev (1973) solved the viscous problem by proposing that random velocity fluctuations, known as turbulence, might act as an effective viscosity, removing angular momentum and driving disk evolution in reasonable timescales. In this case viscosity is parametrized as,

$$\nu = \alpha c_s H \quad (1.3)$$

where c_s is the sound speed and H the hydrodynamical pressure scale height (described in section 1.2.3.2). Typically an α of $\sim 10^{-2}$ is required to match observational constraints of timescales and accretion rates (Armitage 2015). While this prescription is a sensible solution, it still poses the question regarding the origin and strength of turbulent motions. Various hydrodynamical instabilities have been proposed to cause turbulence, with distinct vertical patterns and launching mechanisms (Lesur et al. 2023). Magneto-rotational instability (MRI, Balbus & Hawley 1991) and vertical shear instability (VSI, Urpin & Brandenburg 1998) will produce high values of turbulence in the upper disk and smaller fluctuations near the midplane (Shi & Chiang 2014; Simon et al. 2015). Comparatively, gravitational instability (GI, Lynden-Bell & Pringle 1974) is expected to launch turbulent motions that will be constant throughout the disk vertical structure (Forgan et al. 2012). We will discuss turbulence in depth and the relevance of resolving its value across the vertical structure in chapter 4.

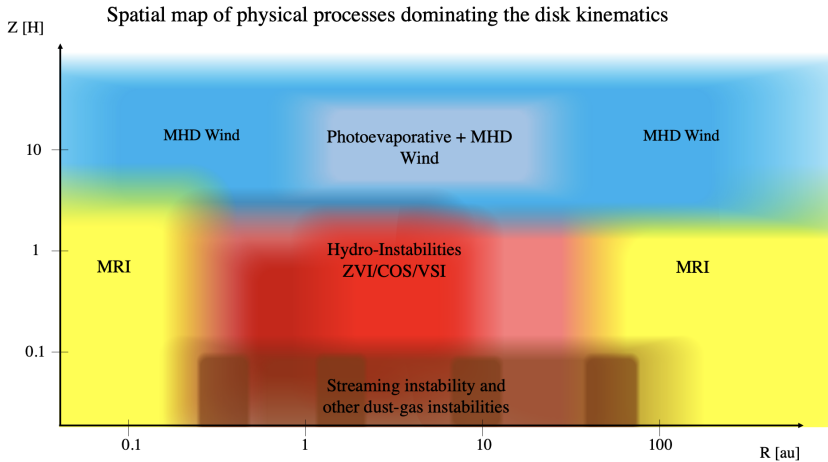


Figure 1.2: Figure from Lesur et al. (2023) indicating the spatial map of dominant physical processes (hydrodynamical instabilities and winds) relevant for the evolution of protoplanetary disks. Distribution of specific instabilities can be model dependent, but in general their effects may be characterized through their local vertical and radial perturbations.

Evolution may also be driven or aided by external torques, specifically, the pres-

ence of magneto-hydrodynamical (MHD) winds could cause a magnetic torque on the disk surface and drive mass loss (Blandford & Payne 1982; Wardle & Koenigl 1993). MHD processes require the disk material to be ionized, as the gas must support electrical currents in order to interact with the magnetic field and launch the wind (Lesur et al. 2023). It has been shown that even for weakly ionized disks, magnetised outflows may be launched resulting in a mass loss rate within the order of measured accretion rates (Bai & Stone 2013; Simon et al. 2013; Bai 2017; Lesur et al. 2014; Gressel et al. 2015). Unfortunately, while many theoretical models predict the effectiveness of MHD winds, observational confirmation has been scarce. Winds have been identified in a number of systems, but determining their nature (MHD or thermal) is still a complication within the field (see discussion in Pascucci et al. 2023). Upcoming facilities such as the Next Generation Very Large Array (ngVLA), could make advances in this matter (Ricci et al. 2021). Figure 1.2 maps the regions where winds may be relevant ($z/r \gtrsim 10$) compared to the previously discussed hydrodynamical instabilities which may drive turbulent motions in disk layers between the midplane and $z/r \sim 8$.

1.2.3 Disk structure

In simple terms a protoplanetary disk consists of material orbiting around the star following (mostly) Keplerian motion. As discussed in previous sections, dust aggregates have their dynamics determined by gravitational and centrifugal forces, together with the drag they feel from the gas (Whipple 1972; Weidenschilling 1977). Gas particles are also subject to gravitational and centrifugal forces, but in addition feel radial and vertical pressure support which will directly depend on the gas temperature (Pinte et al. 2023). Overall, pressure support will create a force pointing outwards from the inner disk, causing the gas to have a slightly sub-Keplerian motion. This velocity difference with respect to the dust particles (that are not pressure supported) will decelerate the dust, causing solids to lose angular momentum and drift towards the inner disk (Whipple 1972; Weidenschilling 1977). To avoid this *radial drift* and fast accretion of the solid reservoir, radial pressure gradients must exist, to accumulate and allow dust growth to happen at locations of pressure maxima (Pinilla et al. 2012a,b). This is particularly relevant for large (mm-cm) solids, as the smaller μm dust will be well coupled to and follow the molecular gas dynamics and structure. Figure 1.3 represents the radial and vertical material distribution and main processes discussed in the following sections.

1.2.3.1 Radial distribution

Radially, the disk can be divided between a hot inner disk ($< 20 \text{ au}$) and a cold outer disk. Infrared telescopes such as the James Webb Space Telescope (JWST) study the emission at several 100 K of the inner disk and many ongoing studies are trying to understand the structure and processes in the terrestrial-planet forming zone, close to the star. These topics, however, are outside the scope of this thesis and we will not refer to them beyond acknowledging their importance towards characterizing the innermost planet-forming zone.

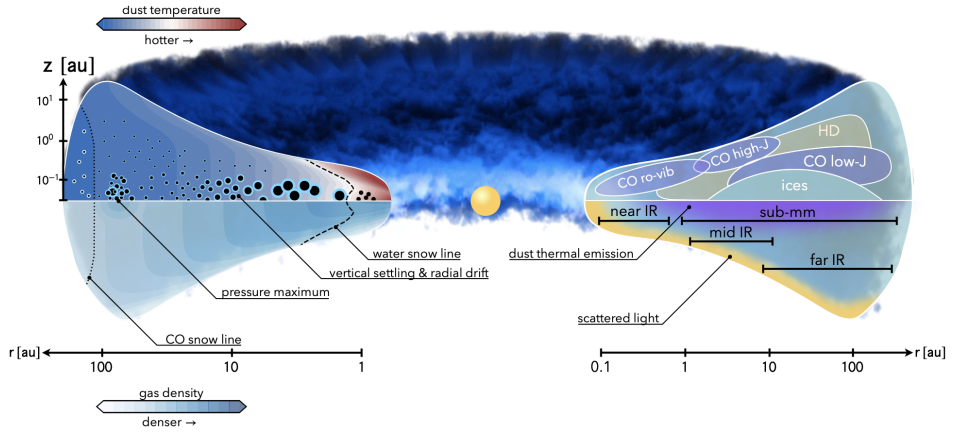


Figure 1.3: Illustration from Miotello et al. (2023) indicating the emission regions, relevant scales, dust temperature and gas density structure in protoplanetary disks. Left side shows the distribution of dust particles in black circles with different sizes represented as symbol size. Right side presents a simplified view of the molecular layering for the main observed gas-phase molecules. In the bottom the main dust thermal and scattered light emission regions are highlighted in purple and yellow.

On the other hand, ALMA observations can access the outer disk at a spatial resolution of a few au (depending on the observing frequency, ALMA Partnership et al. 2015) when observing systems at ~ 150 pc distance (the typical distance of nearby Star-Forming Regions, Gaia Collaboration et al. 2023), obtaining high spatial resolution data of the material beyond ~ 20 au (e.g., Andrews et al. 2018; Öberg et al. 2021b). Several systems have now been observed at the highest resolution possible with ALMA, revealing a plethora of continuum and gas substructures, from axisymmetric rings, cavities and gaps (ALMA Partnership et al. 2015; Huang et al. 2018b) to azimuthally concentrated vortices (Pérez et al. 2018a), spirals (Pérez et al. 2016; Huang et al. 2018c) and extreme asymmetries (van der Marel et al. 2013). Radial substructure is ubiquitous and expected, as it is the physical representation of accumulation of dust grains in pressure maxima, overcoming the radial drift problem (Pinilla et al. 2012b; Testi et al. 2014). By analyzing the morphology, properties and dynamics of these substructures, studies aim to determine their physical or chemical origin (Andrews 2020).

Assuming that substructures are only a lower-order modulation of the radial disk structure, most works assume that the radial distribution of material (surface density, $\Sigma(R)$ profile) follows a radial power-law dependence, typically with an exponential taper at large radii. The precise prescription for the surface density will depend on the governing evolution mechanism and different prescriptions have been proposed in individual disk studies. The most used form is the self-similar solution for a viscously evolving disk (Lynden-Bell & Pringle 1974; Andrews et al. 2011), such that the surface density follows,

$$\Sigma(R) = \Sigma_c \left(\frac{R}{R_c} \right)^{-\gamma} \exp \left[-\frac{R}{R_c} \right]^{2-\gamma} \quad (1.4)$$

where R_c is the characteristic radius and γ the surface density exponent. It is important to note that dust and gas will likely have different radial distributions; indeed the MAPS ALMA large program (Öberg et al. 2021b) showed that molecular emission substructure is rarely coincident with the continuum substructure (Law et al. 2021a). Multiple studies have also shown that gas outer radii are generally many times larger than the dusty mm-disk edge, indicating a more extended distribution for the gas (see discussion in Miotello et al. 2023).

1.2.3.2 Vertical structure

From a theoretical standpoint, disks are well described in their vertical dimension. Hydrostatic equilibrium between the gravitational potential of the star and thermal support will shape the vertical distribution of the gaseous material and of the small dust grains coupled to it (Armitage 2015). In cylindrical coordinates, the hydrostatic equilibrium equation for the vertical direction follows,

$$\frac{1}{\rho} \frac{dP}{dz} = -\frac{d\phi}{dz} \quad (1.5)$$

where ρ is the gas density, P the gas pressure and ϕ the gravitational potential. Strictly speaking, both the central star and the disk material contribute to the gravitational potential, however, in most cases the disk self-gravity is negligible and therefore we consider only the stellar gravitational potential,

$$\phi = -\frac{GM_*}{(r^2 + z^2)^{1/2}} \quad (1.6)$$

For an ideal gas, pressure and density can be related such that $P/\rho = c_s^2 = kT/(\mu m_p)$, where c_s is the sound speed. The differential equation to solve for P is,

$$\frac{1}{P} \frac{dP}{dz} = -\frac{z GM_*}{c_s^2 (r^2 + z^2)^{3/2}} \quad (1.7)$$

which in the most general form can be solved through,

$$P(z) = c_s(z)^2 \rho(z) = C \exp \left(-\int \frac{z GM_*}{c_s^2 (r^2 + z^2)^{3/2}} dz \right) \quad (1.8)$$

where C is an integration constant. The latter equation describes the gas density throughout the vertical extent at each radial position, which will depend on the thermal structure through c_s . Indeed, disks are not isothermal, but it is not possible to analytically determine their thermal gradient, as it will depend on the stellar radiation parameters, dust distribution (which affect in cooling and shielding) and material density. Numerical models that aim to solve this equation must do so self-consistently, assuming a previously computed thermal structure

to iterate from (e.g., D'Alessio et al. 1998, see also Chapter 5 of this thesis). A common approximation to the vertical density distribution is to assume a thin disk such that $z \ll r$ where the disk is vertically isothermal. This simplifies our general equation as c_s will no longer have a vertical dependence, therefore the solution follows,

$$\rho(z) = \rho_c(r) \exp \left[-\frac{z^2}{(2H^2)} \right] \quad (1.9)$$

Here $\rho_c(r)$ is the gas density at the midplane ($z = 0$) and H is known as the gas pressure scale height such that,

$$H = \sqrt{k T r^3 / (\mu m_p G M_*)} = c_s / \Omega \quad (1.10)$$

where T is the midplane temperature, constant across the vertical extent in this approximation and Ω the disk angular velocity. Upcoming sections and chapters in this thesis will discuss observational proof that this is not an adequate solution to the vertical structure, however it is a first-order approximation used in many state-of-the-art hydrodynamical and thermochemical models to set the vertical material distribution.

1.3 Studying the disk vertical structure

As discussed in the previous sections, the vertical structure of disks contains information on key physical disk properties such as the thermal, ionisation and density structure, characteristic hydrodynamical instabilities and winds. However, probing this dimension observationally in large disk samples has only been possible over the past few years. Many of the data-driven advances presented in this section are also addressed in throughout the thesis and will be discussed in depth along the upcoming chapters. To avoid reiterating results, only conclusions from other groups are presented in this section.

1.3.1 Framework from theoretical models

A number of thermochemical models that account for the physics and chemistry of protoplanetary disks have been developed in the past years (e.g., D'Alessio et al. 1998; Bruderer 2013; Woitke et al. 2016), allowing for predictions and analysis focused on the thermal, chemical and density disk structure (for an overview see Dutrey et al. 2014). These models have confirmed that protoplanetary disks should be characterized by vertical and radial temperature and density gradients, affected by varying UV radiation and X-ray intensities, depending on the stellar parameters and dust properties. Indeed, it is important to consider that the dust distribution will strongly affect the gas temperature (Jonkheid et al. 2004, 2007; D'Alessio et al. 2005, 2006) which, while not a main topic of this thesis, should be a focus of future work obtaining observational constraints of the vertical distribution of both molecular gas and dust reservoirs simultaneously. Overall, in the disk vertical

extent, three regions can be characterized as shown in Figure 1.4; (1) the cold, dense and dusty midplane, (2) a warm molecular layer and (3) a hot, ionized and heavily irradiated upper disk (Aikawa & Herbst 1999; Dutrey et al. 2014).

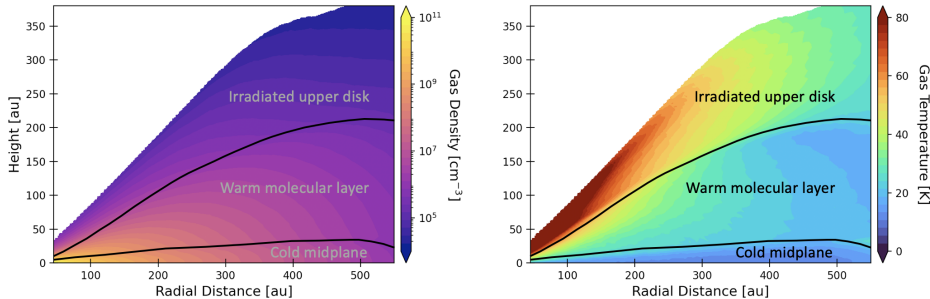


Figure 1.4: Output from thermochemical DALI (Bruderer 2013) models of the disk material surrounding a 1 solar mass star. Left panel shows the gas density distribution and the right panel displays the gas temperature, accounting for stellar, dust and molecular cooling and heating processes. Overlaid are rough estimations of the key vertical regions, the midplane, molecular layer and irradiated upper disk. Details on the model are presented in Chapter 5 of the thesis.

The dense midplane is also considered the “planet-forming zone” as larger (mm-sized) solids will settle towards it (Testi et al. 2014) and form or accrete onto planetesimals through various processes (for a review see Drażkowska et al. 2023). This region is shielded from high-energy stellar radiation through the layers of material above it, which makes it “darker” and colder than the more vertically extended material. Nevertheless, the inner ($\lesssim 10$ au) disk will be extremely hot and the high densities will allow optically thick continuum emission to be used as a probe for the dust and gas temperature in that area (which will be in equilibrium due to collisional coupling, Dutrey et al. 2014), if the spatial resolution is sufficient to avoid beam-dilution effects (Andrews et al. 2018). The outer disk midplane will be extremely cold, therefore dust grains will be covered in icy mantles, that may host a reservoir of volatile rich and organic molecules (Henning & Semenov 2013; Sturm et al. 2023).

Above the midplane, a warmer ($\gtrsim 20$ K) and less dense molecular zone is located. This molecular layer has boundaries loosely defined between the CO freeze-out and photodissociation layer (Aikawa et al. 2002). Conditions in this region have hydrogen densities of $n_H \sim 10^5$ - 10^8 cm $^{-3}$, allowing for multiple gas-phase and gas-grain reactions and leading to the synthesis of molecular species commonly observed in disks such as CO, CN, C $_2$ H, H $_2$ CO, HCN and CS, among others (Aikawa et al. 2002). Finally, a diluted, heavily irradiated and ionized layer is located at the disk surface, resembling the photodissociation regions (PDRs) at the edge of dense clouds (van Dishoeck 2006). Here ions, photostable radicals and polycyclic aromatic hydrocarbons (PAHs) may survive as molecules are photodissociated by the intense UV radiation from the central star. Atomic carbon (CI) or molecules such as C $_2$ H and CN have been proposed to be tracers of the lower boundary for

this zone, given their UV-chemistry origin (Bergin et al. 2016; Cazzoletti et al. 2018; Law et al. 2023a), however there is a lack of observational agreement or understanding about the location and properties of this region (see discussion in Urbina et al. 2024).

1.3.2 Extreme inclination disks

1.3.2.1 Edge-on

Vertical structure can be immediately accessed in edge-on disks, where high inclinations ($\gtrsim 75^\circ$) allow observations to directly probe the 2D radial and vertical material distribution. Protoplanetary disks from evolved systems (Class II, Guilloteau et al. 2016a; Dutrey et al. 2017; Louvet et al. 2018; Ruíz-Rodríguez et al. 2021; Villenave et al. 2020, 2022) and younger stars (Class I/0, Podio et al. 2020; van’t Hoff et al. 2020; Villenave et al. 2023) at high inclinations have been studied at millimeter wavelengths thorough dust continuum and molecular line emission. Figure 1.5 shows an example from dust and gas emission in an edge-on system.

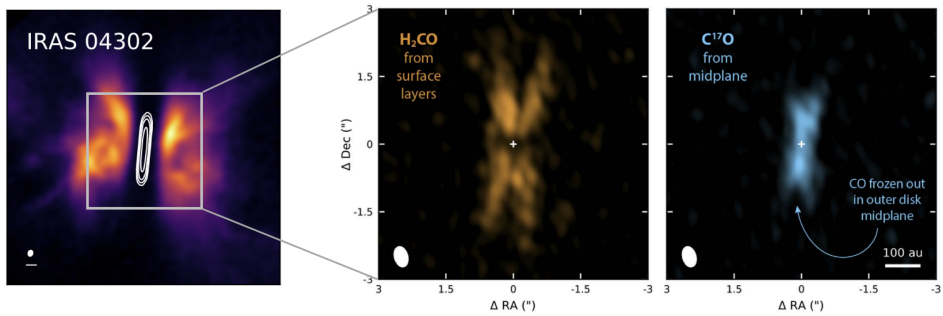


Figure 1.5: Data from edge-on source IRAS 04302. Data on left panel shows the dust continuum traced at mm wavelengths by ALMA (white contours) and the μm grains observed through scattered light (colors) shown in Villenave et al. (2020). The right two panels present molecular emission from H_2CO and C^{17}O studied in van’t Hoff et al. (2020).

Continuum emission data show that the millimeter-sized grains in Class II disks are significantly settled vertically, while earlier epochs show a measurable vertical extent or cannot be characterized due to their large optical thickness (Villenave et al. 2023, 2022). This offers observational evidence for dust settling processes affecting larger grains, while the small μm sized particles are coupled to the gas and trace a much more vertically and radially extended region. Observations of scattered light taken both from ground and space observatories show with exquisite detail the separation between the vertical zones traced by each grain size in edge-on systems (e.g., Padgett et al. 1999; Stapelfeldt et al. 2014).

Constraints from the distribution of molecular gas in edge-on disks have given crucial insight into processes such as CO freeze out (see rightmost panel in Figure 1.5) and allowed for a direct comparison to thermochemical models in order

to better understand processes affecting temperature and density throughout the disk extent (Dutrey et al. 2017; Ruíz-Rodríguez et al. 2021; van’t Hoff et al. 2020). Unfortunately, the sample of edge-on disks is a small fraction of all detected protoplanetary disks and their high inclinations make it extremely complex to compare the observed features to any azimuthal or radial structure. Attempts to deproject the emission and obtain the 3D material distribution at high inclination have been scarce due to their complexity and the need for high spatial resolution and sensitivity (e.g., Dent et al. 2014; Teague et al. 2020).

1.3.2.2 Face-on

On the other side of the inclination spectrum lie face-on disks. These low-inclination objects ($\lesssim 35^\circ$ inclination) show the 2D radial and azimuthal material distribution, but lack the orientation to easily access the vertical structure. There are many examples of such disks, more than for edge-on systems given the broader inclination range, but for this section we focus on TW Hya as a representative of face-on systems hosting a protoplanetary disk with an inclination of $\sim 6^\circ$.

TW Hya

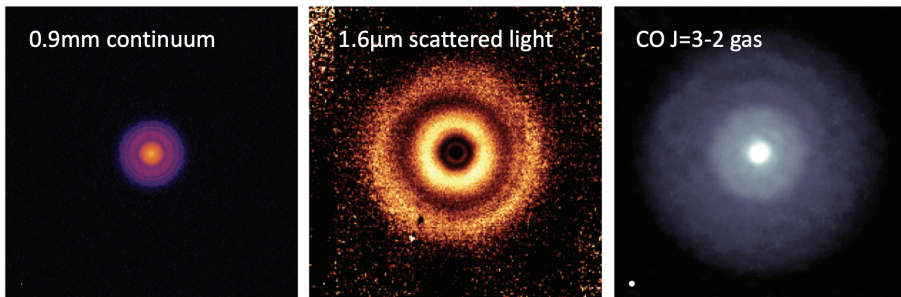


Figure 1.6: Panels with data from continuum (mm ALMA and μm scattered light) and CO gas emission observed in TW Hya. Adapted from Andrews (2020).

TW Hya is one of the most studied systems due to its closeness to earth (~ 60 pc Gaia Collaboration et al. 2023) and bright protoplanetary disk studied in dust (e.g., Kim et al. 2019; Ilee et al. 2022; Macías et al. 2021; Nomura et al. 2016; Wilner et al. 2000; Andrews et al. 2012; Tsukagoshi et al. 2022; Hogerheijde et al. 2016; Jayawardhana et al. 1999) and gas (e.g., Huang et al. 2018a; Walsh et al. 2018; Nomura et al. 2021; Teague et al. 2017; Kastner et al. 2015; Salinas et al. 2016; Yoshida et al. 2022; Rosenfeld et al. 2012; Vlemmings et al. 2019; Bergin et al. 2013; Schwarz et al. 2016; Teague et al. 2016). Adequately constraining its thermal vertical structure has been at the core of many TW Hya studies, as interpretation of the total disk mass (e.g., Calahan et al. 2021), turbulent motions (Teague et al. 2016, 2018b), dynamics (e.g., Rosenfeld et al. 2012) and dust properties (e.g., Macías et al. 2021) all require assumptions on the vertical material distribution and properties. Uncertainties in this dimension may be a reason as to why, for

example, the disk mass estimates using different tracers and approaches yields differences of up to two orders of magnitude between methods (see discussion in Miotello et al. 2023). Indeed, Calahan et al. (2021) discusses the importance of accurately defining the vertical thermal disk structure to obtain reliable results, something they achieve through a detailed fit of various molecular emission profiles. This is the challenge of face-on disk studies, while they display a unique view of radial and azimuthal substructures, interpretation of their physical properties can be hindered due to the unknown vertical properties.

A way of overcoming the challenges of accessing the vertical dimension in face-on disks is to study the kinematics, which, if the disk is not at an inclination of 0° , may offer insight into the vertical structure through its effect on the velocities (Rosenfeld et al. 2013a; Teague 2019a). However, the effect of the disk back surface will be unconstrained and could become, particularly for optically thin tracers, an important source of contamination in the data. Like in the edge-on case, it is not trivial to access all three dimensions when only two (radial and azimuthal here) are displayed clearly.

1.3.3 Mid-inclination disks

The remainder of the protoplanetary disk sample, with observed inclinations between $\sim 35\text{--}70^\circ$ are classified as mid-inclination disks. These are objects where all three dimensions may be probed. As indicated in panel (A) of Figure 1.7, the azimuthal and radial material distribution can be observed from continuum (e.g., ALMA Partnership et al. 2015; Andrews et al. 2018) or intensity-integrated moment 0 molecular emission maps (e.g., Law et al. 2021a). At millimeter wavelengths, the vertical dimension can be directly probed through the emission channel maps, following the methodology presented by Pinte et al. (2018a) which is detailed below and in the sketch of Figure 1.7. If azimuthally symmetric structures are present, scattered light images of mid-inclination disks may also be used to trace the vertical location where μm -sized grains reside (e.g., Avenhaus et al. 2018).

The method of Pinte et al. (2018a) recovers the vertical structure from a given molecule using spatially and spectrally resolved data such that the emission within multiple channel maps is resolved, this allows us to trace the maxima of emission in each channel emission. The recovered maxima is identified in cartesian coordinates such that the x -axis and y -axis fall along the semi-major and semi-minor axis respectively, as defined by the disk position angle (PA). It is assumed that for a same x position, the maxima obtained at y_n (“near” side) and y_f (“far” side) will come from the same vertical height with respect to the disk midplane. For each x position where y_n and y_f values are extracted, the coordinates of the centre of the projected circular orbit passing through the two points are (x_c, y_c) . These projected orbit coordinates relate to the stellar position (x_*, y_*) and maxima coordinates following $x_c = x_*$ and $y_c = (y_f + y_n)/2$. Considering this, for each duo of identified emission maxima at x position, a single radial (r) and height (h) point are computed accounting for the system inclination angle (i) following,

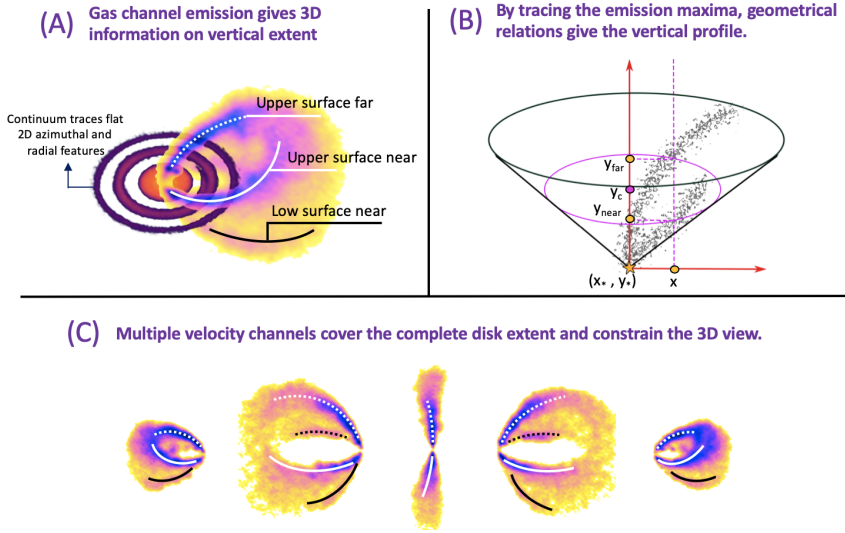


Figure 1.7: Sketch of key coordinates and steps for extracting the vertical disk profiles from emission channel maps of protoplanetary disks following the method of Pinte et al. (2018a). Panel (A) shows the position-angle corrected continuum and CO emission data, where the continuum characterizes the disk midplane and the upper and lower gas surface emission can be identified, tracing the vertical disk extent. Panel (B) presents the geometrical coordinates and assumptions used in the method, as explained in the main text. Panel (C) displays channel map emission at various velocities, where the emission maxima are traced in the upper and lower surfaces, as an example of how multiple channels are used to trace the vertical extent across the disk. Data are taken from the ^{12}CO 2 – 1 emission and 1.3mm continuum of HD 163296 (Öberg et al. 2021b).

$$r = \sqrt{(x - x_c)^2 + \left(\frac{y_f - y_c}{\cos(i)} \right)^2} \quad (1.11)$$

$$h = \frac{y_c - y_*}{\sin(i)}. \quad (1.12)$$

An overview of the methodology and coordinates is presented in Figure 1.7. This methodology has been implemented in public algorithms DISKSURF (Teague et al. 2021b) and ALFAHOR (Paneque-Carreño et al. 2023, see Chapter 3) and used in multiple studies to extract the molecular surfaces of upper and lower sides in a growing sample of disks (Pinte et al. 2018a; Rich et al. 2021; Paneque-Carreño et al. 2021, 2023, 2024; Law et al. 2021b, 2022, 2023a,b, 2024; Urbina et al. 2024; Hernández-Vera et al. 2024). Alternatively, as with the face-on disks, parametric models can be fit in the image plane to account for the vertical distribution together with other molecular emission properties such as linewidth and intensity (Rosenfeld et al. 2013a; Izquierdo et al. 2021). While parametric models can give

good estimates of the overall emission vertical location, they are generally not sensitive to any substructure or asymmetry that may be present in the surfaces.

1.3.4 Applications of vertical structure analysis in mid-inclination disks

The immediate applications of directly measuring the molecular layering in protoplanetary disks are many, depending on the selected tracers, the resolution and the available information from any radial or azimuthal structures. In this section we mention some examples of interest, many will be discussed in upcoming chapters.

By using optically thick CO isotopologues; ^{12}CO , C^{13}O and, if the disk is massive enough, C^{18}O , the temperature structure can be traced through their peak brightness temperature. The brightness temperature (T_b) relates to the effective disk temperature (T_{eff}) as $T_b \sim T_{\text{eff}}(1 - e^{-\tau})$, where τ is the optical depth of the tracer. Recent works have exploited the spatially resolved vertical and radial CO isotopologue profiles to empirically trace the 2D thermal structure (e.g., Pinte et al. 2018a; Law et al. 2021b). This provides strong constraints to benchmark thermochemical models and provides precise temperature measurements, which, for example, are critical in turbulence studies (e.g., Guilloteau et al. 2012; Flaherty et al. 2015, 2017, 2020, see Chapter 4 of this thesis for an application). For observations at lower spatial resolution or emission from less abundant complex molecules where the vertical structure may not be directly extracted, empirical thermal maps may be used to spatially locate these tracers, while their temperature is estimated using alternative methods such as rotational diagrams or hyperfine structure ratios (e.g., Ilee et al. 2021; Bergner et al. 2021).

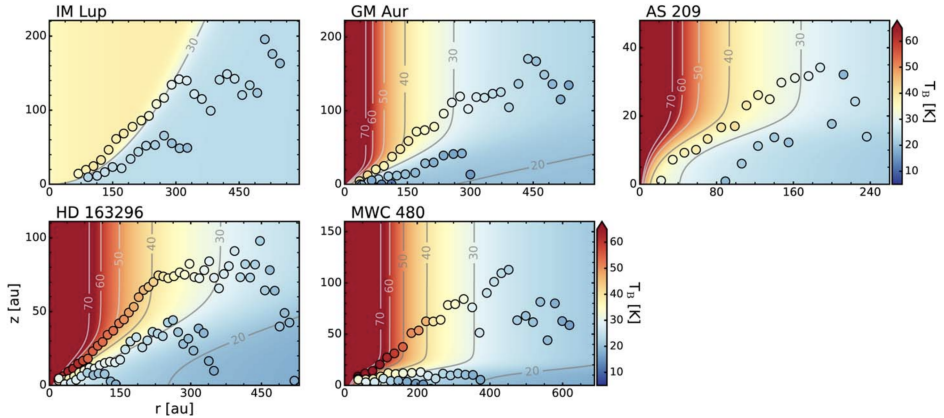


Figure 1.8: Results from empirical temperature maps extracted for the MAPS sample (Öberg et al. 2021b) by Law et al. (2021b). In each panel the circle symbols trace the optically thick CO emission surfaces and the circle colors are the peak brightness temperature extracted from the data. The colored background indicate the parametric fit to the data used to extrapolate the temperature values to other disk regions.

If spatially resolved kinematic information is available, at high spectral resolu-

tion, recent methods allow to separate the radial, azimuthal and vertical components of the material motion (e.g., Teague et al. 2018a; Pinte et al. 2023; Izquierdo et al. 2023). By combining this with the location of the vertical emission surfaces, it is possible to directly trace and test the presence of meridional flows or disk winds (Teague et al. 2019; Galloway-Sprietsma et al. 2023), crucial for understanding ongoing processes and disk dynamics.

Most recently, by tracing the vertical location of atomic carbon, early studies are being conducted to understand the disk layering and location of the hot irradiated surface (Law et al. 2023a; Urbina et al. 2024). In principle, any parameter may be traced in the vertical dimension, for example the ionization structure through observations and characterization of the HCO^+ , DCO^+ and N_2H^+ emission surfaces. Observations of UV-sensitive molecules, such as CN and C_2H will give an overview of the energetic radiation field, which studies have found may be deeper penetrating than previously expected (Ruíz-Rodríguez et al. 2021, see also Chapter 2 of this thesis).

1.4 This thesis

Recognizing the importance of characterizing the vertical protoplanetary disk structure to further understand the conditions and governing processes of planet formation, this thesis presents an in-depth observational and theoretical analysis of this third dimension. An initial question from the beginning of the PhD was if it was possible to extract vertical surfaces for molecules beyond the routinely studied CO, focusing particularly on expected tracers of the upper disk region; CN and C_2H . The existence of vertical substructure, never before characterized in detail, was also studied through the creation of a sensitive algorithm capable of accurately tracing the vertical profiles even in low signal-to-noise data. Finally, comparisons of large observational samples with thermochemical models and parametric prescriptions are done, in order to link our theoretical understanding of disk vertical structure to the observational constraints. Here is an outline of the upcoming chapters and main conclusions of this work,

Chapter 2: Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk. Based on its chemistry, cyanide (CN) emission is predicted to originate in the upper layers of protoplanetary disks, tracing UV-irradiated regions. This hypothesis, however, has been observationally tested only in a handful of disks. Elias 2-27 is a young star that hosts an extended, bright, and inclined disk of dust and gas. The inclination and extreme flaring of the disk make Elias 2-27 an ideal target to study the vertical distribution of molecules. We analyse CN $N = 3 - 2$ emission in two different transitions $J = 7/2 - 5/2$ and $J = 5/2 - 3/2$ and compare it to CO isotopologue emission. Our results show that the vertical location of CN and CO isotopologues in Elias 2-27 is layered and consistent with predictions from thermochemical models. We characterize the optical depth and column densities for CN, ^{13}CO and C^{18}O . Overall, the inferred CN column densities, low optical depth ($\tau \leq 1$), and location near the disk surface

are consistent with thermochemical disk models in which CN formation is initiated by the reaction of N with UV-pumped H_2 . This study highlights the importance of tracing the vertical location of various molecules to constrain the disk physical conditions.

Chapter 3: Directly tracing the vertical stratification of molecules in protoplanetary disks. This work focuses on showing the power of the method from Pinte et al. (2018a) to extract vertical surfaces of multiple molecular lines in a sample of protoplanetary disks. The ALFAHOR code is presented in this work, which is an implementation of the method that obtains accurate vertical profiles even for low signal-to-noise molecules implementing an interactive masking procedure. Our sample of disks consists of Elias 2-27, WaOph 6, and the five sources targeted by the MAPS ALMA Large Program (Öberg et al. 2021b). The set of molecules studied includes CO isotopologues in various transitions, HCN, CN, H_2CO , HCO^+ , C_2H , and $\text{c-C}_3\text{H}_2$. We are able to extract vertical profiles for ten different molecules and transitions in HD 163296. In the rest of the sample it is possible to vertically locate between four and seven lines. Thermal structure, gas pressure scale heights, substructure and modulations in the vertical profiles and relations to the chemical origin of each observed molecule are discussed. Overall, we show that it is possible to trace the vertical locations of multiple molecular species and relate this information to a wide variety of physical and chemical disk properties. The vertical layering of molecules is in agreement with theoretical predictions in some systems, but not in all. Therefore, dedicated physical-chemical models are needed to further study and understand the diversity of the emission surfaces.

Chapter 4: High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C_2H emission. Constraining turbulence in disks is key to understanding their evolution via the transport of angular momentum. Measurements of turbulence through its line-broadening effect rely on knowledge of the thermal conditions for the molecular emission. Combining the information on the physically resolved temperature structure that can be obtained from the vertical structure analysis, we present a new way of directly measuring turbulence without the need of complex radiative transfer or thermochemical models. This method is benchmarked using CN and C_2H molecular emission from the protoplanetary disk of IM Lup. Our analysis retrieves high turbulence of Mach 0.4-0.6 at $z/r \sim 0.25$. Considering previous estimates of low turbulence near the midplane, this may indicate for the first time evidence of a vertical gradient in the disk turbulence, which is a key prediction of magneto rotational instabilities that may be occurring in the IM Lup disk.

Chapter 5: Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion. The growing sample of mid-inclination disks with measured CO emission surfaces grows and a fundamental but unanswered question is how these vertical profiles connect to their host properties. In this chapter we address this question by using thermochemical models to study the protoplanetary

disk parameters that most affect the recovered CO $J = 2 - 1$ emission surfaces. The modelling predictions are benchmarked against data of CO emission from nineteen disks. We find that the CO emission surface is most affected by the total disk mass (M_d) and volatile carbon abundance. A z/r - M_d relationship is derived, which varies depending on the carbon abundance. In order to reconcile total disk mass estimates from the characteristic z/r and the values obtained based on dust continuum analysis, a volatile carbon depletion of 10-100 (with respect to the ISM) is needed for the majority of our sources.

The main results and conclusions of this thesis are the following;

1. Vertical emission surfaces of molecules in protoplanetary disks can be directly extracted from ALMA observations of gas emission in mid-inclination disks. This is possible even for optically thin and low signal-to-noise molecular tracers. (*Chapters 2, 3, 4*)
2. The disk thermal structure follows a radial and vertical gradient. This can be empirically probed using optically thick tracers such as ^{12}CO and ^{13}CO . The physical conditions of the gas (e.g., turbulence and density) may be inferred by combining the thermal structure with information on the spatial location from various molecules. (*Chapters 2, 3, 4*)
3. CO isotopologues show a clear vertical layering, with ^{12}CO being the most vertically extended tracer and both ^{13}CO and C^{18}O $J = 2 - 1$ tracing similar regions. (*Chapters 2, 3*)
4. CN $3 - 2$ and C_2H $4 - 3$ emit from a vertically constrained and mostly optically thin slab high up in the disk. This is in agreement with theoretical predictions and makes them ideal tracers of the conditions and location of the upper disk layers. (*Chapters 2, 4*)
5. Vertical emission surfaces of various molecular tracers display modulations and peaks (vertical sub-structure). In the case of CO isotopologues these are correlated with the radial location of millimetre continuum gaps and kinematic perturbations. (*Chapter 3*)
6. Turbulence may have higher values in the upper disk layers than the mid-plane. The empirically-derived thermal structure can be combined with spatially resolved emission from optically thin molecules to directly measure turbulence across the disk extent using a simple parametric model. (*Chapter 4*)
7. Total disk mass and volatile carbon depletion can be probed through the vertical location of the CO emission surface using a $z/r - M_d$ relationship. (*Chapter 5*)
8. Most protoplanetary disks show indications of volatile carbon depletion, between 1-2 orders of magnitude with respect to the ISM. T Tauri disks are more carbon depleted than Herbig systems. (*Chapter 5*)

1.4.1 Future prospects

Studies of vertical disk structure in large samples have only just begun, to date only ~ 20 disks have vertical CO surfaces characterized and ~ 8 (Paneque-Carreño et al. 2023; Law et al. 2024) have measured vertical profiles of more than three different molecules. The overall work from this thesis has shown that it is possible to use ALMA observations to observationally study the vertical molecular layering and relate it to a number of physical processes.

Future work must focus on expanding the sample of disks with characterized molecular surfaces and combine the chemical information with knowledge on the dust grain distribution to accurately characterize disk processes. This requires high spatial and spectral resolution observations of molecules beyond CO, which is typically time consuming due to the low signal-to-noise of less abundant tracers. Looking forwards to the ALMA Wideband Sensitivity Upgrade, in the upcoming years it will be possible to do these studies in less times and larger samples. Small μm -sized dust, as traced by scattered light images, plays a key role in regulating the thermal and radiation fields towards the disk. Combining information from the solid and molecular material distributions will allow us to obtain a much better overview of the disk conditions.

Characterizing turbulence in disks or localizing features related to winds through tracers of the upper disk atmosphere will also be an interesting avenue of research in the coming years. Both of these processes have been suggested to drive disk evolution, but the complexity of detecting them has made them difficult to study. Through the analysis of vertical structure in mid-inclination disks a new avenue of observational constraints for these theories opens. In particular, high spatial and spectral resolution observations of CN $3-2$ and $\text{C}_2\text{H } 4-3$ in ALMA Band 7, together with atomic Carbon at higher frequencies, should be key targets for this goal.

This thesis has shown that CO surfaces, combined with other methods, may be good probes of disk mass and volatile carbon depletion, other molecules must also be studied to see how their location may be exploited to learn about their host's properties. It is expected that UV tracers might be strongly affected by stellar parameters, or maybe less abundant CO isotopologues could be more sensitive to other parameters beyond the mass. Dedicated thermochemical models that test these hypothesis will be useful as the number of disks with molecular surfaces grows.

Overall, the possibility of studying the planet-forming material distribution across all three dimensions offers unique insight into the process of forming planets. Observational constraints are now catching up to the questions posed by theoretical models, which must be revised in order to explain the observed features. In the same way that for the past decade studies have focused on explaining the existence of radial and azimuthal substructure, we must now look at the third dimension and digest the information that comes from it. The techniques and results from this thesis have laid the foundations for many future studies that will for sure answer the questions we have left open.

Chapter 2

Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk

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Astronomy & Astrophysics, 666, A168, (2022)

Abstract

Context: Cyanide (CN) emission is expected to originate in the upper layers of protoplanetary disks, tracing UV-irradiated regions. This hypothesis, however, has been observationally tested only in a handful of disks. Elias 2-27 is a young star that hosts an extended, bright, and inclined disk of dust and gas. The inclination and extreme flaring of the disk make Elias 2-27 an ideal target to study the vertical distribution of molecules, particularly CN.

Aims: Our aim is to directly trace the emission of CN in the disk around Elias 2-27 and compare it to previously published CO isotopolog data of the system. The two tracers can be combined and used to constrain the physical and chemical properties of the disk. Through this analysis we can test model predictions of CN emission and compare observations of CN in other objects to the massive, highly flared, asymmetric, and likely gravitationally unstable protoplanetary disk around Elias 2-27.

Methods: We analyzed CN $N = 3 - 2$ emission in two different transitions $J = 7/2 - 5/2$ and $J = 5/2 - 3/2$, for which we detect two hyperfine group transitions. The vertical location of CN emission was traced directly from the channel maps, following geometrical methods that had been previously used to analyze the CO emission of Elias 2-27. Simple analytical models were used to parameterize the vertical profile of each molecule and study the extent of each tracer. From the radial intensity profiles we computed radial profiles of column density and optical depth.

Results: We show that the vertical location of CN and CO isotopologs in Elias 2-27 is layered and consistent with predictions from thermochemical models. A north–south asymmetry in the radial extent of the CN emission is detected, which is likely due to shadowing on the north side of the disk. Combining the information from the peak brightness temperature and vertical structure radial profiles, we find that the CN emission is mostly optically thin and constrained vertically to a thin slab at $z/r \sim 0.5$. A column density of 10^{14} cm^{-2} is measured in the inner disk, which for the north side decreases to 10^{12} cm^{-2} and for the south side to 10^{13} cm^{-2} in the outer regions.

Conclusions: In Elias 2-27, CN traces a vertically elevated region above the mid-plane, very similar to that traced by ^{12}CO . The inferred CN column densities, low optical depth ($\tau \leq 1$), and location near the disk surface are consistent with thermo-chemical disk models in which CN formation is initiated by the reaction of N with UV-pumped H_2 . The observed north–south asymmetry may be caused by either ongoing infall or by a warped inner disk. This study highlights the importance of tracing the vertical location of various molecules to constrain the disk physical conditions.

2.1 Introduction

Protoplanetary disks are the formation sites of planetary systems. Studying the dust and gas components of these disks is crucial for understanding the origin and composition of planets (Andrews 2020). Analyzing the radial and vertical distribution of molecular tracers within a protoplanetary disk offers spatially located information on the temperature gradient, abundances, and physical conditions of a system (e.g., Law et al. 2021a,b; Guzmán et al. 2021). To conduct these studies, high spectral and spatial resolution observations are required, a task that has been possible in recent years with the Atacama Large Millimeter/submillimeter Array (ALMA). To date, high-resolution studies have been biased toward a few of the brightest and largest sources in the dust continuum (Andrews et al. 2018; Öberg et al. 2021b) and/or toward studying the most abundant and brightest molecular tracers, mostly common CO isotopologs (Ansdell et al. 2018; Long et al. 2017; Barenfeld et al. 2016; Miotello et al. 2017; Piétu et al. 2014; van der Marel et al. 2015, 2016). Less abundant molecules have also been studied in some sources at lower spatial and/or spectral resolution (Kastner et al. 2018; Bergner et al. 2018; Miotello et al. 2019; Anderson et al. 2019; Bergner et al. 2019; Le Gal et al. 2019; Garufi et al. 2021; Ilee et al. 2021; Guzmán et al. 2021). These studies have shown the potential of other tracers to give us information not only on chemical abundance and spatial location, but also on temperature profiles, density, ionization, atomic ratios, and kinematics (see Öberg et al. 2021b; Öberg & Bergin 2021b, for a complete overview and review).

Studying various molecular tracers is key to completing our understanding of the disk structure, which can be vertically divided into three distinct zones: 1) a hot atmosphere mainly populated by atomic gas, heavily irradiated by energetic UV photons and X-rays from the star, as well as cosmic rays from the environment; 2) a warm molecular layer where most of the chemical interactions occur and molecules may reside in gas phase; and 3) a cold midplane where larger grains of dust are found and some simple molecules may be present in gas phase, although most of the molecules are found in ice form coating the dust grains (Aikawa et al. 2002; Bergin et al. 2007; Henning & Semenov 2013; Dutrey et al. 2014). To gain information on the whole disk structure, we must characterize the emission from molecules residing in the various layers (e.g., van Zadelhoff et al. 2001; Law et al. 2021b).

Cyanide (CN) is a molecule that is abundant enough to be bright and observable in relatively short integration times (Kastner et al. 2008; van Terwisga et al. 2019). Theoretically, its main formation pathway is the reaction of N with vibrationally excited H_2 , through UV pumping of H_2 , which occurs in the uppermost regions of the disk atmosphere (Cazzoletti et al. 2018; Visser et al. 2018). This enables CN to be a unique tracer of the upper disk structure and UV radiation from photons of wavelengths $< 105 \text{ nm}$ (Bergner et al. 2021; Heays et al. 2017). CN also has multiple hyperfine structure transitions, which come from the splitting of energy levels by nuclear magnetic interactions. Studying the hyperfine structure components allows us to directly determine various physical properties, such as the density and optical depth of the emission (e.g., Goldsmith & Langer 1999; Loomis

et al. 2018; Facchini et al. 2021). The study of multiple CN hyperfine transitions has been possible in TW Hya (Kastner et al. 2014; Teague et al. 2016; Teague & Loomis 2020), V4046 Sgr (Kastner et al. 2014), and more recently in HD 163296 (Bergner et al. 2021).

Individual analyses of resolved sources have shown ring-like CN emission in disks (van Terwisga et al. 2019; Teague & Loomis 2020; Bergner et al. 2021). This was predicted by Cazzoletti et al. (2018) as a consequence of CN formation mediated by the balance of excited H_2 , via far-ultraviolet (FUV) pumping and the collisional de-excitation of H_2 . More recently, using models of UV radiation, Bergner et al. (2021) show that the radial extent and morphology of the CN emission in various systems is in agreement with the variations in the UV flux from photons with wavelengths of 91-102 nm. Observational studies are consistent with theoretical predictions that CN emission traces zones of UV radiation, regions at about $z/r \sim 0.2 - 0.4$ (Teague & Loomis 2020; Ruíz-Rodríguez et al. 2021; Bergner et al. 2021). However, the height of the emission in observations has mostly been determined indirectly through models (Bergner et al. 2021) or temperature estimates (Teague & Loomis 2020). To the best of our knowledge, a direct measurement of the CN emitting layer in a protoplanetary disk of a Class II stellar source has only been done in the edge-on system known as the Flying Saucer (Ruíz-Rodríguez et al. 2021).

In this study we present new CN observations of the disk surrounding Elias 2-27, a Class II young stellar object (Andrews et al. 2009, 2018), which has been proposed to host a massive ($\sim 17\%$ of the stellar mass, Veronesi et al. 2021) protoplanetary disk currently undergoing gravitational instability (GI) (Pérez et al. 2016; Huang et al. 2018c; Paneque-Carreño et al. 2021). Elias 2-27 is located in the star-forming region of ρ Oph, at a distance of 115.8 pc (Gaia Collaboration et al. 2018). Dust continuum observations at multiple wavelengths show a symmetric double-spiral morphology (Pérez et al. 2016; Huang et al. 2018c; Paneque-Carreño et al. 2021), with signatures of dust trapping along the spirals (Paneque-Carreño et al. 2021). Spectral line studies have been challenging, even with bright tracers like isotopologs of CO $J = 2 - 1$, due to the heavy cloud absorption that affects the system (Pérez et al. 2016; Andrews et al. 2018; Pinte et al. 2020). For this reason, previous attempts to observe CN $N = 2 - 1$ were unsuccessful (Reboussin et al. 2015). Recently, Paneque-Carreño et al. (2021) presented C^{18}O and ^{13}CO $J = 3 - 2$ data that are much less affected by absorption, showing that higher energy transitions can be used to characterize the gas structure and kinematics of the source.

Thanks to the inclination of the system (56.2° , Huang et al. 2018b) Elias 2-27 is a prime target to study both the radial distribution and the vertical location of any molecular tracer. A study of the vertical structure of Elias 2-27 was done using C^{18}O and ^{13}CO data by Paneque-Carreño et al. (2021), directly tracing the emission from the channel maps and applying geometrical methods to obtain the emitting surface (following the method outlined in Pinte et al. 2018a). In the CO isotopolog data an asymmetry in the vertical structure between the east and west sides of the disk was found and the origin of this variation was proposed to be ongoing infall (Paneque-Carreño et al. 2021). We expect CO isotopologs to trace

the intermediate layer of the disk (Bergin et al. 2007; Dutrey et al. 2014), and CN to contain information on the upper layers of the disk (Cazzoletti et al. 2018).

Using the disk structure as traced with CN we can compare the distribution of CN against the asymmetries found in CO isotopologs. The constraints provided on the location of the CN emission in Elias 2-27 can be compared with theoretical models of CN (Cazzoletti et al. 2018) and previous observations of other systems (Teague & Loomis 2020; Ruíz-Rodríguez et al. 2021; Bergner et al. 2021). Finally, combining the information on the emission and location of the available tracers, we can study the overall temperature, column density, and distribution of molecules in the source.

As Elias 2-27 is the first system to show strong evidence, in multiple tracers, of being gravitationally unstable (Pérez et al. 2016; Paneque-Carreño et al. 2021) it is also an excellent test-case for predictions of GI chemistry (Ilee et al. 2011; Evans et al. 2015). In particular, CN has been predicted to be a good tracer of GI due to the temperatures along the GI spirals. The temperature in the spirals depends on how massive the disk is, but can reach values of up to ~ 400 K (inner ~ 20 au, Evans et al. 2015); at these high temperatures CN would be destroyed due to its reaction with NH_3 (Evans et al. 2015) or H_2 (Visser et al. 2018). However, in the outer parts of the disk, the spirals may have more moderate temperatures and reach values that would lead to CN being desorbed from the dust grains in the midplane. The desorption temperature of CN is around 120 K (Evans et al. 2015); therefore, if this temperature is reached and CN is emitted from the midplane, it may trace the spiral arms as seen in the dust continuum.

The paper is organized as follows. Section 2 describes the imaging procedure and main observed features. Section 3 details the analysis of the vertical location of the CN emission, comparing it to the available CO tracers in Elias 2-27. Section 4 presents the results obtained from CN emission, and we study the asymmetries in the emission extent of the disk. Section 5 describes the derived temperature structure, abundance, and optical depth of the disk emission. Section 6 discusses the implications of our findings and section 7 lists our main conclusions.

2.2 Observations

2.2.1 Self calibration and imaging

We present the analysis of CN $v = 0$, $N = 3 - 2$ in $J = 7/2 - 5/2$ ($E_u = 32.67$ K) and $J = 5/2 - 3/2$ ($E_u = 32.63$ K) emission of the disk around Elias 2-27. The data are part of ALMA programs 2016.1.00606.S and 2017.1.00069.S, and were obtained simultaneously with C^{18}O and ^{13}CO ($J = 3 - 2$) spectral line observations presented in Paneque-Carreño et al. (2021) and also used in this work. The calibration, imaging, and initial analysis of C^{18}O and ^{13}CO is described in Paneque-Carreño et al. (2021). Additionally, we use archival ^{12}CO $J = 2 - 1$ data obtained as part of the DSHARP program (Andrews et al. 2018). Calibration and imaging details for ^{12}CO can be found in the original DSHARP papers (Andrews et al. 2018; Huang et al. 2018c).

The spectral windows for the CN $v = 0$, $N = 3 - 2$ observations are centered at 340.248 GHz ($J = 7/2 - 5/2$) and 340.014 GHz ($J = 5/2 - 3/2$), respectively, with a spectral resolution of 0.2 MHz. For the $J = 5/2 - 3/2$ data we measured two peaks of line emission in the border channels, at 340.035 GHz and 340.031 GHz. This corresponds to the blended emission from hyperfine transitions $F = 3/2 - 1/2$ and $F = 5/2 - 3/2$ (340.035 GHz) and emission from hyperfine transition $F = 7/2 - 5/2$ (340.031 GHz). The CN $J = 5/2 - 3/2$ fine structure group has two other hyperfine components that we do not detect, $F = 5/2 - 5/2$ (340.008 GHz) and $F = 3/2 - 3/2$ (340.019 GHz), which are the transitions with the lowest relative intensities within the group (0.054 each, where a value of 1 is the total intensity of the group; Hily-Blant et al. 2017, and references therein). In the CN $J = 7/2 - 5/2$ group the emission we measure is the blended contribution from hyperfine components $F = 7/2 - 5/2$, $F = 9/2 - 7/2$ (both 340.247 GHz) and $F = 5/2 - 3/2$ (340.248 GHz). In this group we do not detect emission from the lowest relative intensity components $F = 5/2 - 5/2$ (340.261 GHz) and $F = 7/2 - 7/2$ (340.265 GHz), (relative intensity of 0.027 each, where 1 is the total intensity of the group; Hily-Blant et al. 2017, and references therein). As the CN data were obtained simultaneously with Band 7 continuum (0.89 mm) observations, we applied the self-calibration solutions of that continuum dataset to the CN measurements (for details see Paneque-Carreño et al. 2021).

Previous CO data show that Elias 2-27 presents extended large-scale emission (Paneque-Carreño et al. 2021). We checked for any large-scale structure in the CN transitions by imaging the whole field of view available for CN using a robust parameter of 2.0. We did not detect any large-scale emission up to a sensitivity of $2.2 \text{ mJy beam}^{-1}$. Even with the non-detection of large-scale structure, we performed the final CN imaging using **uvrange** to ensure we were imaging emission only from disk scales. Additionally, **uvtaper** was applied to obtain a roughly round beam, which facilitates the analysis and comparison between transitions.

The CN $J = 7/2 - 5/2$ emission was imaged with a robust parameter of 1.3 and we used **uvrange** to only consider baselines larger than 34 m, excluding any possible emission from scales larger than $6.5''$ (750 au, at 115 pc). We applied **uvtaper** of $0.175'' \times 0''$ and obtained a final beam of $0.29'' \times 0.29''$ (34 au, at 115 pc). CN $J = 5/2 - 3/2$ was imaged with robust parameter 1.8, applying **uvrange** to use only baselines over 35 m (excluding emission larger than $6''$) and with **uvtaper** of $0.18'' \times 0.01''$ to achieve a final beam of $0.3'' \times 0.3''$ (35 au, at 115 pc).

2.2.2 Emission morphology and line ratios

For easier identification, hereafter we refer to the blended CN $J = 7/2 - 5/2$ emission as CN-1 and to the $J = 5/2 - 3/2$ group (two emission peaks) as CN-2; the blended emission at 340.035 GHz and 340.031 GHz is labeled hf1 and hf2, respectively. The integrated intensity maps of each CN transition are shown in the top row of Figure 2.1, together with a 240 GHz high-resolution continuum image of Elias 2-27 (Andrews et al. 2018). The bottom row shows the integrated spectra of the observations. This figure shows that the CN emission has an asymmetrical distribution between the north and south sides of the disk in all transitions. The

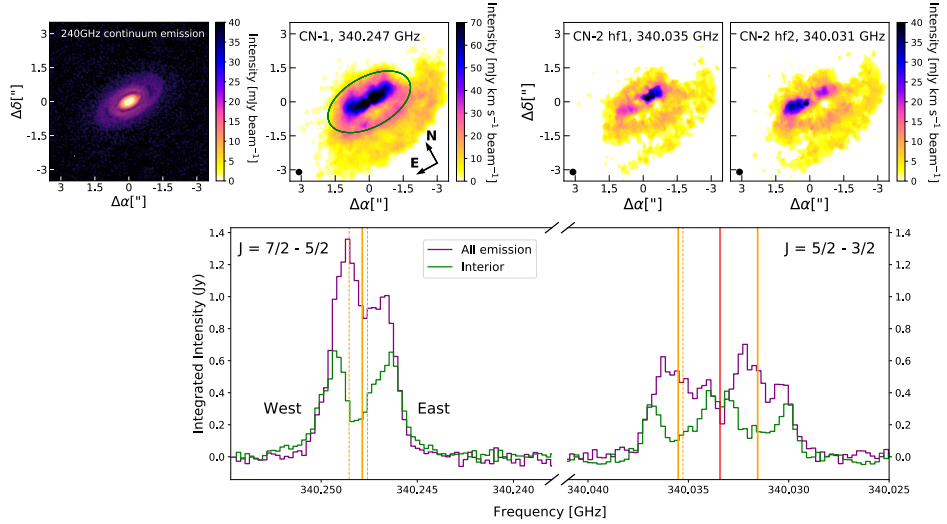


Figure 2.1: Continuum and CN datasets for Elias 2-27. Top row: High-resolution 240 GHz dust continuum emission (left). The subsequent panels (from left to right) show the integrated intensity (zeroth moment) for CN $J = 7/2 - 5/2$ (CN-1), and the CN $J = 5/2 - 3/2$ hyperfine group transitions at ~ 340.035 GHz (CN-2 hf1) and ~ 340.031 GHz (CN-2 hf2). The frequency of each group is shown at the top of each panel and the ellipses in the bottom left corners show the beam size. In the left panel the green ellipse indicates the region within 230 au from the center (interior region), assuming a flat geometry. Bottom row: Disk integrated spectrum for the whole emitting region (in purple) and for only the interior region (in green). The orange vertical lines indicate the hyperfine transition frequencies that are blended in each peak. When there are multiple transitions, the solid vertical line indicates the one with the higher relative intensity (values in Table 4.1). The red vertical line is the separation between the CN-2 hyperfine groups

emission is centrally peaked and elongated along the major axis; however, toward the north there is not much emission beyond the bright inner region. On the south side of the disk, the emission extends up to $\sim 2''$ in the sky plane from the center and shows arc-like features. The CN-2 integrated emission (mom0) maps were computed by visual identification of the two hyperfine lines in the integrated spectrum, and a separation between them was set at 340.033 GHz (see red line in Fig. 2.1, bottom panel). Relative to their respective central frequencies, CN-2 hf1 lacks redshifted emission (spatially located on the east side) and CN-2 hf2 is missing blueshifted emission (spatially located on the west side). The differences observed in the central emission between the east and west sides of CN-2 hf1 and hf2 (top right panels of Figure 2.1) are likely artificial and due to the channel selection when computing the zeroth moment map.

Two spectra are displayed for each transition group (bottom panel in Figure 2.1). The purple spectrum is from the complete emitting region of the disk; the green spectrum was obtained from the region within 230 au of the star, considering a flat geometry. In all groups the purple spectrum shows a higher intensity toward redshifted frequencies with respect to the central frequency of the strongest transition (solid orange vertical line). This peak of emission corresponds spatially to the west side of the disk and the asymmetry is not seen in the spectrum from the interior region. We can visually assess that beyond the interior region there is further emission in the south of the disk that is more azimuthally extended toward the west side. Therefore, the flux difference in the spectrum is tracing an emission asymmetry between the east and west sides of the disk at large radii. From CO observations it is known that Elias 2-27 is largely affected by cloud absorption on the east side of the disk (Pérez et al. 2016; Huang et al. 2018c); however, we do not see a flux difference in the CN emission when considering only the interior region. We hence consider it unlikely that the flux asymmetry of CN at large scales (>230 au) is caused by cloud absorption. The visually identified emission extension difference between north and south is studied in detail in Section 4.

Table 4.1 shows the molecular line data from the literature and the measured integrated fluxes for the detected CN transitions and CO lines that are used in the remainder of this work. In Appendix B we explain the procedure to determine the integrated flux and associated errors for each tracer, and the integrated emission maps and spectra are presented for each CO line (Figure 2.B.1). We compare the integrated flux ratios of the CN emission to the expected ratio values, obtained from the relative intensities (R.I.s, see Table A.1 in Hily-Blant et al. 2017) and the Einstein emission coefficient (A_{ul}) of each hyperfine component. The R.I. value is normalized so that within each fine structure group the total sum of all individual values equals unity (Hily-Blant et al. 2017). Our table shows the R.I. values only for the transitions that are detected; therefore, the values within each group do not sum to unity. We separated the CN-2 emission into hf1 and hf2; however, they are both from the same fine structure group $J = 5/2 - 3/2$ and can be easily compared. The emission labeled hf1 has two blended components; their R.I.s sum to 0.448. CN-2 hf2 has only one hyperfine transition that accounts for 0.445 of the group intensity. Therefore, the expected intensity ratio of the two components is $\text{hf1/hf2} = 0.448/0.445 = 1.01$. From the integrated emission values

Table 2.1: Molecular line data, values from CDMS catalog (Müller et al. 2001)

Species	J Transition	F Transition	Frequency (GHz)	E_u (K)	A_{ul} (s^{-1})	g_u	R.I. [*]	Int. Flux ^{**} (Jy km s $^{-1}$)
^{12}CO	$J = 2 - 1$		230.5380000	16.59	6.91×10^{-7}	5		29.61 ± 1.28
^{13}CO	$J = 3 - 2$		330.5879653	31.73	2.19×10^{-6}	14		22.26 ± 0.09
C^{18}O	$J = 3 - 2$		329.3305525	31.61	2.17×10^{-6}	7		4.45 ± 0.06
CN-1	$J = 7/2 - 5/2$	$F = 7/2 - 5/2$	340.247590 ^a	32.67	3.797×10^{-4}	8	0.307	3.55 ± 0.07
		$F = 9/2 - 7/2$	340.247861 ^a	32.67	4.13×10^{-4}	10	0.417	
		$F = 5/2 - 3/2$	340.248544	32.67	3.67×10^{-4}	6	0.222	
CN-2 hf1	$J = 5/2 - 3/2$	$F = 3/2 - 1/2$	340.035269 ^b	32.63	2.89×10^{-4}	4	0.167	1.49 ± 0.08
		$F = 5/2 - 3/2$	340.035507 ^b	32.63	3.23×10^{-4}	6	0.281	
CN-2 hf2	$J = 5/2 - 3/2$	$F = 7/2 - 5/2$	340.0315494	32.63	3.85×10^{-4}	8	0.445	1.62 ± 0.08

Notes. ^(*) Relative intensity values for hyperfine CN transitions obtained from Hily-Blant et al. (2017) and references therein. ^(**) Integrated flux values and their uncertainties for the CN lines calculated from the emission spectra in Figure 2.1, and in the same way for CO isotopologs from Figure 2.B.1 ^(a) Value in CDMS catalog is 340.247700 for both; new value from Teague & Loomis (2020) ^(b) Value in CDMS catalog is 340.0354080 for both; new value from Teague & Loomis (2020).

we calculate that $hf1/hf2 = 1.49/1.62 = 0.92 \pm 0.07$ (the error obtained considering the propagation of uncertainties listed in Table 4.1). The ratio calculated from observational constraints is very close to the theoretical prediction and suggests that CN-2 is optically thin emission.

To compare CN-1 with CN-2 we take into account the ratio of the Einstein coefficients, as the emission is from different fine structure groups (Hily-Blant et al. 2017). The total relative intensity for the blended CN-1 emission is 0.946. To calculate the expected intensity ratio with CN-2 hf2 we calculate $(0.946/0.445) \times (4.13 \times 10^{-4}/3.85 \times 10^{-4})$, where the second term is the Einstein coefficient ratio. For multiple blended transitions we use the coefficient value of the hyperfine component with the highest relative intensity in the group. The expected ratio of CN-1 to CN-2 hf2 is then 2.28; for CN-1 to the full CN-2 emission (both peaks) the expected ratio is 1.14. From the integrated intensity, the observational ratios are 2.19 ± 0.12 and 1.14 ± 0.05 . As in the comparison between CN-2 peaks, the theoretical and observational values are very similar, indicating that overall CN emission is likely to be optically thin. It is important to note that when the flux ratios are close to unity they do not provide a strong discriminant between optically thick and thin regimes, even if the theoretical prediction matches the observed values, as is the case here. In section 5 we present an independent way to determine the optical depth and physical properties of the CN emission.

2.3 Vertical structure analysis

2.3.1 Height of CN emission

A selection of the channel maps showing the emission from each CN transition is displayed in Figure 2.2. We note that for CN-2 the top row shows emission from hf1 and the bottom row from hf2 transitions. For the complete map with all available channels, see Figures 2.A.1 and 2.A.2 for CN-1 and CN-2, respectively. The systemic velocity of the system is determined to be $V_{LSR} \sim 1.95 \text{ km s}^{-1}$ (Paneque-Carreño et al. 2021). From the channel maps we identify that the emission does not come from the midplane, but rather originates from a constrained and flared vertical layer. This can be deduced from the separation between the emission from the lower and upper layers, which were visually identified (see Figure 2.2) and indicate the vertical location of the gas emission with respect to the disk midplane, as observed from our line of sight. These layers can be visually identified from the channel maps aided by the prior information on the CO distribution (Paneque-Carreño et al. 2021) and the geometry of the system (Huang et al. 2018c). To extract the radial vertical profile we applied the method developed by Pinte et al. (2018a), which directly traces the emitting surface from the channel maps. This was done by following the maxima of emission along the upper layer in channels where it is possible to identify the far and near sides of the upper layer (for a detailed sketch see Figures 2 and 3 of Pinte et al. 2018a). This method was used for the extraction of the $C^{18}O$ and ^{13}CO vertical emitting layer in Elias 2-27 (Paneque-Carreño et al. 2021) and in various works, for other sources and/or CO isotopologs (e.g., Law et al. 2021b; Rich et al. 2021; Leemker et al. 2022).

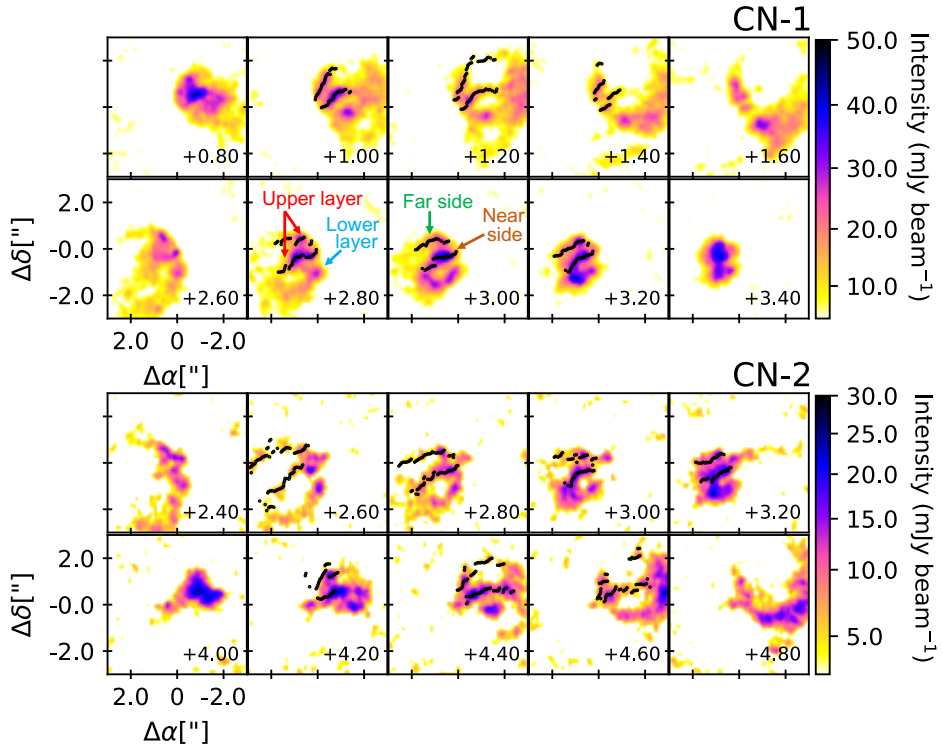


Figure 2.2: Selection of channel maps for CN-1 (top) and CN-2 (bottom) emission. The number in the top right corner of each panel shows the channel velocity (systemic velocity is 1.95 km s^{-1}), and the ellipse in the bottom left corner the beam size. For the channels used to derive the vertical profile, black dots trace the peak intensity locations along the upper layer of emission. Upper and lower layers of emission, as well as far and near sides of the emission are identified for reference in the bottom panels of the CN-1 emission. A complete panel of the channel map emission is presented in Appendix A for each transition.

The channels used for this analysis are those between (and including) $1.0\text{--}1.4 \text{ km s}^{-1}$ and $2.8\text{--}3.2 \text{ km s}^{-1}$ in CN-1, $1.0\text{--}1.2 \text{ km s}^{-1}$ and $2.6\text{--}3.2 \text{ km s}^{-1}$ for CN-2 hf1, and $4.2\text{--}4.6 \text{ km s}^{-1}$ and $6.0\text{--}6.4 \text{ km s}^{-1}$ for CN-2 hf2. The selection of channels was done through visual inspection, choosing those where it was possible to identify the upper layer on the near and far sides. Each selected channel was rotated to correct for the disk position angle and to work in Cartesian coordinates for the extraction of the emission maxima (for details, refer to Figure 2 in Pinte et al. 2018a). From the rotated channel emission, we masked the near and far sides of the upper layer. The pixel of peak intensity is automatically identified from the pixels within the mask, sampling every quarter of the beam along the disk major axis. Figure 2.2 shows the retrieved peak intensity values (black dots) of the upper layer in some of the selected channels. The height of the emission at a given radial

distance is retrieved by applying geometrical relations to the Cartesian location of the emission maxima (for details refer to Pinte et al. 2018a).

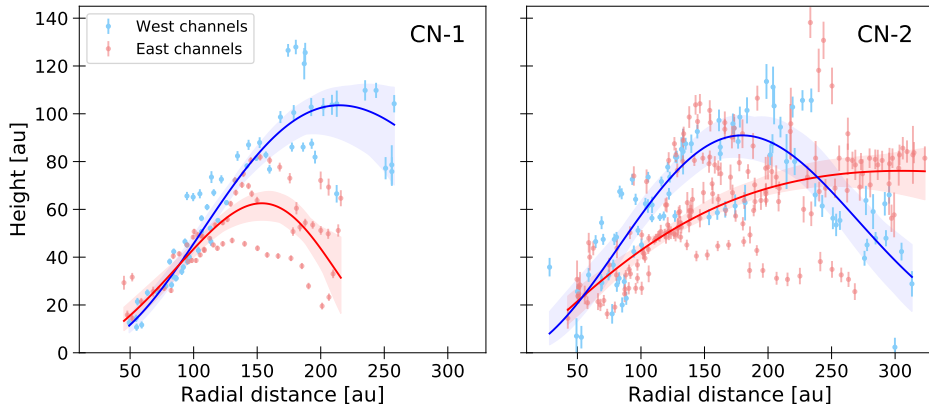


Figure 2.3: Vertical location of emission from CN-1 (left) and CN-2 (right) transitions, using data obtained from the channel map analysis of the emission. The dataset is separated between the east (red dots) and west (blue dots) sides of the disk, as defined by the semi-minor axis. The solid blue and red curves trace the best-fit exponentially tapered model of each side. The colored regions show the uncertainty of the model, obtained from the spread of the posterior values from our MCMC analysis.

It has been shown for the CO isotopologs that the emission from the east side of the disk appears to be coming from a layer closer to the midplane than the west side of the disk (Paneque-Carreño et al. 2021). Considering this, we divided the data analysis for CN between east and west sides of the disk, as defined by the projected minor axis. Figure 2.3 shows the extracted vertical profiles of each CN transition. The data are fitted using an exponentially tapered power law defined as

$$z(r) = z_0 \times \left(\frac{r}{100 \text{ au}} \right)^\phi \times \exp \left[\left(\frac{-r}{r_{\text{taper}}} \right)^\psi \right], \quad (2.1)$$

where r is the radial distance from the star along the midplane. The best-fit parameters of the final model are obtained from the median value of the posteriors using a Markov chain Monte Carlo (MCMC) simulation (Goodman & Weare 2010) as implemented by `emcee` (Foreman-Mackey et al. 2013). The best-fit values of each parameter and its uncertainties (16th and 84th percentile uncertainties derived from the posteriors) are shown in Table 2.2.

Figure 2.4 shows the extracted data points separated by disk sides and hyperfine structure. It is apparent that the data from the west side of the disk are consistent between the various transitions, and the best-fit vertical profiles of CN-1 and CN-2 trace the same region, within their uncertainties. The vertical structure from the east side of the disk shows a large scatter in the extracted data, which makes the results vary largely between the CN-1 and CN-2 emission. The scatter

Table 2.2: Best-fit model parameters of exponentially tapered vertical profiles from channel analysis. The data are presented in Figure 2.3.

Transition	side	z_0 [au]	ϕ	r_{taper} [au]	ψ
CN-1	W	$59.5^{+16.78}_{-9.07}$	$2.25^{+0.24}_{-0.27}$	$196.53^{+35.86}_{-38.39}$	$1.96^{+0.69}_{-0.47}$
CN-1	E	$46.0^{+4.54}_{-2.15}$	$1.54^{+0.21}_{-0.14}$	$195.2^{+6.16}_{-11.18}$	$4.27^{+1.02}_{-1.08}$
CN-2	W	$66.13^{+12.1}_{-5.79}$	$1.59^{+0.43}_{-0.29}$	$216.37^{+28.37}_{-38.53}$	$2.54^{+0.65}_{-0.53}$
CN-2	E	$67.77^{+13.61}_{-14.5}$	$1.3^{+0.23}_{-0.2}$	$229.03^{+124.85}_{-66.01}$	$0.96^{+0.29}_{-0.14}$

may be caused by environmental conditions as the signatures of absorption and ongoing infall from the CO emission are all on the east side of the disk (Paneque-Carreño et al. 2021). Considering the well-defined surface of the west side in all CN transitions and the lack of a strong east–west asymmetry, for the remainder of this work the best-fit vertical profile from the west is used as representative of the CN distribution in the whole disk.

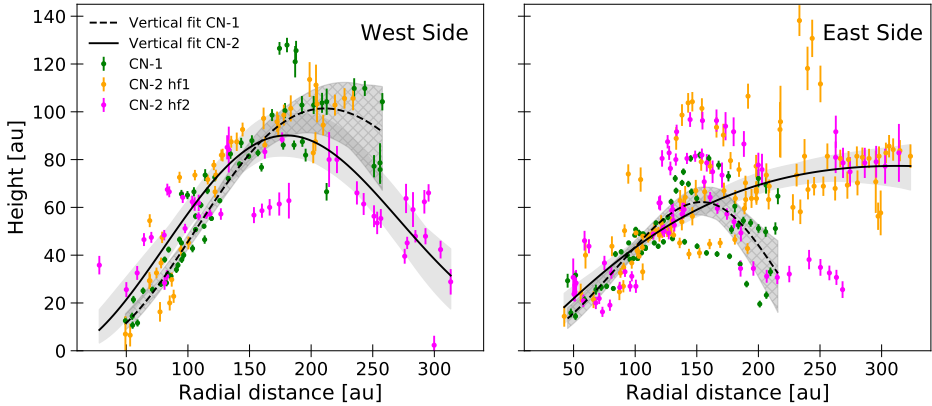


Figure 2.4: Same data as shown in Figure 2.3, but the panels are separated by the west and east sides of the disk. The colored data show the identified CN hyperfine transitions. The solid and dashed black curves show the best-fit vertical models for CN-1 and CN-2, respectively. The light gray region identifies the uncertainties in the best-fit vertical profile, obtained from the spread of the posterior values of the MCMC model.

2.3.2 CN versus CO emission

The vertical distribution of the emission from different molecular layers in Elias 2-27 allows us to characterize the various chemical processes occurring in the disk and to estimate the 2D temperature structure of the system (e.g., Pinte et al. 2018a; Law et al. 2021b). We compare the CN tracers with previous CO isotopolog observations (Paneque-Carreño et al. 2021) and additionally present the

results from extracting the vertical structure of the high-resolution $^{12}\text{CO } J = 2 - 1$ DSHARP data (Andrews et al. 2018). We do this comparison only on the west side, due to the cloud contamination that heavily affects the east side in all CO tracers, particularly $^{12}\text{CO } J = 2 - 1$ (Pérez et al. 2016; Huang et al. 2018c).

Figure 2.5 presents the comparison of the derived vertical structures of each molecule for the west side of the disk. As expected from disk chemical models (Bergin et al. 2007; Dutrey et al. 2014), the molecule that traces closest to the midplane is C^{18}O , followed by ^{13}CO for most of the radial extent. The emitting surfaces of the ^{12}CO and CN transitions seem to be tracing almost the same layer up to ~ 120 au. The right panel of Figure 2.5 shows the z/r measurements of each tracer. The mean values in each case are 0.53, 0.33, and 0.26 for ^{12}CO , ^{13}CO , and C^{18}O , respectively. For the CN tracers the mean values across the radial extent for both tracers is 0.45. In the discussion (section 6) we analyze and compare this value to what has been derived for other Class II sources. Overall, our results are consistent with CN emission tracing the uppermost layers of the disk, which in Elias 2-27 seem to be significantly vertically extended.

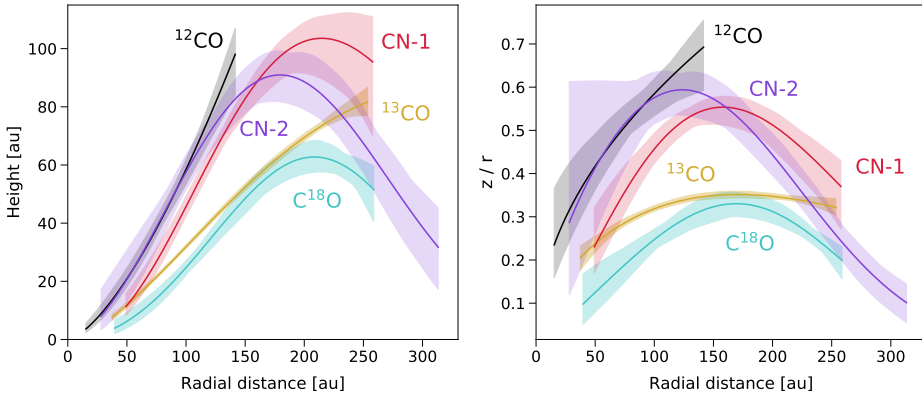


Figure 2.5: Height (left panel) and z/r (right panel) profiles for the available CO isotopologs and CN transitions in Elias 2-27. The CN emission is separated by a hyperfine group. Solid lines show the best-fit exponentially tapered vertical profile and the shadowed regions show the uncertainty on the best-fit model, derived from the spread of the posteriors in each tracer. Due to the absorption and asymmetries that affect Elias 2-27, the data corresponds to measurements only from the west side of the disk (for all tracers).

We note that the radial extent of the derived vertical profiles is always smaller than the radial extent of the emission of each tracer. This can be seen from the selected CN channels, shown in Figure 2.2, where the black dots tracing the upper layer do not reach the border of the channel emission. In particular for ^{13}CO and C^{18}O , the radial extent of the emission, as traced in the integrated intensity map, is ~ 650 and ~ 500 au, respectively (Paneque-Carreño et al. 2021). Therefore, the CO isotopolog emission is roughly two times more extended radially than the farthest radial distance up to where we are able to trace the vertical structure. This occurs because we trace the upper layer of emission directly from the channel

maps and only up to radial distances where we can separate the upper and lower layers. At the border of the disk this is not possible. In the case of ^{12}CO , which has the smallest radial extent, we are not able to trace farther out due to the coarse spectral resolution and cloud absorption, which does not allow us to separate the emitting layers beyond ~ 140 au. As we are not able to sample farther radial distances in the ^{12}CO emission, the location of the “turnover” in the height profile is not measured, contrary to the other molecules, and it is unclear if at larger radii ^{12}CO and CN would continue tracing similar locations.

2.3.3 Lack of envelope or large-scale emission

Considering the high z/r values and vertical extension that we derive in Elias 2-27, we analyze the CN emission using a position-velocity (PV) diagram to see if there is any indication of non-Keplerian velocities that may be associated with winds or other effects in the high disk atmosphere (Arce & Sargent 2006). Figure 2.6 shows the PV diagram along the major axis of the disk, for each of the CN transitions. Overlaid is the expected velocity profile, considering also the best-fit model for the vertical profile and a stellar mass of $0.46M_{\odot}$, as derived by Veronesi et al. (2021). There is no indication of non-Keplerian motion, and we have already discarded any large-scale emission from the emission maps (section 2), as seen in CO isotopologs (Paneque-Carreño et al. 2021); therefore, the disk has intrinsically vertically extended CN emission. It is still plausible that winds or larger-scale structures are present in Elias 2-27, but, due to its high critical densities, CN may not be emissive enough to be detected.

2.4 Asymmetric distribution of CN emission

The most striking feature from the PV diagram analysis is the extent of the emission to the west side (negative offset), which is larger than on the east side (positive offset). This was discussed in section 2 and relates to the extension difference seen between the north and south regions of the disk, which is not perfectly symmetric in its azimuthal extent with respect to the disk major axis. In the south the radially extended emission stretches azimuthally more toward the west than the east.

To study the north–south radial extent asymmetry, the emission of each tracer is adequately deprojected using the corresponding vertical structure previously derived (Figures 2.3 and 2.4). Azimuthally averaged intensity profiles and stacked spectra are obtained directly from the integrated intensity maps using the `get_2D_profile` function from `gofish` (Teague 2019b) and sampling in radial bins of $0.1''$ (one-third of our beam). The data analysis is separated between the north and south sides of the disk as defined by the major axis. Figure 2.7 presents the integrated intensity maps and respective intensity profiles for each CN transition. We note that the analysis of CN-2 considers both hyperfine transitions.

The intensity profiles from the north side of the disk show lower values than the south side in both transitions, at all radii. For CN-1 the 98% flux radius

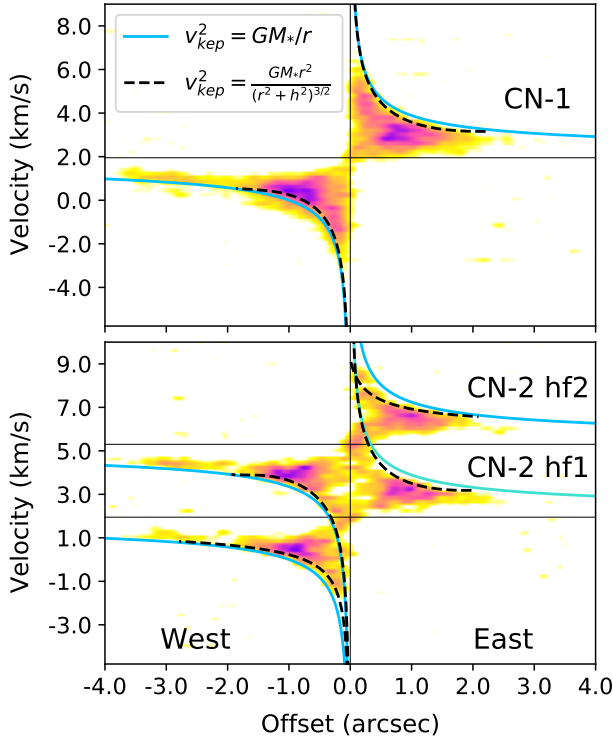


Figure 2.6: Position-velocity diagrams along the semi-major axis of the disk ($PA = 118.8^\circ$) for CN-1 (top) and CN-2 (bottom, with two hyperfine group transitions). The offset is positive toward the east side of the disk and negative toward the west. The horizontal lines give the systemic velocity ($\sim 1.95 \text{ km s}^{-1}$), shifted for CN-2 hf2 emission to $\sim 5.3 \text{ km s}^{-1}$. The blue curve shows the expected Keplerian velocity curve assuming a flat disk geometry. The dashed black line is the expected Keplerian velocity considering the derived best-fit model for the vertical profile of each tracer. Both models consider a stellar mass of $0.46 M_\odot$, as derived in Veronesi et al. (2021). The east and west sides of the disk are indicated in the bottom panel for reference.

of the north side emission is $202.8 \pm 11.6 \text{ au}$ and for CN-2 $179.6 \pm 11.6 \text{ au}$ (errors correspond to the radial bin size). Figure 2.7 shows the respective radial contour of the 98% flux radius overlayed on the integrated intensity map of each tracer. We do not resolve any structure from the north side intensity profiles, but beyond 300 au there is a small bump in emission in both transitions. This bump is likely due to the “tail” of the emission that extends slightly toward the north on the southeast side of the disk, and can be seen in the integrated intensity maps (Fig. 2.7).

Theoretical (Cazzoletti et al. 2018) and observational (Teague & Loomis 2020; van Terwisga et al. 2019; Bergner et al. 2021) studies have shown that the radial profile of CN is expected to present a ring-like feature, which may become shallower or more peaked depending on the disk’s physical properties (Cazzoletti et al. 2018).

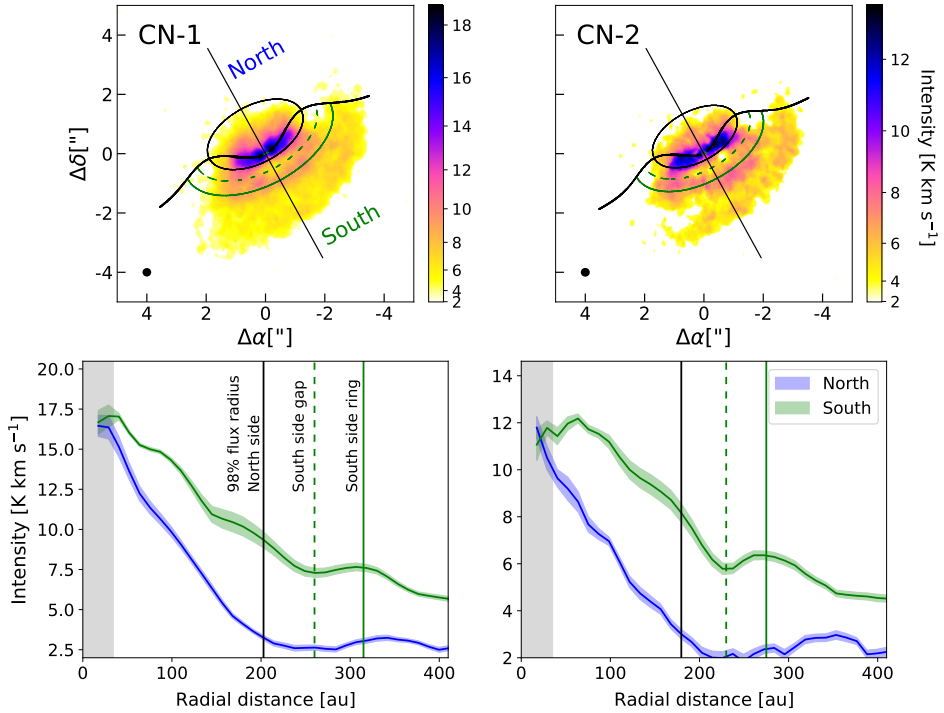


Figure 2.7: Azimuthal and radial analysis of the CN emission. Top row: Integrated intensity of each CN transition. The minor and major axis are marked considering the exponentially tapered vertical profile of the disk. The black elliptical contour marks the north quadrant’s 98% flux radius, derived from the intensity profile analysis. The north and south regions are shown in the colors that are used for the intensity radial profiles. The dashed and continuous green contours respectively indicate the location of the gap and ring detected in the south side emission. Bottom row: Intensity profiles derived from the integrated intensity map of each transition. The blue curve traces the north side emission and the green curve the south side emission. The vertical black lines show the location of the north emission 98% flux radius. The vertical green lines show the location of the identified gap (dashed) and ring (solid) in the south side emission. The gray vertical shaded area indicates a one-beam distance from the center. The colored shaded regions show the uncertainty of the intensity profile within each radial bin, obtained as the standard deviation of the data over the number of beams within the radial bin.

The integrated intensity maps show a band-like emission in the south, and we identify local maxima and minima from the south profile that we relate to the presence of at least one gap and one ring in each transition. The location of these structures are determined through scrutiny of the radial intensity profile and, when overlayed in the integrated emission maps, there is excellent agreement between the identified locations and the observed band-like structures (top row Fig. 2.7). For CN-1 the gap is located at 260 au and the ring at 315 au. In CN-2 we determine a position of 230 au for the gap and 275 au for the ring. The

small differences in the location of gaps and rings between the two transitions are likely due to the differences in the vertical profiles that are used for deprojecting the emission. We note that in the inner 200 au there may also be tentative gaps and/or rings; however, we are not able to visually assess them in the integrated emission maps with high confidence and do not classify them. The south profile also shows a possible dip in emission in the inner disk, which is expected for CN and is due to the high temperatures near the star that causes CN to be destroyed through its reaction with H_2 (Visser et al. 2018).

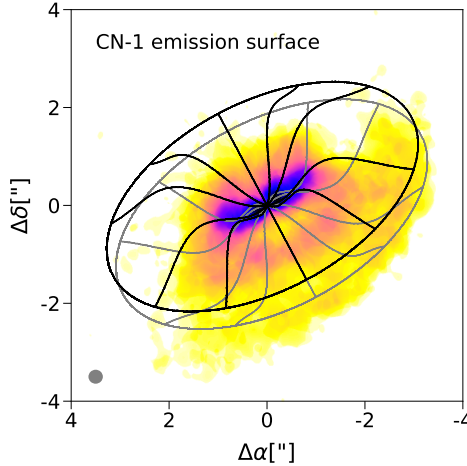


Figure 2.8: Integrated intensity of CN-1. Overlaid are the emission surfaces using the exponentially tapered vertical profile and assuming symmetry between the upper (black) and lower (gray) layers.

Figure 2.8 displays the expected emission surfaces for the upper and lower layers from the best-fit exponentially tapered height profile, assuming they are symmetric. The maximum radial extent in the two surfaces is 400 au which is comparable to the sampled radii in the intensity profiles (Fig. 2.7). Figure 2.8 shows that the extended emission in the southernmost part of the disk is not explained by a projection effect of the lower layer, as it is expected to extend only slightly beyond the upper layer. A lack of emission in the north is also observed.

2.5 Physical properties

To measure the system properties and abundance parameters, we can compute rotational diagrams (Goldsmith & Langer 1999). We used this approach for the CO isotopologs and CN hyperfine group transitions. The analysis of a rotational diagram relates the transition’s theoretical properties, particularly the upper state energy, to the measured quantities obtained from the flux of the emission. If several transitions of the same tracer with varied upper state energies are available, this method allows an estimate of both the excitation (or rotation) temperature and

the column density of the tracer. As only one transition of each molecule in CO and CN-1, together with the two CN-2 hyperfine group transitions that are too close in their upper energy values (see Table 4.1) are available, we are not able to simultaneously fit for the temperature and the total column density of each tracer, as was done in previous works (e.g., Goldsmith & Langer 1999; Loomis et al. 2018; Facchini et al. 2021). Therefore, we fit only the total column density and use an estimate for the rotational temperature, as is done by Facchini et al. (2021).

For optically thick tracers, such as ^{12}CO and ^{13}CO , the brightness temperature is coincident with the kinetic temperature. This approach was used in previous works to determine the 2D radial and vertical temperature structure of disks (Pinte et al. 2018a; Law et al. 2021b; Ilee et al. 2022). We constrained that CN comes from a vertical layer, close to ^{12}CO and higher than ^{13}CO (Fig 2.5), so we use the peak brightness temperature profiles of these two CO isotopologs as upper and lower limits for the kinetic temperature in the region from where CN emits. C^{18}O traces a layer just below ^{13}CO , so the ^{13}CO brightness temperature profile can be used as an estimate of the kinetic temperature of the region where C^{18}O emits. We used the online tool RADEX (van der Tak et al. 2007) to estimate the minimum H_2 number density needed for the rotation temperature to equal the derived kinetic temperature. For ^{12}CO , ^{13}CO and C^{18}O densities on the order of 10^5 cm^{-3} are sufficient. In the case of CN, the number density must be at least 10^8 cm^{-3} . Models predict that at the location of CN emission the number density is $10^6\text{-}10^8 \text{ cm}^{-3}$ (Cazzoletti et al. 2018). RADEX simulations show that these lower H_2 densities result in lower CN rotation temperatures of 20-40 K assuming a kinetic temperature of $\sim 40 \text{ K}$. These values are within the range that is sampled assuming the ^{12}CO and ^{13}CO temperature profiles as upper and lower limits (see Fig. 2.9).

The brightness temperature profiles are computed from peak brightness temperature maps and are shown in Figure 2.9. Due to the asymmetries and cloud absorption, only the west side emission is considered for CO isotopologs and only the south side emission is considered for CN transitions. ^{12}CO traces between 35-60 K, ^{13}CO has a peak temperature of $\sim 28 \text{ K}$, and C^{18}O varies with a mean temperature value of 11.9 K. The CN tracers have mean values of 9.4 K for CN-1 and $\sim 7.1 \text{ K}$ for CN-2. All mean brightness temperature values are calculated considering radial distances beyond 40 au to avoid effects of beam smearing in the innermost radii. We note that these profiles do not necessarily correspond to the kinetic and/or rotation temperature at the location of the molecules; this is only true for optically thick tracers. Indeed, ^{12}CO and ^{13}CO show high brightness temperatures above the freeze-out temperature for CO ($\sim 21 \text{ K}$, van Zadelhoff et al. 2001; Bisschop et al. 2006). The low brightness temperatures of C^{18}O and both CN transitions are likely caused by the low optical depth of both molecules, which is why these values are not accurate representations of their kinetic temperature. The RADEX simulations of CN result in similar brightness temperatures (10.5 K and 7.8 K for CN-1 and CN-2, respectively) compared to our measurements when the column density of CN is $\sim 6 \times 10^{13} \text{ cm}^{-2}$ and the kinetic temperature 40 K. We note that if the number density is very low in the upper disk layers, CN may be subthermally excited (van Zadelhoff et al. 2003), which would also result in low

brightness temperatures.

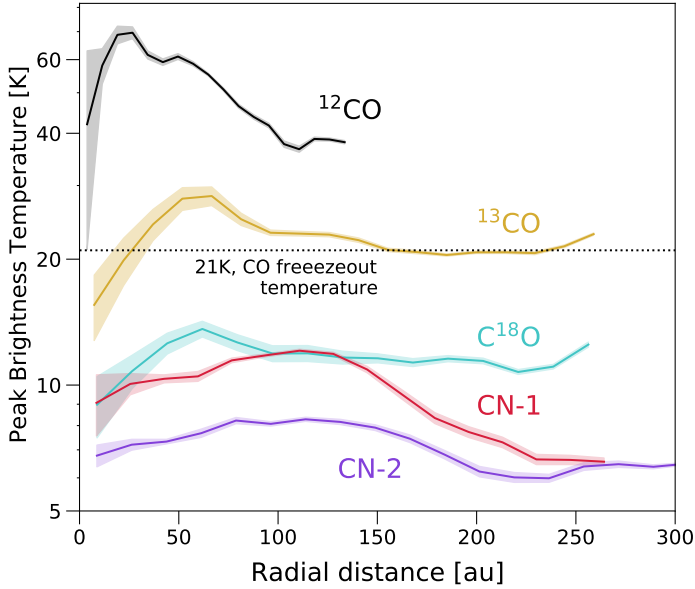


Figure 2.9: Azimuthally averaged peak brightness temperature profiles of each tracer available for Elias 2-27. The data are extracted only from the west side of the disk to avoid the high absorption effects of the east. In the case of CN the data are only from the south side, due to the additional north-south emission asymmetry. The shadowed colored regions show the uncertainty in the azimuthal averaging of the peak brightness temperature maps, obtained by dividing the standard deviation by the number of independent beams in each radial bin area.

With the temperature profiles of ^{12}CO and ^{13}CO as estimates of the kinetic temperature in the region where the molecules under study are located, we can obtain an estimate of the total column density and also calculate the optical depth profiles of each tracer. To do this we must first calculate the column density from the upper state (N_u) of each transition using the integrated intensity profiles (obtained in Figure 2.7) and the parameters of each transition (see Table 4.1). For optically thin emission ($\tau \ll 1$):

$$N_u = \frac{4\pi S_\nu \Delta\nu}{A_{ul} \Omega h c}. \quad (2.2)$$

Here $S_\nu \Delta\nu$ corresponds to the integrated flux density, Ω is the area over which the flux was integrated, and $S_\nu \Delta\nu$ is obtained from the integrated intensity profiles of Figure 2.7, where the profile has been derived from radial bins. The intensity value from the radial profile must be multiplied by the area of the radial annuli used in each bin and divided by the beam area to obtain the correct flux density units. Each radial annulus has an area Ω . The other parameters are the Einstein emission coefficient of the transition A_{ul} , the speed of light c , and the Planck constant h .

If the optical depth (τ) of the emission is non-negligible, then a correction factor C_τ must be applied to the upper state column density,

$$C_\tau = \frac{\tau}{1 - e^{-\tau}}. \quad (2.3)$$

The column density of the upper state can then be related to the total column density (N_T), considering the correction factor, through

$$\frac{N_u}{g_u} C_\tau = \frac{N_T}{Q(T_{rot})} e^{-E_u/kT_{rot}}, \quad (2.4)$$

where g_u is the upper state degeneracy, E_u is the upper state energy, and k is the Boltzmann constant. The value of the partition function $Q(T_{rot})$ is estimated at each temperature by interpolating with a cubic spline from the values of the CDMS catalog (Müller et al. 2001), as is done in Facchini et al. (2021). Finally, the optical depth of the emission may also be estimated from the upper state column density measurement following

$$\tau_{ul} = \frac{A_{ul} c^3}{8\pi\nu^3 \Delta\nu} N_u (e^{h\nu/kT_{rot}} - 1). \quad (2.5)$$

Here $\Delta\nu$ is the line width, which is calculated assuming that the broadening from turbulence is negligible and where the thermal broadening is calculated from the temperature and the molecular weight of the molecule under study, and ν is the line central frequency. All the other parameters have been defined previously. Equation 5 allows us to express C_τ in terms of N_u , and therefore to solve equation 4 for N_T , considering the optical depth properties of the molecules.

Figure 2.10 shows the results for the total column density N_T (top row) and optical depth (bottom row) profiles in ^{13}CO , C^{18}O , and CN tracers. The temperature profile used for the CO isotopologs is only the ^{13}CO profile and the calculation considers the temperature profile uncertainties for the fit. For CN we considered a temperature range, where the upper limit is given by the ^{12}CO temperature profile and the lower limit by the ^{13}CO temperature profile. As the ^{12}CO temperature is only constrained up to ~ 130 au, we consider the last temperature value, 38 K, as a constant value for the remainder of the radial extent. The assumption of constant temperature in the outer radii is based on the temperature profiles of ^{13}CO and C^{18}O that display roughly constant temperature profiles from ~ 100 au outward (see Fig. 2.9). For the calculation of the CN physical parameters, we do not consider the CO temperature profile errors as they are within the sampled range of temperatures.

Both CN tracers have column densities of 10^{14} cm^{-2} in the inner disk that then drop to 10^{13} cm^{-2} in the south side outer disk and even lower in the north. On the north side the column density has a steep decline, reaching values below 10^{13} cm^{-2} beyond 150 au. Likewise, the optical depth of the north side emission rapidly goes to values below unity in the inner 100 au, indicating that the emission is optically thin. The south side of the disk displays a slowly radially decreasing column density which is always within the same order of magnitude, 10^{13} cm^{-2} . We note that CN-2 displays a localized decrease in the column density of the south

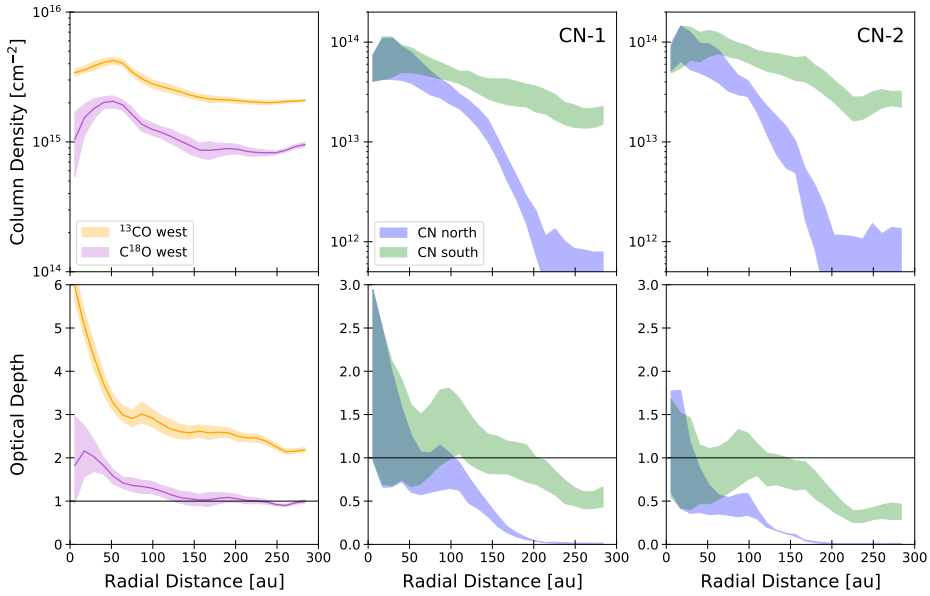


Figure 2.10: Azimuthally averaged emission properties for CO isotopologs and CN. Top row: Column density profiles for each analyzed tracer. Shown together in the leftmost panel are ^{13}CO and C^{18}O . Middle and right panels: Column density profile of each CN hyperfine group, separated between north and south sides of the disk. Bottom row: Optical depth profile for each molecule, following the same order as the top row. The horizontal black lines indicate the optical depth of $\tau = 1$. In all panels, the shaded regions show the uncertainty on the model.

side at ~ 230 au, which coincides with the location of the tentative gap reported in section 4. Regarding the optical depth values of the south side, they are close to unity and show a localized increase at ~ 100 au. Therefore, beyond ~ 150 au CN is optically thin in the whole disk; however, the emission may be marginally optically thick on the south side, particularly inward of ~ 100 au.

For the CO isotopolog emission, our results trace a total column density of $\sim 10^{15} \text{ cm}^{-2}$ for ^{13}CO and C^{18}O ; however, ^{13}CO has a factor of 2-3 higher values. Studies have shown that CO column densities vary between systems depending on the stellar parameters, disk size, and mass (Miotello et al. 2016). Within an order of magnitude, our derived values are in agreement with previous observational and theoretical results (Miotello et al. 2016, 2018; Facchini et al. 2021). The optical depth values of ^{13}CO are above unity, corroborating our initial assumption that it is optically thick. C^{18}O shows marginally optically thin emission from ~ 100 au outward.

2.6 Discussion

2.6.1 Origin of CN emission and comparison to theoretical models

The main formation mechanism of CN is thought to be the reaction of N with vibrationally excited H_2 pumped by UV radiation, making CN a tracer of the upper layers of a disk. (Cazzoletti et al. 2018; Visser et al. 2018). Our analysis of CN transitions in Elias 2-27 spatially locates the molecule in a constrained uppermost layer of the disk, with $z/r \sim 0.45$ in all tracers. The disk is sufficiently flared that we can identify the upper and lower layers of emission in the channel maps (see Fig. 2.2), and from there directly trace the vertical surface of emission. To our knowledge this is the first time that a direct measurement has been made for CN emission in a disk of moderate inclination, where it is also possible to analyze the radial and azimuthal distribution of material. Previous works have relied on temperature estimates (e.g., Teague & Loomis 2020) or have been conducted in edge-on systems, lacking information on the azimuthal distribution (Ruíz-Rodríguez et al. 2021).

A key feature predicted by models and detected in previous observations of CN is a shallow ring-like structure in the intensity and column density profiles of the disk that is not related to any gas or dust surface density features, but due to chemistry (Cazzoletti et al. 2018; van Terwisga et al. 2019; Teague & Loomis 2020; Ruíz-Rodríguez et al. 2021; Bergner et al. 2021). Both of the analyzed CN transitions show a ring of emission in the south side intensity profiles at 315 au and 275 au. Additionally, the optical depth profiles show a feature at ~ 100 au, where tentative bumps in the radial intensity profile may also be identified (see Fig. 2.7). All of these features are detected on the south side of the disk. From the north emission we do not retrieve any features, even in the inner (< 200 au) region where there is strong CN emission.

Emission of CN is predicted to be optically thin, with typical column densities of $\sim 10^{14} \text{ cm}^{-2}$, and to be spatially constrained to a thin layer in the upper disk by physical-chemical models (Cazzoletti et al. 2018; Visser et al. 2018). Our results confirm these predictions in most of the radial extension; however, in the inner ~ 100 au some emission may be marginally optically thick ($\tau = 1-2$, see Fig. 2.10). This could be due to Elias 2-27 hosting a massive gravitationally unstable disk. In agreement with T Tauri models (Cazzoletti et al. 2018), the column density of CN in Elias 2-27 declines less than an order of magnitude on the south side of the disk for both transition groups. The rapid decline in column density on the north side is discussed in section 6.3, and we do not associate it with a chemical process, rather to an effect of the disk environment. Overall, our results of morphology and chemical and physical conditions are in agreement with theoretical predictions for CN emission originating from UV radiation.

Elias 2-27 is likely a gravitationally unstable disk (Paneque-Carreño et al. 2021), and studies focusing on the chemistry of GI disks suggest that CN may be a good tracer of GI spirals (Evans et al. 2015). CN emission originating from the spirals should be observed at the midplane because it would be produced by

the desorption of CN from the dust grains along the spirals. CN emits from tens of au above the midplane; therefore, we are not able to compare the dust continuum structure with the CN emission because they are not spatially co-located and there is no signature of any emission from the midplane. This does not rule out self-gravity or that there is no desorption in the midplane. It is possible that, if CN emission originating from GI is present, it is invisible due to the bright emission arising from the higher disk layers or lack of sensitivity in the outer disk. Another option is that, as the spirals are traced between 50 and 200 au (Pérez et al. 2016; Huang et al. 2018c; Paneque-Carreño et al. 2021) and CN is marginally optically thick in this region, it is not possible to observe emission down to the midplane.

2.6.2 Comparison with resolved emission in other systems

Cyanide has been detected in several Class II systems, both in spatially unresolved (see surveys by, Reboussin et al. 2015; Guilloteau et al. 2013, 2016b) and resolved emission (e.g., van Terwisga et al. 2019; Teague & Loomis 2020; Ruíz-Rodríguez et al. 2021; Bergner et al. 2021). There have been various indirect and direct methods employed to measure the vertical location and physical conditions of CN. Overall, there seems to be agreement on the CN conditions in Class II systems. Studies on TW Hya (Kastner et al. 2014; Teague & Loomis 2020) and the Flying Saucer (Ruíz-Rodríguez et al. 2021) both characterize CN column densities between 10^{13} and 10^{14} cm $^{-2}$. In the MAPS dataset (Öberg et al. 2021b) the CN column densities peak at 10^{15} cm $^{-2}$ for most disks (IM Lup, GM Aur, AS 209, HD 163296, MWC 480); however, the azimuthally averaged column densities are $\sim 10^{13}$ cm $^{-2}$ for most of the radial extent (Bergner et al. 2021). These column density values are in agreement with what we derive in Elias 2-27 (see section 5). MAPS also finds marginally optically thick CN emission in the inner disk (Bergner et al. 2021), in agreement with our results.

Even though the column density and optical depth values are in agreement with previous works and theoretical predictions, the distribution of the CN emission in Elias 2-27 is peculiar. In particular, the vertical extent is much higher than the estimated values for all other Class II sources. Indirect estimates using temperature profiles (TW Hya, Teague & Loomis 2020) or UV-radiation models (MAPS collaboration, Bergner et al. 2021) trace the emitting surface of CN at $z/r \sim 0.2$. The CN region in the Flying Saucer disk (Ruíz-Rodríguez et al. 2021), which is the only one to have been modeled directly, shows vertically symmetric CN emission arising from an intermediate molecular layer, lower than ^{12}CO . Ruíz-Rodríguez et al. (2021) also measure very low kinetic temperatures in the CN region (≤ 15 K), which they attribute to the low mass of the star ($0.57 M_{\odot}$) and extended CN emission, proposing deep X-ray radiation as the origin of the CN. It is interesting to note that Elias 2-27 has a comparable stellar mass of $0.46 M_{\odot}$ (Veronesi et al. 2021) to the Flying Saucer, but a very different vertical structure.

In the case of Elias 2-27 CN arises from a high layer of $z/r \sim 0.45$, indicating that this disk is more vertically extended than previously studied Class II systems. The vertical distribution of CN in Elias 2-27 is similar to that of the Class I source IRAS 04302+2247, where the CN vertical extent traces $z/r \sim 0.4$ (see Fig.

2 and discussion within Podio et al. 2020). Unfortunately, CN observations in IRAS 04302+2247 are contaminated due to the continuum oversubtraction and absorption, and therefore we do not have further information to compare with our results.

Comparison of the CO vertical structure in Elias 2-27 with other Class II disks shows that the mean z/r values for Elias 2-27 are much higher than those found in the MAPS sample, for all CO isotopologs (Law et al. 2021b). The differences in the ^{13}CO and C^{18}O values may be due to the higher transition ($J = 3 - 2$) used in this work; however, for ^{12}CO the same transition as in MAPS is used ($J = 2 - 1$). A tentative relation between z/r and the CO radial extent has been proposed such that higher z/r values relate to more extended disks (Law et al. 2021b, 2022). Elias 2-27 has an extended CO disk, consistent with this trend, although this relation also finds that vertically extended CO disks ($z/r > 0.3$) have mean ^{12}CO brightness temperatures < 30 K (Law et al. 2022). As shown in section 5, the brightness temperature of ^{12}CO varies in the range 35-60 K. A larger sample of objects with varied disk and stellar properties is needed to determine if Elias 2-27 is indeed an outlier or if there are more systems with hot and vertically extended gas emission.

2.6.3 Asymmetric CN, further evidence for infall or a warp?

The CN emission of Elias 2-27 shows an extreme asymmetry between the flux and density profiles on the north and south sides of the disk. This was not seen in previous observations of CO emission (Paneque-Carreño et al. 2021); however, it is similar to the morphology of available NACO L'-band observations (see Fig. 12 in Launhardt et al. 2020). Figure 2.11 displays the integrated intensity maps for the studied CO isotopologs and CN-1 emission for a comparison of the different radial and azimuthal locations. The east side of the disk shows radially extended CO emission and lack of ^{12}CO , particularly in the northeast quadrant. We propose two scenarios to explain the CN asymmetric emission that are also compatible with the various CO brightness and vertical extent asymmetries.

A decrease in CN production can be linked to the presence of small grains on the north side disk atmosphere, which would shield the surface layers from FUV radiation and reduce the CN emission. An enhanced presence of small grains can be explained by a high dust-to-gas ratio in this region (Nomura et al. 2021) or by the infall of small grains. Infall is the mechanism proposed to be ongoing in Elias 2-27, due to the large-scale emission and variations between the east and west sides observed in ^{13}CO and C^{18}O (Paneque-Carreño et al. 2021). If material is still accreting onto the system, it would explain the vertical differences between east and west and also the north-south extension asymmetry seen in CN.

A second hypothesis to explain the asymmetry is the presence of a warp in the dust disk that creates a shadow and affects the FUV and X-ray radiation received by the north side of the disk (Young et al. 2021). A warped structure is thought to be responsible for the vertical asymmetries detected in the CO emission and the strong kinematical residuals (Paneque-Carreño et al. 2021; Young et al. 2022; Rowther et al. 2022). CN is expected to be a good tracer of the presence

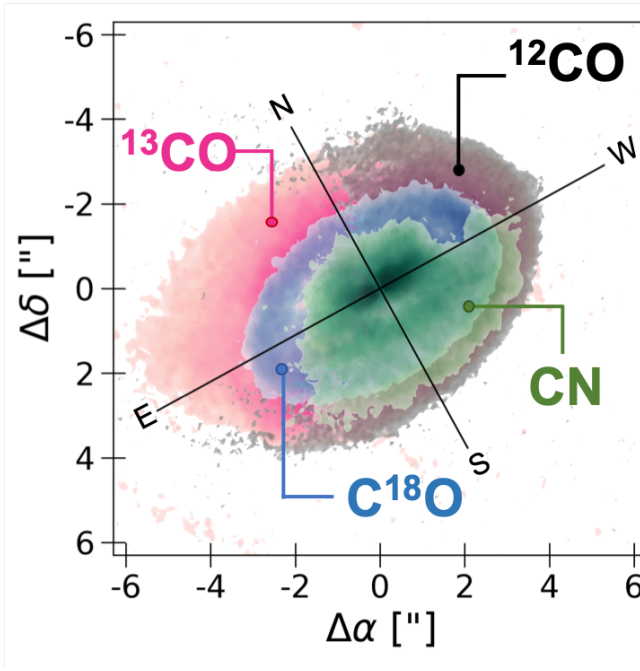


Figure 2.11: Integrated intensity maps for the tracers studied in this work: $^{13}\text{CO } J=2-1$, $^{13}\text{CO } J=3-2$, $\text{C}^{18}\text{O } J=3-2$, and $\text{CN } J=7/2-5/2$ (CN-1).

of a warp, through asymmetric distribution of its emission (Young et al. 2021). If there is a warped inner disk then we can characterize its inclination direction based on the south–north CN asymmetry, and estimate that it will be aligned with the disk major axis. The presence of a warp will not necessarily affect the CO abundance, although it is expected to affect the CO temperature. Previous studies have shown that the south side of the disk shows brighter CO emission (Pérez et al. 2016; Paneque-Carreño et al. 2021), which would be in agreement with the shadowing of the north side by an inner warp (Young et al. 2021). With our current data we are unable to distinguish between the two proposed scenarios (infall or warp).

Asymmetric CN emission, as reported in this work, has not been observed in any of the resolved Class II observations (van Terwisga et al. 2019; Teague & Loomis 2020; Ruíz-Rodríguez et al. 2021; Bergner et al. 2021); however, there is a similar case in the Class I protobinary source, Oph-IRS 67 (Artur de la Villarmois et al. 2019). Oph-IRS 67 has CN emission traced only toward the south of the disk. This emission likely originates from a photon-dominated region (PDR) beyond the circumbinary disk (Artur de la Villarmois et al. 2019). In addition to CN, the asymmetry in Oph-IRS 67 is also traced in $\text{c-C}_3\text{H}_2$, DCN, and H_2CO . It is possible that external radiation could also affect the emission of Elias 2-27. However, we do not have any evidence of PDR regions beyond the disk that could affect the emission. Obtaining observations of PDR sensitive tracers could be

useful to further study the asymmetry.

2.7 Conclusions

We presented an extensive analysis of CN $v=0$, $N=3-2$, $J=7/2-5/2$, and $J=5/2-3/2$ emission in Elias 2-27. We also made use of previously published CO isotopolog observations to characterize the vertical stratification and physical properties of the disk (temperature, column density, and optical depth). Through this study Elias 2-27 becomes one of the few Class II systems with a detailed study of the vertical structure and chemical properties of its protoplanetary disk. Our main conclusions are the following:

1. CN originates at a high vertical location from the disk midplane. It traces a region similar to ^{12}CO , at least up to a radial distance of ~ 150 au. CN emits from a vertically constrained and mostly optically thin slab. This is in agreement with theoretical predictions that its main formation mechanism is the reaction of N with UV excited H_2 .
2. We trace a strong CN emission asymmetry between the north and south sides of the disk. The extent of CN on the south side goes beyond 400 au, while the 98% flux radius of the north side is 180-200 au. A ringed structure at 230-275 au is observed in the south emission, as predicted by chemical models and similar to observations of CN in other systems. No structure is observed on the north side of the disk emission.
3. The observed CN asymmetry may be explained by either ongoing infall or a warped inner disk. With the current data and models we are not able to confirm or reject either scenario.
4. Elias 2-27 is a peculiar Class II source and the studied asymmetries share a strong resemblance with some Class I objects. It has vertically extended ($z/r > 0.3$) CN and CO isotopolog emission, with high ^{12}CO brightness temperatures and asymmetric CN distribution.
5. Highly inclined sources such as Elias 2-27 are excellent systems to directly trace and analyze the disk structure and properties. Using optically thick tracers, such as ^{12}CO and ^{13}CO , we can determine the kinetic temperature structure. Combining the temperature profiles with information on the spatial location of various molecules we can recover the physical conditions of the gas.

In summary, this study shows the vertical layering and structure of molecules in Elias 2-27. This is an excellent test case for the importance of simultaneous analysis of multiple tracers to obtain constraints on temperature, column density, and optical depth variations. The favorable inclination and high S/N make it possible to study the 3D disk structure so the emission can be traced radially, azimuthally, and vertically. Future observations with additional tracers, for example

HCN, which is UV and temperature sensitive, or $\text{c-C}_3\text{H}_2$ and DCN, which can trace PDR regions, will allow us to fully study the vertical distribution and better understand the origin of the asymmetries in Elias 2-27.

Acknowledgements

This paper makes use of the following ALMA data: #2013.1.00498.S, #2016.1.00606.S and #2017.1.00069.S. ALMA is a partnership of ESO (representing its member states), NSF (USA), and NINS (Japan), together with NRC (Canada), NSC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO, and NAOJ. Astrochemistry in Leiden is supported by the Netherlands Research School for Astronomy (NOVA), and by funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 101019751 MOLDISK). L.P. gratefully acknowledges support by the ANID BASAL projects ACE210002 and FB210003, and by ANID, – Millennium Science Initiative Program – NCN19_171. This project has received funding from the European Union’s Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 823823, (RISE DUSTBUSTERS).

Appendix

2.A Channel maps

In this section we present the complete channel maps for each of the CN transitions. Figure 2.A.1 shows the CN-1 emission, which has only one hyperfine group transition. Figure 2.A.2 shows the emission of the two hyperfine group structures of CN-2, imaged with respect to the frequency of CN-2 hf1, 340.0354080 GHz (Müller et al. 2001). The systemic velocity of Elias 2-27 is estimated to be 1.95 km s^{-1} (Paneque-Carreño et al. 2021).

2.B CO isotopolog observations

Figure 2.B.1 shows the integrated intensity maps and spectra for the CO isotopologs used in this study. The detailed analysis of these data are presented in Andrews et al. (2018) and Huang et al. (2018c) for ^{12}CO and in Paneque-Carreño et al. (2021) for ^{13}CO and C^{18}O . The heavy contamination and absorption in the northeast is visually identified in all tracers, least affecting C^{18}O .

We obtain the integrated fluxes and uncertainties of each tracer (shown in Table 4.1) from the spectra in the emitting and line-free regions. For the total integrated flux we use an elliptical mask that encircles all of the emission, determined using a curve of growth method on the integrated intensity maps. This mask also determines the region from where the plotted spectra is derived (in Fig-

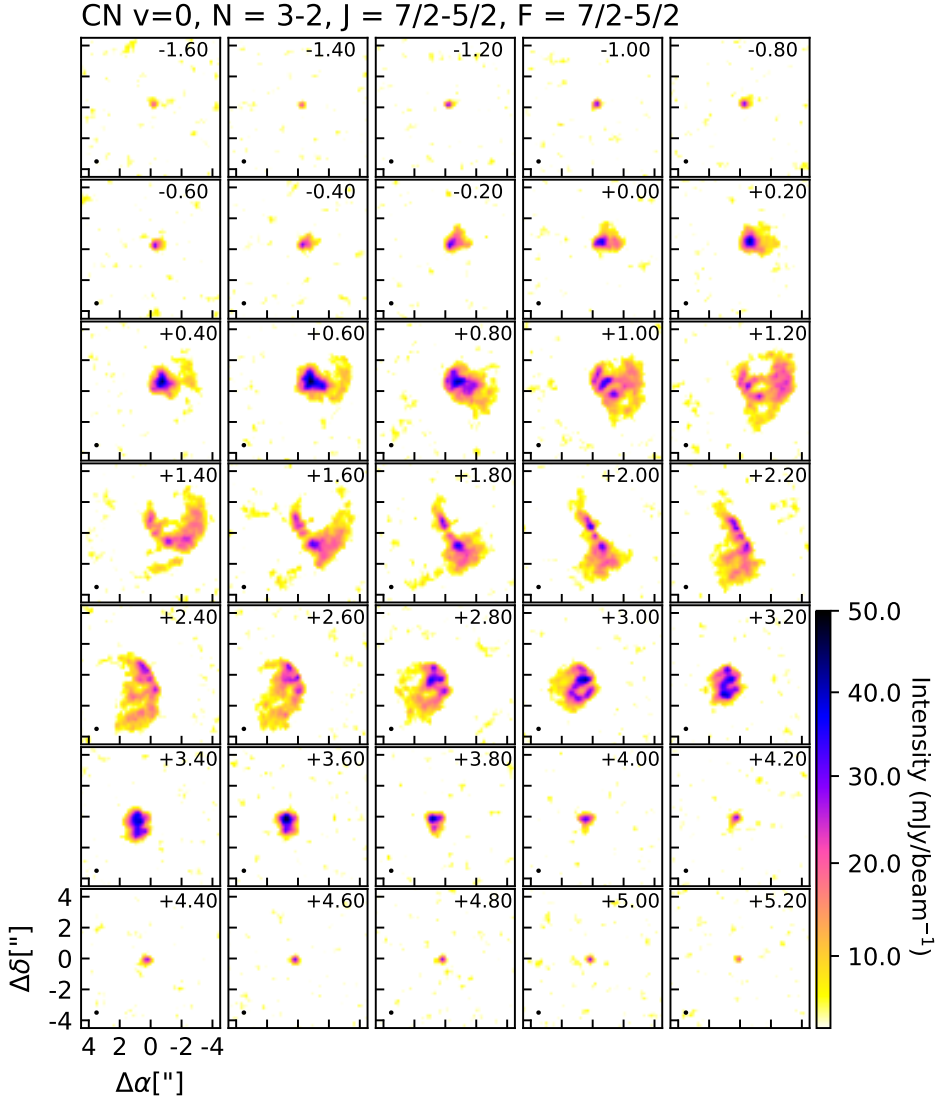


Figure 2.A.1: Complete channel map emission for $\text{CN } J = 7/2 - 5/2$. In each panel the channel velocity is given in the upper right corner and the beam size of the emission is shown by a black ellipse in the bottom left corner.

ures 2.1 and 2.B.1). The uncertainties are derived from the standard deviation of the integrated flux retrieved from 20 line-free regions.

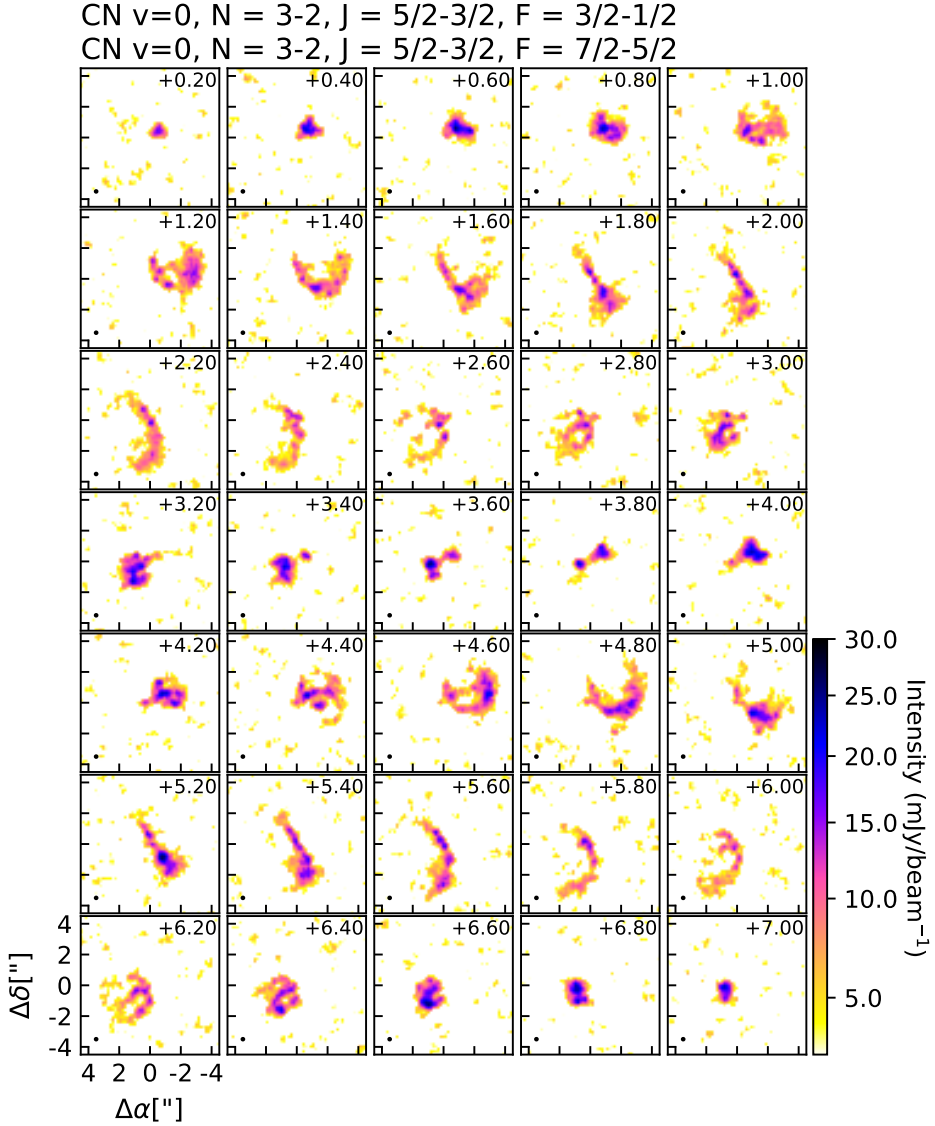


Figure 2.A.2: Complete channel map emission for CN $J = 5/2-3/2$. In each panel the channel velocity is given in the upper right corner and the beam size of the emission is shown by a black ellipse in the bottom left corner. This transition shows two consecutive hyperfine group transitions.

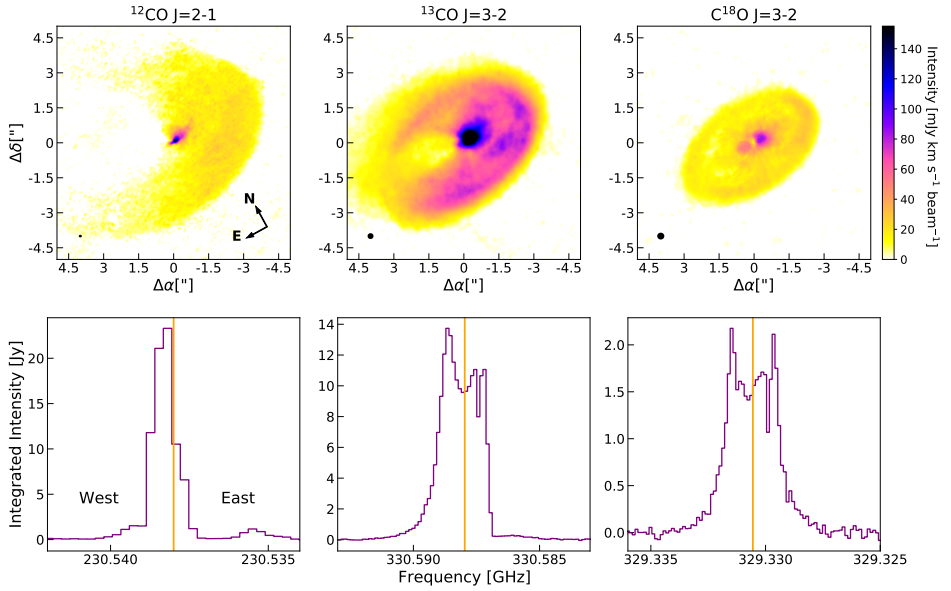


Figure 2.B.1: CO isotopolog emission data used in this study. The top row shows the zeroth moment maps for each CO isotopolog. The beam size is shown in the bottom left corner of each panel. The bottom row displays the spectrum of each tracer. ^{12}CO has a resolution of 0.35 km s^{-1} , while ^{13}CO and C^{18}O have a resolution of 0.111 km s^{-1} . The orange vertical line gives the rest frequency in each case.

Chapter 3

Directly tracing the vertical stratification of molecules in protoplanetary disks

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Astronomy & Astrophysics, 669, A126 (2023)

Abstract

Context: The specific location from where molecules emit in a protoplanetary disk depends on the system properties. Therefore, directly constraining the emitting regions radially, azimuthally, and vertically is key to studying the environment of planet formation. Due to the difficulties and lack of high resolution observations, most of the current observational constraints for the vertical distribution of molecular emission rely on indirect methods.

Aims: We aim to directly trace the vertical location of the emitting surface of multiple molecular tracers in protoplanetary disks. Our sample of disks includes Elias 2-27, WaOph 6, and the sources targeted by the MAPS ALMA Large Program. The set of molecules studied includes CO isotopologues in various transitions, HCN, CN, H₂CO, HCO⁺, C₂H, and c-C₃H₂.

Methods: The vertical emitting region is determined directly from the channel maps by tracing the location of emission maxima along the upper surface. This method has been used in previous studies, but here we implement an accurate masking of the channel emission in order to recover the vertical location of the emission surface even at large radial distances from the star and for low-S/N lines. Parametric models are used to describe the emission surfaces and characterize any structure within the vertical profile.

Results: The vertical location of the emitting layer is obtained for ten different molecules and transitions in HD 163296. In the rest of the sample it is possible to vertically locate between four and seven lines. Brightness temperature profiles are obtained for the entire sample and for all CO isotopologues. IM Lup, HD163296, and MWC 480 ¹²CO and ¹³CO show vertical modulations, which are characterized and found to be coincident with dust gaps and kinematical perturbations. We also present estimates of the gas pressure scale height in the disks from the MAPS sample. Compared to physical-chemical models, we find good agreement with the vertical location of CO isotopologues. In HD 163296, CN and HCN trace a similar intermediate layer, which is expected from physical-chemical models. For the other disks, we find that UV flux tracers and the vertical profiles of HCN and C₂H are lower than predicted in theoretical models. HCN and H₂CO show a highly structured vertical profile, possibly indicative of different formation pathways in the case of H₂CO.

Conclusions: It is possible to trace the vertical locations of multiple molecular species that in turn trace a wide variety of physical and chemical disk properties. The distribution of CO isotopologues is in agreement with theoretical predictions, and the emission is found at a wide range of vertical heights, $z/r = 0.5-0.05$. The vertical location of CO may be inversely related to the stellar mass. Other molecular lines are mostly found at $z/r \leq 0.15$. The vertical layering of molecules is in agreement with theoretical predictions in some systems, but not in all. Therefore, dedicated physical-chemical models are needed to further study and understand the diversity of the emission surfaces.

3.1 Introduction

Planets form in disks of dust and gas that surround young stars. In recent years the spatial resolution and sensitivity achieved by instruments such as the Atacama Large Millimeter/submillimeter Array (ALMA) has allowed us to characterize these objects in detail. A key feature that we can only now properly study is the disk vertical structure, if data at an adequate resolution are available. Protoplanetary disks have a vertical extent that depends on the system properties, such as the stellar mass and radiation field, but also on the disk temperature structure and surface density distribution (Bell et al. 1997; D’Alessio et al. 1998; Aikawa & Herbst 1999; van Zadelhoff et al. 2001; Walsh et al. 2010; Fogel et al. 2011; Rosenfeld et al. 2013b). The vertical extent of a disk is set by hydrostatic equilibrium: the balance between stellar gravity and pressure support (Armitage 2015). Tracing of the vertical structure can be used to detect deviations from equilibrium that can be related to meridional flows in the presence of planets (Morbidei et al. 2014; Szulágyi et al. 2022), shadowing due to warped structures (Nealon et al. 2019), or infall of material (Hennabelle et al. 2017), among other factors. While larger, millimetre-sized, grains are expected to be settled in the midplane of disks, molecular and scattered light observations can be used to recover the vertical structure of the disk (e.g. Pinte et al. 2018a; Avenhaus et al. 2018; Villenave et al. 2020; Law et al. 2021b).

Studying the vertical location of various molecular tracers is particularly powerful for accurately mapping the disk structure thanks to the sensitivity of line emission to temperature, radiation, and density variations. Several works have used the excitation temperature of line emission to infer the expected vertical location of a given molecule (e.g. van Zadelhoff et al. 2001; Dartois et al. 2003; Teague & Loomis 2020; Bergner et al. 2021; Ilee et al. 2021). This indirect approach is promising, but it relies on physical-chemical models and assumptions about the disk conditions at the location of the emission. Direct tracing of molecular emission layers is fundamental for comparisons with current models. Previous studies have focused on edge-on disks to do this (e.g. Podio et al. 2020; van’t Hoff et al. 2020; Villenave et al. 2020; Ruíz-Rodríguez et al. 2021). However, with the development of new analysis techniques, it is now possible to directly extract the vertical surfaces from moderately inclined ($35\text{--}60^\circ$) sources (e.g. Pinte et al. 2018a; Paneque-Carreño et al. 2021; Rich et al. 2021; Law et al. 2021b, 2022). Analysing systems that host moderately inclined disks allows us to study them in three dimensions, as it is also possible to trace the azimuthal and radial distribution of material.

Of the handful of moderately inclined systems with direct extraction of their vertical surfaces, the vast majority have been analysed using only CO isotopologue emission (Pinte et al. 2018a; Paneque-Carreño et al. 2021; Rich et al. 2021; Law et al. 2021b; Leemker et al. 2022; Law et al. 2022). The exceptions are AS 209, HD163296, and MWC 480, where the vertical location of HCN and C₂H emission was constrained in the inner ~ 150 au (Law et al. 2021b). However, the emission extends to over 300 au (Law et al. 2021a), and therefore a large portion of the vertical structure is still unconstrained. For Elias 2-27, the vertical location of

CN has also been directly measured from the channel maps; additionally, by comparing the location of CN emission to that of CO isotopologues, its density and optical depth conditions were constrained (Paneque-Carreño et al. 2022). ^{12}CO and ^{13}CO emission is expected to trace optically thick slabs of material in distinct vertical regions, while C^{18}O likely traces closer to the midplane and CO freeze-out region (van Zadelhoff et al. 2001; Miotello et al. 2014). Through the study of CO isotopologues, it is possible to trace the temperature gradient in the vertical direction (Law et al. 2021b) and study CO abundance variations (Zhang et al. 2021).

Tracing the location of less abundant molecules can offer complimentary constraints on the disk structure and the physical-chemical processes that construct the environment conditions of planet formation. Emission from CN, HCN, and C_2H is expected to originate from UV-dominated regions (Aikawa et al. 2002; Cazzoletti et al. 2018; Visser et al. 2018; Bergner et al. 2021; Guzmán et al. 2021). For these molecules, models predict that the emission should arise from elevated regions (van Zadelhoff et al. 2003; Cazzoletti et al. 2018; Cleeves et al. 2018; Bergner et al. 2021; Guzmán et al. 2021). HCO^+ is a molecular ion. Its abundance is expected to be dominant in the CO molecular layer, and, combined with the CO isotopologue distribution, it can be used to study the disk ionization (Aikawa et al. 2021). Formaldehyde (H_2CO) has two main formation pathways, gas-phase chemistry (Loomis et al. 2015) and grain-surface chemistry through the hydrogenation of CO ices (Hiraoka et al. 1994; Fuchs et al. 2009). H_2CO could be a better tracer of cold gas in the outer disk if it originates from desorption processes off the dust grains; however, the emission may also arise from warmer and higher layers if gas-phase chemistry is dominant in its formation (Guzmán et al. 2021; Loomis et al. 2015). Direct tracing of the vertical location of the H_2CO emission could shed light on the dominant mechanism leading to the formation of H_2CO .

In this work we recover the location of the emitting regions for a sample of seven disks, using data from the Molecules with ALMA at Planet-forming Scales (MAPS) ALMA Large Program (#2018.1.01055.L, Öberg et al. 2021b; Czekala et al. 2021) and archival ALMA data of Elias 2-27 (#2016.1.00606.S and #2017.1.00069.S; P.I. L. Pérez) and WaOph 6 (#2015.1.00168.S; P.I. G. Blake). The data selected for all the disks have sufficient signal-to-noise ratios (S/N) and resolution (spectral and spatial) to recover the vertical structure from multiple CO isotopologues and additional molecular tracers in each system. Elias 2-27 and WaOph 6 have spiral structures in the dust emission that have been studied at high angular resolution (Andrews et al. 2018; Huang et al. 2018c) and may be originated by gravitational instabilities (Pérez et al. 2016; Huang et al. 2018c; Paneque-Carreño et al. 2021; Veronesi et al. 2021). IM Lup, GM Aur, HD 163296, MWC 480, and AS 209 are sources studied by the MAPS collaboration, and each present a variety of dust and gas substructure (Öberg et al. 2021b; Law et al. 2021a). Our complete sample is composed of a broad range in stellar parameters ($0.5 - 2 M_\odot$) and disk substructures (spirals, rings, and gaps). The goal of this study is to offer observational constraints on the vertical location of the emission for a wide molecular reservoir, in a heterogeneous sample, and to relate the measured system properties to theoretical predictions.

The remainder of this paper is organized as follows. Section 2 details the data that were used and the methodology for extracting the vertical profiles. Section 3 presents our results: we first highlight the case of HD 163296, where we obtain vertical and radial profiles for ten molecules; then we show the CO emission location for all disks and study vertical modulations. This is followed by results on the radial brightness temperature profiles and an estimate of the disk gas pressure scale height. Finally, we present results for multiple molecules, other than CO, and detail our findings on the structured vertical profiles of HCN and H₂CO. Section 4 presents a discussion of our main results, comparing our observational constraints to theoretical estimations, and in Sect. 5 the main conclusions of this study are highlighted.

3.2 Observations and method

3.2.1 Data

In this work we use the publicly available data from the MAPS ALMA Large Program (Öberg et al. 2021b). For each disk in the sample we download the image cubes that were produced accounting for the incorrect default flux scaling of the CLEAN residual map (Jorsater & van Moorsel 1995), named from now onwards JvM corrected cubes (Czekala et al. 2021). An initial visual assessment is done to determine if a specific molecular emission from a disk can be used for extracting the vertical structure from the channel maps, following the methodology detailed in Sect. 2.2. Reasons for rejecting a molecule can be low S/N or lack of resolution to identify a Keplerian morphology in the channel emission. Table 3.1 shows the details of the selected files for each tracer, corresponding to those molecules for which it is possible to conduct our analysis in at least three disks. The dataset used may be identified by either the robust parameter or the beam size. For each molecule, the selected robust or beam size is the same for all disks in the MAPS sample. For datasets selected based on the robust parameter the difference in beam value between major and minor axis is typically of order $\leq 0.02''$. Between sources there is also a slight beam size difference of $\leq 0.02''$. At a distance of ~ 120 au this represents a difference of ~ 2.5 au; therefore, we consider beam size variations negligible in our calculations of the vertical profile. In addition to the information presented in Table 3.1, for HD 163296 we also study CN ($N = 1 - 0$, 113.499 GHz) and c-C₃H₂ ($J = 7_{07} - 6_{16}$, 251.314 GHz). The selection of these data is done by the beam size, $0.5''$ for CN and $0.3''$ for c-C₃H₂. A detailed study on HD 163296 is presented in Sect. 3.1.

To the MAPS sample, we add publicly available data of Elias 2-27 and WaOph 6. In both sources we study ¹²CO $J = 2 - 1$ emission from The Disk Substructures at High Angular Resolution Project (DSHARP, Andrews et al. 2018). We also include ¹³CO and C¹⁸O $J = 3 - 2$ data of Elias 2-27 from ALMA programmes #2016.1.00606.S and #2017.1.00069.S (P.I. L. Pérez). Calibration and imaging procedures of Elias 2-27 can be found in Andrews et al. (2018) and Paneque-Carreño et al. (2021). For WaOph 6 we include archival data of ALMA programme

Table 3.1: Selected files for molecules in MAPS sample disks.

Molecule	Transition	Freq. [GHz]	robust	beam ^a ["]
¹² CO	$J = 2 - 1$	230.538	0.5	~0.13
¹³ CO	$J = 2 - 1$	220.398	0.5	~0.13
C ¹⁸ O	$J = 2 - 1$	219.560	0.5	~0.13
¹³ CO	$J = 1 - 0$	110.201	0.5	~0.26
HCN	$J = 3 - 2$	265.886	-	0.30
C ₂ H	$N = 3 - 2$	262.040	-	0.15
H ₂ CO	$J = 3_{03} - 2_{02}$	218.222	-	0.30
HCO ⁺	$J = 1 - 0$	89.188	0.5	~0.32

Notes. ^(a) For molecules that were selected based on the robust parameter, the beam value corresponds to the mean value of all sources. In all $J = 2 - 1$ transitions the typical deviation from the mean value between sources is 6.7% and in the $J = 1 - 0$ transitions it is 8.3%

#2015.1.00168.S (P.I. G. Blake) and the ALMA Large Program DSHARP (Andrews et al. 2018). After self-calibration we can detect emission from ¹²CO, ¹³CO, C¹⁸O, HCN, CN, and HCO⁺ $J = 3 - 2$ in WaOph 6. Due to the moderate spatial resolution of the dataset (0.3-0.4"), in this study we only analyse ¹²CO, ¹³CO, and HCO⁺ data, where we can confidently study the vertical distribution of the disk. The integrated moment maps for all molecules observed in WaOph 6 and details on the self-calibration steps are found Appendix A.

Overall, our sample consists on two Herbig and four T-Tauri stars (Öberg et al. 2021b; Andrews et al. 2018). There are three disks with spirals, and four with rings and gaps (Huang et al. 2018b,c). Additionally, various sources show distinct kinematical features such as signatures of late infall in GM Aur (Huang et al. 2021) and Elias 2-27 (Paneque-Carreño et al. 2021) and possible planetary perturbations in HD 163296 (Pinte et al. 2018b; Teague et al. 2018a; Izquierdo et al. 2022; Teague et al. 2021a) and MWC 480 (Teague et al. 2021a).

3.2.2 Method

3.2.2.1 Vertical profile extraction

To extract the emission surfaces we use the geometrical method outlined in Pinte et al. (2018a) as applied in Paneque-Carreño et al. (2021). Knowing the central star position and geometrical properties, the vertical profile of the upper emitting layer can be recovered directly from the channel map observations by tracing the location of the maxima of emission along each channel, assuming that they are tracing the isovelocity curve. For the MAPS sample, the data have been centred and aligned following the location of the continuum peak emission (Öberg et al. 2021b), where we assume the central star is located. This same centring has been

performed on the Elias 2-27 and WaOph-6 datasets, and therefore we consider the centre of the image as the stellar location. If the inclination, flaring, and resolution of the disk allow the identification of upper and lower surfaces, it is possible to confidently trace both vertical profiles independently. In cases when the surfaces cannot be visually identified separately we assume that the peak of emission of the channel map comes from the upper surface, which is expected to be brighter than the lower surface.

From the extracted location of the maxima, geometrical relations can be used to obtain the vertical profile of the emission (see Pinte et al. 2018a, for more details). To trace the maxima we use our own implementation of the method (ALgorithm For Accurate Height Over Radius, ALFAHOR), which relies on masking each channel through visual inspection to identify separately the near and far sides of the emission from the upper layer (see Fig. 3.1 for clarification). The masks are selected after the channel map emission has been rotated, using the position angles indicated in Table 5.3, such that the bottom side of the disk emission is towards the south. The maxima of emission are retrieved automatically, but only from sampling the pixels within the masks. The masks are selected with as conservative margins as possible to avoid a bias in the recovered structure and there are no particular criteria regarding maximum outer radius or any other value¹. In this work, we only study the upper layer of emission, but in those cases where the lower layer can be identified (as can be observed for ^{12}CO in Fig. 3.1) it would be possible to additionally trace the vertical extent of the lower layer.

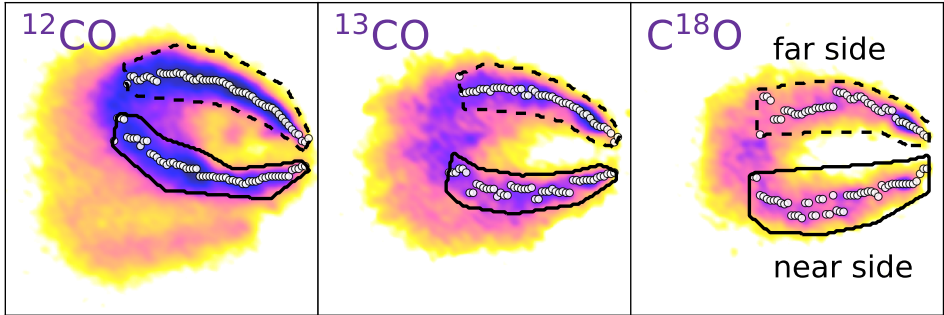


Figure 3.1: Rotated 7.86 km s^{-1} channel map emission of the $J = 2 - 1$ transition of CO isotopologues in HD 163296. Overlaid are the regions masked as far and near sides of the upper surface in dashed and solid black lines, respectively. White dots trace the emission maxima within the masked regions.

Previous work for some of the disks and molecules in our sample (Law et al. 2021b) used a publicly available implementation of the Pinte et al. (2018a) method, DISKSURF (Teague et al. 2021b). In DISKSURF the search of the emission maxima can be blind or constrained with initial expected values of the minimum and maximum z/r , the minimum S/N and selected channels. While this allows

¹A repository with the mask and code developed for this study can be found at <https://github.com/teresapaz/alfahor>.

Table 3.2: Studied systems, their properties, and the analysed molecules in each case.

Star ^a	M _* [M _⊙]	L _* [L _⊙]	Distance [pc]	Inclination [deg]	PA [deg]	Studied Molecules ^b
IM Lup	1.1	2.57	158	47.5	144.5	¹² CO, ¹³ CO, C ¹⁸ O, HCN, HCO ⁺ , H ₂ CO
GM Aur	1.1	1.2	159	53.2	57.2	¹² CO, ¹³ CO, C ¹⁸ O, HCN, HCO ⁺ , H ₂ CO
AS 209	1.2	1.41	121	35.0	85.8	¹² CO, ¹³ CO, C ¹⁸ O, HCN, HCO ⁺ , H ₂ CO, C ₂ H
HD 163296	2.0	17.0	101	46.7	133.3	¹² CO, ¹³ CO, C ¹⁸ O, HCN, CN, HCO ⁺ , H ₂ CO, C ₂ H, c-C ₃ H ₂
MWC 480	2.1	21.9	162	37.0	148.0	¹² CO, ¹³ CO, C ¹⁸ O, HCN, HCO ⁺ , H ₂ CO, C ₂ H
Elias 2-27	0.46	0.91	116	56.7	118.8	¹² CO (2 − 1), ¹³ CO (3 − 2), C ¹⁸ O (3 − 2), CN (7/2 − 5/2)
WaOph 6	1.1	0.68	123	47.3	174.2	¹² CO (3 − 2), ¹² CO (2 − 1), ¹³ CO (3 − 2), HCO ⁺ (3 − 2)

Notes. ^(a) Stellar and disk parameters taken from Öberg et al. (2021b) for the 5 disks in the MAPS sample and from Huang et al. (2018b) and Andrews et al. (2018) for Elias 2-27 and WaOph 6, except for stellar masses. The stellar mass is estimated dynamically in Veronesi et al. (2021) for Elias 2-27 and in Law et al. (2022) for WaOph 6. ^(b) The transitions of each molecule for the disks of the MAPS sample are detailed in Sect. 2.1. For Elias 2-27 and WaOph 6 the J transition of each molecule is shown in parenthesis.

for a systematic search and characterization of the channel emission, in some cases pixels from the bottom surface are incorrectly classified as located in the upper surface, and the other way around. This induces noisier vertical profiles, as there is a large data spread caused by the contamination of pixels from the lower surface of the disk. The S/N cutoff is also problematic when dealing with emission from less abundant molecules. By masking the channels after visual inspection, we reach locations of lower S/N and avoid contamination from the lower surface, obtaining a more accurate description of the vertical profile. Our implementation has been tested and illustrated in previous works (Paneque-Carreño et al. 2021; Leemker et al. 2022) and in this analysis we also compare it to the results of Law et al. (2021b) using DISKSURF (see Appendix B). Our results are consistent for bright tracers such as ^{12}CO and ^{13}CO , particularly in the inner region (<200 au). However, through our methodology we are able to trace a larger inventory of molecules to further radii.

For each disk and molecule we obtain the maxima from the channel maps by sampling every quarter of the beam semi-major axis in cartesian coordinates, after correcting for the disk position angle (PA). From all the obtained data points (see the Appendix B figures with all of the retrieved data points for each disk and tracer) we present the vertical profiles and the associated dispersion as the average value and the standard deviation within radial bins as wide as the beam semi-minor axis. In some disks, due to low S/N, there are fewer data points. To avoid biases due to lack of sampling, we only consider the data from radial bins where there are at least two independent data points. For Elias 2-27 it has been shown that there are azimuthal asymmetries in the vertical extent (Paneque-Carreño et al. 2021), but we do not find any indication of this behaviour in any of the other disks and molecules of our sample. Therefore, all of the data points are considered to compute the radial profiles. In the case of Elias 2-27 only the data points from the west side are considered. Table 5.3 details for each system the molecular emission from which we are able to produce vertical profiles.

Each emission surface in each disk and isotopologue can be parametrized using an exponentially tapered power law defined as

$$z(r) = z_0 \times \left(\frac{r}{100 \text{ au}}\right)^\phi \times \exp \left[\left(\frac{-r}{r_{\text{taper}}}\right)^\psi \right]. \quad (3.1)$$

The best fit values for z_0 , ϕ , r_{taper} , and ψ in each system are found by using a Markov chain Monte Carlo sampler as implemented by emcee (Foreman-Mackey et al. 2019). For the fitting procedure, we consider all data points. If convergence is not reached for r_{taper} and ψ , or if r_{taper} is much larger than the radial extent of the profiles, we assume a simple power-law profile and fit only for z_0 and ϕ . Table 3.B.1 presents the computed parameters of the exponentially tapered or single power laws for each disk and CO isotopologue.

3.2.2.2 Brightness temperature calculation

The brightness temperature (T_b) profiles are obtained from the peak intensity (I) using the complete Planck law. The relationship between both parameters is the

following,

$$T_b = \frac{h\nu}{k} \ln^{-1} \left(1 + \frac{2h\nu^3}{Ic^2} \right), \quad (3.2)$$

where h is the Planck constant, k the Boltzmann constant, c the speed of light and ν the frequency of the emission. The temperature profiles are computed from the azimuthally averaged peak intensity maps. To accurately de-project the data, we used either the best-fit power-law model or the exponentially tapered power-law model of each molecule. The azimuthally averaged peak intensity profile is obtained using the GoFish package (Teague 2019b), a $\pm 30^\circ$ wedge across the semi-major axis (as done in Law et al. 2021a) and radial bins half the size of the beam semi-major axis.

3.3 Results

3.3.1 The special case of HD 163296

HD 163296 stands out from the rest of the sample, as it is the disk where we were able to trace the emission layer for the highest number of tracers (see Table 5.3). For instance, it is the only system from the MAPS sample where we could obtain vertical profiles for CN and c-C₃H₂. HD 163296 is also a system of interest due to the detection of at least two planetary signatures at 94 and 261 au (Pinte et al. 2018b; Teague et al. 2018a, 2021a; Izquierdo et al. 2022).

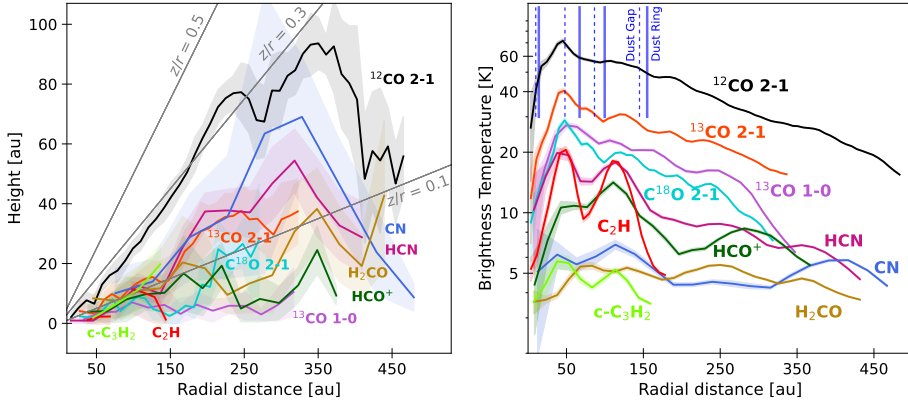


Figure 3.2: For HD 163296, vertical emission profiles (left panel) and azimuthally averaged peak brightness temperature profiles (right panel) for various tracers, beyond CO isotopologues. Solid coloured lines show the mean value in each profile and shaded regions the 1σ data dispersion. The vertical blue lines in the right panel indicate the location of the millimetre continuum gaps and the ring detected by Huang et al. (2018b).

Figure 3.2 presents the emission surface and brightness temperature profiles of each studied molecule. The emission surface of ¹²CO has the highest z/r and traces

a value of 0.3 up to ~ 350 au where it has a turning point and steeply declines. The emission surfaces of CN, HCN and $^{13}\text{CO } J=2-1$ are located in the interval of $z/r \sim 0.1-0.3$. $\text{c-C}_3\text{H}_2$ and H_2CO trace close to $z/r \sim 0.1$. C_2H also follows $z/r \sim 0.1$, but its emission surface rapidly declines at $r \sim 100$ au. This is in agreement with the C_2H vertical profile derived in Law et al. (2021b) for HD 163296. Below $z/r \sim 0.1$ is the emission of HCO^+ , $^{13}\text{CO } J=1-0$, and C^{18}O (only for the inner ~ 150 au in the case of C^{18}O). Beyond ~ 200 au, the vertical profile of C^{18}O elevates and traces a region closer to $^{13}\text{CO } J=2-1$.

The right panel of Fig. 3.2 shows our results for the brightness temperature profiles of each tracer. By comparing molecules found at similar vertical locations, but with different brightness temperatures, we can estimate the optical depth of the emission (not presented in this work, but see Paneque-Carreño et al. 2022, for an example). In the case of optically thick tracers, the brightness temperature will be a probe of the kinetic temperature of the studied region.

As expected, due to its location, high abundance, and optical depth, ^{12}CO has the highest brightness temperature. CN, HCN, and $^{13}\text{CO } J=2-1$ emit from the same vertical region. However, $^{13}\text{CO } J=2-1$ has a temperature of ~ 20 K, HCN is found at ~ 10 K, and CN at ~ 5 K. We expect $^{13}\text{CO } J=2-1$ to be marginally optically thick, while theoretical models and observational constraints (Cazzoletti et al. 2018; Bergner et al. 2021) predict that CN and HCN are likely optically thin, which would lead to a lower brightness temperature, as measured in this work. For the $z/r \sim 0.1$ molecules, we trace similar temperatures for $\text{c-C}_3\text{H}_2$ and H_2CO at $T_b \sim 5$ K and a higher temperature for C_2H , with a strong dip at 75-85 au. This dip is also seen in the HCN and $\text{c-C}_3\text{H}_2$ profiles and coincides with a gap found in the line emission of these molecules (Law et al. 2021a). Finally, in the molecules closer to the midplane, $^{13}\text{CO } J=1-0$ and C^{18}O have a similar $T_b \sim 18$ K. HCO^+ has a lower temperature profile, indicating it is likely optically thin with $T_b \sim 8$ K.

Besides optical depth differences, Leemker et al. (2022) show that differences in the spectral resolution may lead to variations in the extracted brightness temperature. Lower spectral resolution data will result in lower brightness temperature ranging from 10-60% depending on the resolution difference (see Appendix A.3 in Leemker et al. 2022). From the MAPS data, all observations of Band 6 (211-275 GHz) have a velocity resolution of 0.2 km s^{-1} whereas observations taken in Band 3 (84-116 GHz) have a resolution of 0.5 km s^{-1} . Therefore, CN, HCO^+ , and $^{13}\text{CO } J=1-0$ would likely have higher brightness temperature profiles if we compared them at the same spectral resolution as the rest of the tracers. The brightness temperature of all molecules shows a steep turnover in the inner 50 au, which is likely due to effects of beam smearing. At the source distance, the beam major axis of each tracer takes a value between 13-30 au and 50 au in the case of CN. Additional perturbations in the temperature profiles may be due to line flux subtraction from the continuum emission, as we are using the continuum-subtracted datasets. The dust features are indicated in the top of the right panel of Fig. 3.2 for reference.

3.3.2 CO isotopologue vertical structure of the full sample

The extracted emission surfaces of the CO isotopologues from the complete sample of disks are presented in Fig. 3.3. As explained in Sect. 2.2, we are able to trace the emitting layer out to a larger radial extent than the previous work on the MAPS sample (Law et al. 2021b). The main difference is in the $\text{C}^{18}\text{O } J = 2-1$ emission, which at larger radii is observed to trace a region very similar to $^{13}\text{CO } J = 2-1$. This is seen in all disks where both isotopologues are available and is in agreement with previous IM Lup (Pinte et al. 2018a) and Elias 2-27 (Paneque-Carreño et al. 2021) analysis. We are also able to compute a vertical profile for $^{13}\text{CO } J = 1-0$, which mostly traces a layer below $^{13}\text{CO } J = 2-1$, except in MWC 480 and AS 209 where both transitions are very close to the midplane.

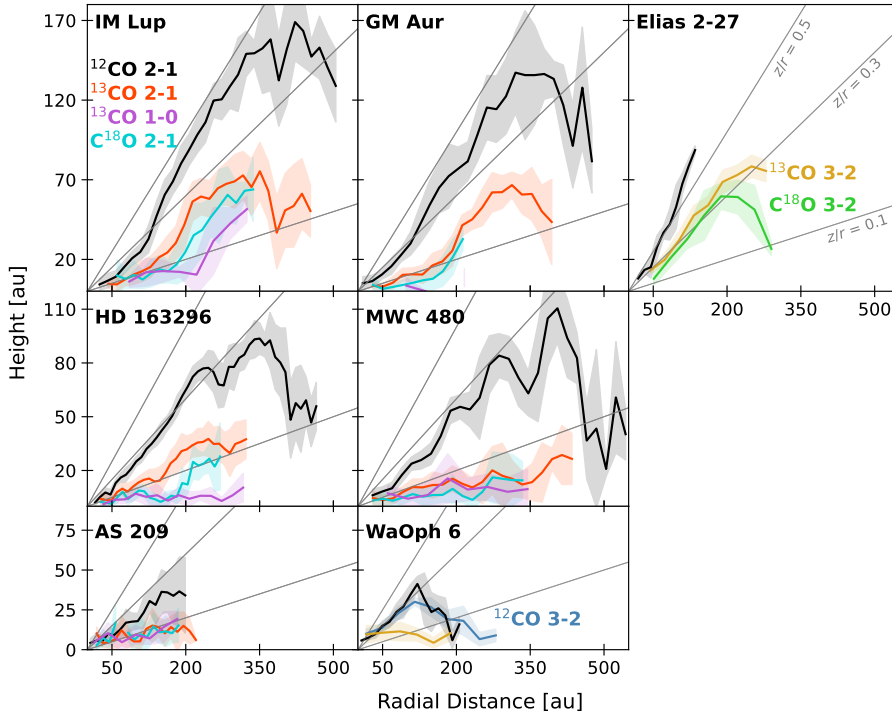


Figure 3.3: Vertical profiles for CO isotopologues as extracted from the channel maps of each disk. The shaded region shows the dispersion of the data points, and the solid coloured line traces the average values within each radial bin. Note that Elias 2-27 and WaOph 6 were observed at a higher transition ($J = 3 - 2$) in some CO isotopologues. Solid grey lines show a constant z/r of 0.1, 0.3, and 0.5. Each row has a different vertical extent.

The sample is divided into three groups, indicated by the three separate rows of Fig. 3.3. This classification depends on the z/r values that the ^{12}CO traces and the radial extension of the emission. IM Lup, GM Aur and Elias 2-27 are the

most vertically extended disks, with $z/r \geq 0.3$. HD 163296 and MWC 480, the two Herbig Ae disks, have a ^{12}CO vertical profile that traces $z/r \sim 0.3$. Finally, AS 209 and WaOph 6 are the flattest and least radially extended disks in our sample, with $z/r \sim 0.1\text{--}0.3$.

In some cases, such as for ^{12}CO in Elias 2-27, we lack sampling of the outer regions due to cloud absorption (Pérez et al. 2016; Paneque-Carreño et al. 2021). In this case the obtained best-fit for the vertical profile (methodology described in Sect. 2.2) follows a single power law. However this description of the data may only be valid in the inner ~ 100 au of the disk. For C^{18}O and ^{13}CO ($J = 1\text{--}0$) it is necessary to fit with a single power-law model in all disks due to the flat morphology or lack of turnover in the measured profile. It is important to emphasize that this does not mean there is no turnover as our parametric description is only valid up to the sampled radial location.

3.3.2.1 Modulations in the surface and correlation to kinematical and dust features

Even though the data can be fitted using a power law, the vertical profiles in Fig. 3.3 show modulations or ‘bumps’. This behaviour is identified in the ^{12}CO surface of HD 163296, MWC 480 and IM Lup. To trace the deviations from the possibly smooth vertical profile, a reference profile is assumed, which we refer to as the ‘baseline’ (see Fig. 3.4). This baseline does not coincide with the previously derived best-fit power-law or exponential profiles, which are not considered for this analysis because they cut through some of the features seen in Fig. 3.3. It is important to note that the retrieval of vertical modulations will strongly depend on the assumed baseline, which we cannot know with certainty without dedicated modelling and understanding of the properties of each disk.

We assume a baseline that traces the averaged vertical profile such that it follows a positive gradient at all radial locations. If there is a turnover, after which modulations are observed, we allow the baseline to follow only negative gradients, from the location where no further positive gradients are found. The final baseline profile is subtracted from all the data points and we compute the binned residuals. It is assumed that data with lower vertical values with respect to the baseline trace modulations and we fit Gaussians at these locations. The amount of Gaussian features to be fitted and the initial guess on the radial location are determined through visual inspection of the residual data points. The best-fit surface is obtained by simultaneously fitting multiple Gaussians to the assumed baseline. The fit is done considering all of the retrieved data points from the channel map analysis, the binned data are only used to determine the baseline and to aid visual inspection. This process is schematically shown in Fig. 3.4.

The ^{12}CO and ^{13}CO $J = 2 - 1$ isotopologues are analysed for HD 163296, MWC 480 and IM Lup, which are the disks and tracers where this behaviour is most clearly identified. C^{18}O is also analysed for HD 163296 and MWC 480, but as no modulations are found in IM Lup the analysis is not shown in this section. Detailed plots and values for each tracer and disk can be found in Appendix B. The best-fit models of ^{12}CO and ^{13}CO are shown overlaid on the data in Fig. 3.5,

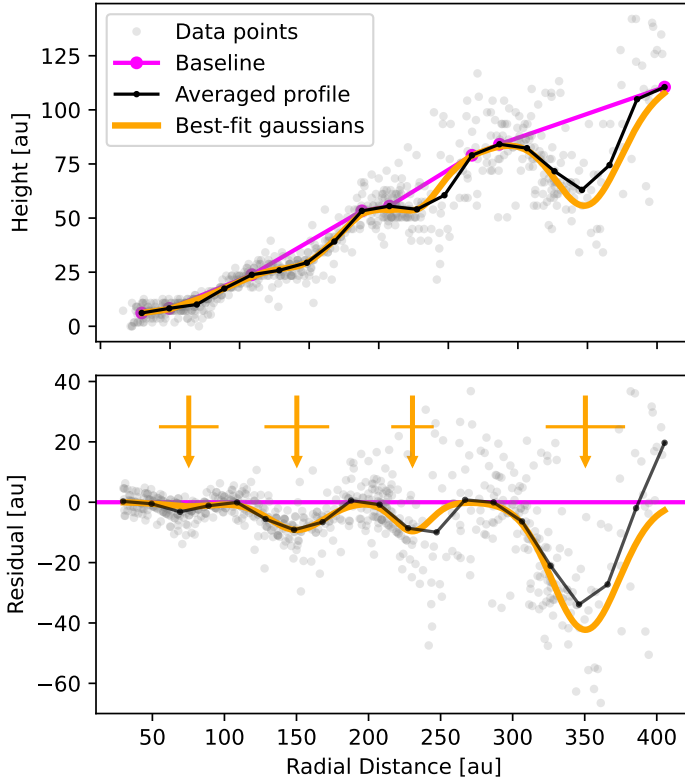


Figure 3.4: Example of baseline and best-fit Gaussian modulation extraction for the MWC 480 ^{12}CO dataset

where we compare the locations of the modulations in different tracers with the location of the dust rings and gaps found in ALMA millimetre continuum emission images (Huang et al. 2018b) and reported kinematic features (Teague et al. 2021a; Izquierdo et al. 2022).

HD 163296 displays a tight correlation between all of the modulations in both tracers. Additional analysis of the C^{18}O emission in HD 163296 also finds modulations at similar radial locations as the inner three structures reported in ^{12}CO and ^{13}CO . In MWC 480 we find a feature in ^{12}CO and C^{18}O that does not seem to have a correspondent in ^{13}CO , at 150 au. IM Lup has a strong feature at 393 au that is recovered in both tracers; however, the other modulations do not relate between isotopologues. Contrary to the other disks, IM Lup does not have visually identifiable drops in the vertical height in the inner 300 au and the features we obtain are broader than in the other systems. It may be that in this case we are tracing the flaring of the inner disk that due to our linear baseline is not considered properly in our reference surface model.

It is found that HD 163296 and MWC 480 present a strong correlation be-

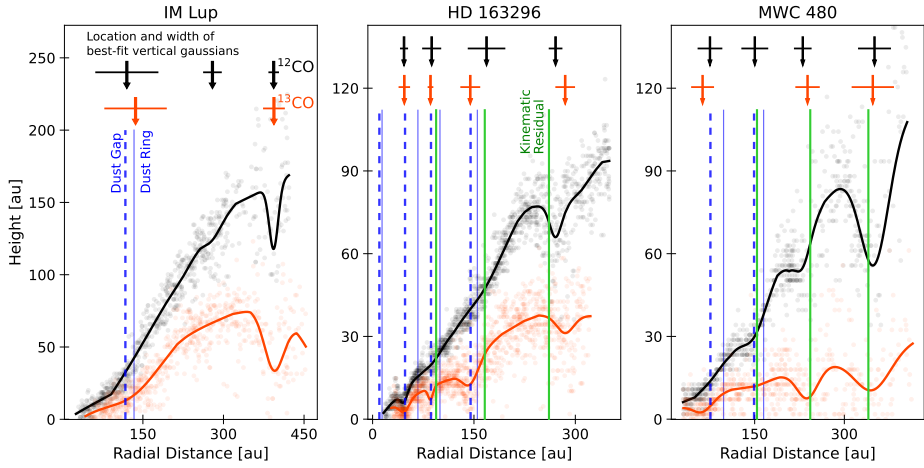


Figure 3.5: Data corresponding to $^{12}\text{CO } J = 2 - 1$ (in black) and $^{13}\text{CO } J = 2 - 1$ (in orange) for three disks where modulations in the vertical surface are detected. Coloured dots indicate the extracted data from the channel maps for each tracer. Continuous lines trace the best-fit surface considering the reference baseline and a number of fitted Gaussians. The location and width of the Gaussians for each molecule are signaled at the top of each panel. Vertical blue lines trace the dust structure from Huang et al. (2018b). Vertical green lines show the reported kinematic residuals from Teague et al. (2021a) and Izquierdo et al. (2022).

tween the location of millimetre continuum emission gaps (Huang et al. 2018b) and vertical modulation in the gas emission. A correlation is also found between the radial location of kinematic deviations detected in residuals from the velocity maps (Teague et al. 2021a; Izquierdo et al. 2022) and the vertical modulations traced in both HD 163296 and MWC 480. In contrast, there is no relation between the emission gaps and rings traced from the integrated emission maps (Law et al. 2021a) in either CO isotopologue for any of the disks. An additional caveat to these results may be that the extraction of the emission surfaces assumes a smooth Keplerian motion of the material (Pinte et al. 2018a) and strong deviations could be responsible for the features we detect, precisely quantifying this effect will be studied in a future work. However, the vertical modulations are recovered for the complete azimuthal range, they are not localized in azimuth as is the case for planetary kinks (e.g. Pinte et al. 2018a; Pérez et al. 2018b; Izquierdo et al. 2021). Considering that the emission surfaces extracted for ^{12}CO and ^{13}CO are expected to be related to the surfaces of $\tau = 1$, it is likely that the recovered modulations trace actual physical perturbations and decreases in the emitting surface or column density of CO. We comment on this further in Sect. 4.

In an analysis of vertical modulations, Law et al. (2021b) studied the inner ~ 100 au for the MAPS sample, and our results recover all of the features previously reported in HD 163296 and MWC 480. The depths and widths of our features slightly differ in some cases from the previous characterization due to the differ-

ences in extracting the vertical profile and in computing the assumed surface. The depth of each modulations is computed in the same way as in Law et al. (2021b). We consider the height value of the assumed surface at the feature location ($z(r_0)$) and the height depletion caused by the Gaussian feature (Δz), which is equivalent to the fitted amplitude. The ratio between these numbers results in a percentual description of the depletion from the assumed surface value. Higher depth values indicate a larger relative decrease in the scale height value. Our results show that, for features that are found in both tracers at similar locations, the relative depth in ^{13}CO is larger than ^{12}CO for all cases. Exact values are found in Appendix B.

3.3.2.2 Brightness temperature profiles

As done in HD 163296, we obtain the brightness temperature profiles for the CO isotopologue emission of the complete sample. In particular, for Elias 2-27 we use only the emission from the east side, due to the elevation and brightness asymmetries (Pérez et al. 2016; Paneque-Carreño et al. 2021). WaOph 6 and AS 209 also have strong absorption and a brightness asymmetry. Therefore, for the azimuthal profiles we only considered the south and west sides, respectively. The rest of the systems have their profiles extracted using a $\pm 30^\circ$ wedge across the semi major axis.

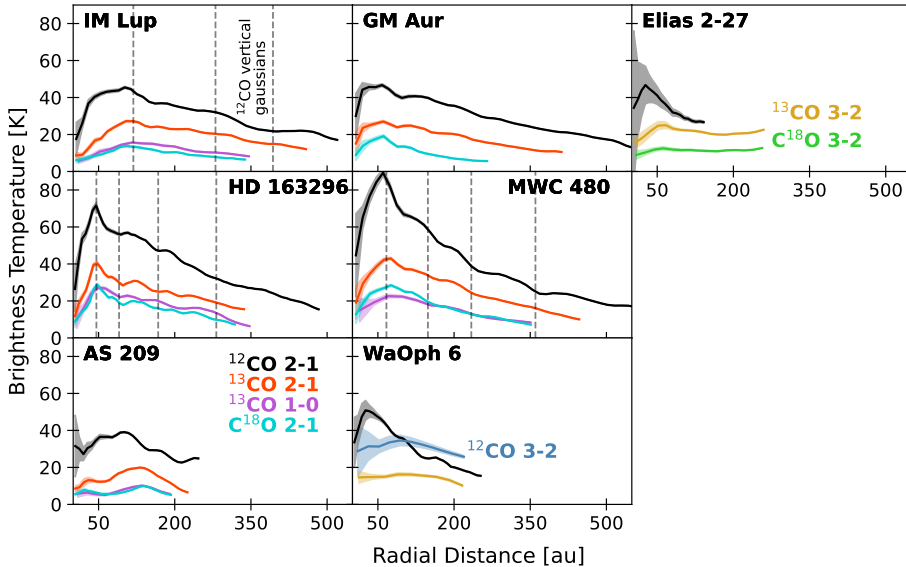


Figure 3.6: Brightness temperature profiles of the CO isotopologue emission in each disk. The solid line indicates the mean value and the shaded region the standard deviation within each radial bin, divided by the number of beams in each annulus. The vertical and radial scales are the same in each panel. Dashed vertical lines in IM Lup, HD 163296, and MWC 480 indicate the location of the vertical modulations determined in this work for ^{12}CO .

Figure 3.6 shows the results for each system and CO isotopologue. The ordering in the panels matches Fig. 3.3. The most vertically extended disks are in the top row, the intermediate disks in the middle row and the smaller, flatter disks in the bottom. All disks show a slowly decreasing temperature profile towards larger radii. Elias 2-27, HD 163296, MWC 480 and WaOph6 show a steeper slope in the temperature decrease of ^{12}CO . HD 163296 and MWC 480 also display higher temperatures for all isotopologues, which is expected as they are both warm Herbig disks orbiting more luminous stars. In all disks from the MAPS sample ^{13}CO $J = 1 - 0$ and C^{18}O $J = 2 - 1$ trace the same brightness temperatures, which are mostly below the CO freeze-out value ($\sim 21\text{K}$). This happens particularly at radii beyond 80 au for the Herbig stars, but at all radii for IM Lup, GM Aur and AS 209. We note that, as discussed previously, the spectral resolution of ^{13}CO $J = 1 - 0$ is lower than that of the other transitions, which may artificially result in lower brightness temperatures (Leemker et al. 2022). Very low brightness temperatures may also be indicative of low optical depths of the studied isotopologues and do not represent the kinetic temperature of the gas at that location. High optical depth tracers, such as ^{12}CO are expected to have brightness temperature profiles that are better tracers of the kinetic temperature at their location.

The vertical dashed lines in Fig. 3.6 show the location of the modulations in the vertical surface of ^{12}CO for IM Lup, HD 163296 and MWC 480 (see Sect. 3.2.1). While the temperature profiles do not show such strong features, slight modulations are distinguished that may be coherent with the locations of the vertical modulations. We tentatively detect relations between dips in the brightness temperature profiles of ^{12}CO and the location of the vertical modulations. Future detailed modelling of each source must be conducted to determine if the variations in the temperature profile are sufficient to explain the drops in the CO emission layer and determine the causes.

Even though the measured ^{12}CO vertical profiles of each disk are different and allow the classification of the sample in three categories based on vertical extension, the brightness temperature profiles of ^{12}CO are very similar. Considering only the disks from the MAPS sample, there is a clear difference in the ^{12}CO temperatures of T Tauri and Herbig Ae stars, as has already been reported in Law et al. (2021b). However, within the T Tauri stars, the vertical extent of the ^{12}CO emission in the disks is twice as large in IM Lup and GM Aur than in AS 209. WaOph6 and Elias 2-27 are also T Tauri stars and both show a warmer ^{12}CO inner disk than the other low mass stars from the MAPS sample.

3.3.2.3 Calculation of disk scale height

We have presented the vertical location of several CO isotopologues in a sample of disks. However, this emission surface depends on several physical-chemical conditions. A more transverse characterization of a disk's vertical structure is given by the gas pressure scale height (H), which can be used to compare theoretical models with observations. In order to derive this information, we design a simple single layer model. Despite the simplicity of the model, this allows us to provide first quantitative estimate of the material distribution. Assuming that the disk is

vertically isothermal it is possible to relate the scale height to the total volumetric gas density (ρ_{gas}) and the surface density of the disk (Σ) through

$$\rho_{\text{gas}}(z) = \Sigma \frac{e^{-z^2/2H^2}}{\sqrt{2\pi}H}. \quad (3.3)$$

We expect our derived vertical profile of ^{12}CO to trace the region where the emission becomes optically thick ($\tau \geq 1$) or where CO becomes self-shielding. For ^{12}CO ($J = 2 - 1$) at a temperature of 40-60K this occurs when the vertically integrated column density of ^{12}CO reaches the critical value $N_{\text{CO,crit}} \simeq 5 \times 10^{16} \text{cm}^{-2}$ (resulting in $\tau_{\text{CO}} \sim 1$, values obtained using the RADEX online simulator, van der Tak et al. 2007). As we are studying CO column density, we assume a constant $x(\text{CO})$ abundance of 2.8×10^{-4} with respect to H_2 in the disk (Lacy et al. 1994; Zhang et al. 2021), such that $\Sigma_{\text{CO}} = \Sigma x(\text{CO})$. Therefore, we can relate our derived vertical ^{12}CO location (z_{CO}) to the scale height of the disk and critical column density following

$$N_{\text{CO,crit}} = \frac{\Sigma_{\text{CO}}}{\sqrt{2\pi}H} \int_{z_{\text{CO}}}^{+\infty} \exp\left(-\frac{z^2}{2H^2}\right) dz. \quad (3.4)$$

To solve Eq. (4) we used a change in variable such that $z' = z/H$ and obtained an equation that can be solved numerically at each radial location where we have information on the ^{12}CO emitting layer (z_{CO}), to obtain the disk scale height if the emission is optically thick:

$$\int_{z_{\text{CO}}/H}^{+\infty} e^{z'^2/2} dz' = \frac{N_{\text{CO,crit}} \sqrt{2\pi}}{\Sigma_{\text{CO}}}. \quad (3.5)$$

Considering the surface density best-fit parameters derived from models in Zhang et al. (2021), we obtain the scale height profiles from our measurements for the disks in the MAPS sample. We note that the CO depletion profiles from Zhang et al. (2021) are not considered because they are obtained for C^{18}O and C^{17}O , and therefore we would have to make assumptions on the isotope ratios to convert them into ^{12}CO depletion profiles, adding an additional uncertainty (Miotello et al. 2014). This analysis is not done for Elias 2-27 and WaOph 6 as we do not have a model of the surface density and replicating the study of Zhang et al. (2021), which involves thermochemical modelling and radiative transfer, is beyond the scope of this work. Figure 3.7 shows our estimation for the scale height based on the best-fit parametrization of ^{12}CO surfaces, compared to the scale height profiles from the best-fit models studied in Zhang et al. (2021). Our results are in agreement with the models and with the canonical assumption of $H/R = 0.1$ for a standard irradiated disk beyond $\sim 100 \text{au}$ (see Eq. 5 in Lodato et al. 2019).

For IM Lup and HD 163296 there are also estimates on the pressure scale height from the location of the scattered light surfaces (Ginski et al. 2016; Avenhaus et al. 2018; Rich et al. 2021). Our values for the gas pressure scale height are below these estimates in both cases. The results show a layering where the ^{12}CO emitting surface is the most vertically extended, followed by the scattering surface and then the gas pressure scale height (see Fig. 3.C.2). The latter is in agreement

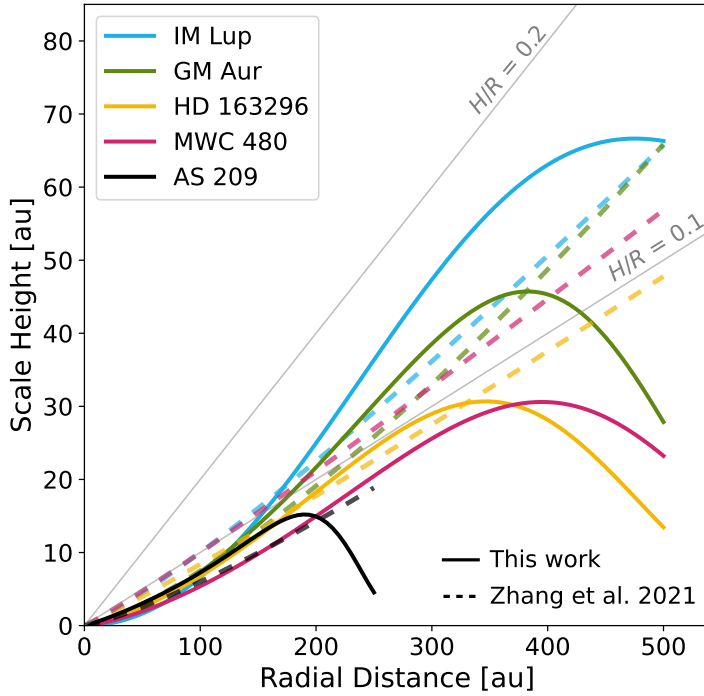


Figure 3.7: Derived gas pressure scale height (H) for each of the disks in the MAPS sample (in solid coloured lines) from our analysis of the ^{12}CO emitting surface. Dashed lines show the predicted scale height for each disk from Zhang et al. (2021). Solid grey lines show the location of constant H/R at 0.1 and 0.2.

with expectations from theoretical models, where the gas pressure scale height is estimated to be 3–4 times lower than the scattering surface (Chiang et al. 2001; Ginski et al. 2016). Our results display a difference of only 1.5–2 between the scattering surface and the gas pressure scale height. We note that the estimates we obtain of the pressure scale height strongly depend on the assumed density profile and CO abundance ($x(\text{CO})$). Low densities (Σ_{CO} below or close to the assumed CO critical density) push the pressure scale height to large values, up to a factor of a few, with respect to the derived CO emission layer. This indicates that if we would consider a depletion factor in the CO abundance then the H/R value would increase.

To test the robustness of our method we perform 2D thermochemical models with DALI (Bruderer 2013), using the gas surface density prescription of Zhang et al. (2021) and creating mock channel maps to retrieve the ^{12}CO $J = 2-1$ vertical profile (z_{CO}) for applying our methodology. The model details can be found in Appendix C.3 and the results of our test are displayed in Fig. 3.8. We observe that, as expected in our model, the emitting layer we retrieve for ^{12}CO from the mock channel maps is located at a similar height than the CO optical depth of $\tau_{\text{CO}} \geq 1$.

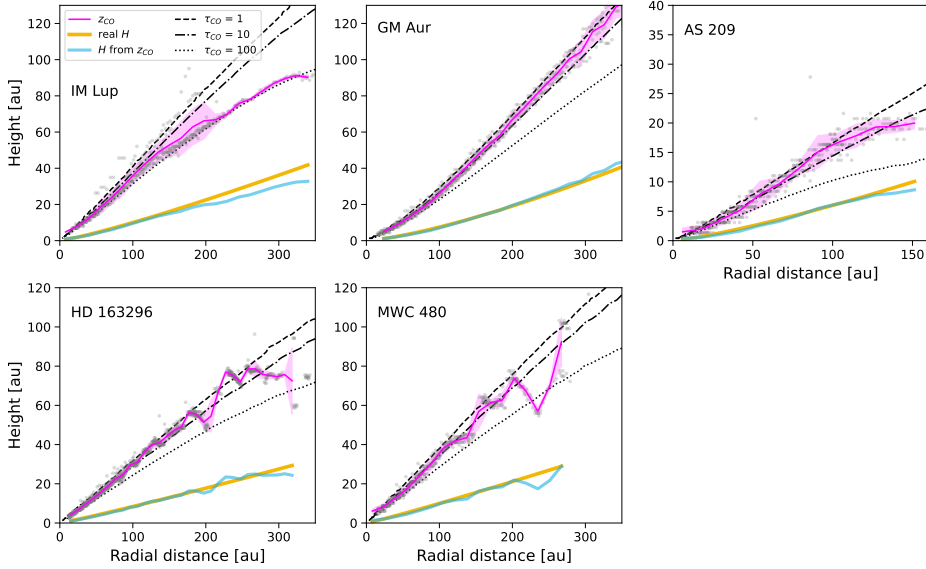


Figure 3.8: Results on the vertical location for ^{12}CO (pink line) and the inferred pressure scale height (blue line). The ^{12}CO vertical location is obtained with ALFAHOR through the analysis of mock channel maps generated from a DALI model that uses the surface density prescription from Zhang et al. (2021) for each disk. Points extracted from the synthetic channel maps are shown in grey for comparison with the average value (z_{CO}). The inferred pressure scale height is calculated following Eq. 5. The pressure scale height used as input for the DALI models (H) is shown for comparison (yellow line). Dashed, dot-dashed, and dotted lines show the model location of the CO millimetre optical depths (τ_{CO}) 1, 10, and 100, respectively.

The optical depth value is an output of the DALI models and is calculated at each radial point by vertically integrating towards the disk midplane the sum of line and dust opacities and then subtracting the dust only integrated opacity value. In some cases, the measured vertical profile for ^{12}CO emission traces a location closer to the disk midplane; therefore, it traces an optically thicker region reaching values of $\tau_{\text{CO}} \sim 100$. This difference in the expected location of the ^{12}CO emission does not seem to be related to any projection effects, such as disk inclination (see Fig. 3.C.4). IM Lup is the system that traces higher τ_{CO} in the outer disk and is also the source with the highest disk mass and radial extent (see Table 5.1). The resulting synthetic channel maps in this system are harder to trace in the outer radii than for the other sources, due to sudden brightness variations in the emission. The effect of this difficulty is reflected by the spread in the data points at 150–200 au and low sampling further out (see Fig. 3.8). Additionally, HD 163296 and MWC 480 show features in the model vertical structure that seem like the modulations studied in the previous section; however, it is uncertain if this is an actual physical effect or a structure that appears due to the coarser model resolution in the outer disk region. A future study focused on thermochemical

models will aim at understanding the parameters that affect the exact location of the emission. The models shown in this section are just first approximations to future theoretical work and are not analysed in detail here.

Using the extracted vertical profiles from the models, we apply our method to obtain the pressure scale height and recover an almost exact match to that of the scale height used as input for each source (see Fig. 3.8). Differences between the inferred pressure scale height and the model input value are most apparent in the outer regions ($r \geq 250$ au), where the emission comes from more optically thick zone (most apparent in IM Lup as mentioned before; see Fig. 3.8). A plot relating the conversion factor between the ^{12}CO emitting layer and the gas pressure scale height, for different τ_{CO} values can be found in Appendix C.

While this observationally driven derivation of H should be considered as an approximate first trial on describing the disk pressure scale height using the location of CO emission, our initial test with thermochemical models show it is a good approximation. We expect this method to hold if the gas in the disk follows Keplerian rotation, ^{12}CO emission is optically thick and the vertical distribution is similar to a Gaussian profile. Under these assumptions, our estimate shows that all systems have scale heights between H/R of 0.1-0.2 (Fig. 3.7), which is in agreement with theoretical predictions. An important caveat to our comparison with DALI models is that we have tested our method (Eq. 5) with a model that uses a Gaussian distribution for the vertical profile (see Appendix C for details), which is our initial assumption for inferring the pressure scale height (Eq. 3). While our tests are an important check to assure that our method is consistent, future work must focus on the errors that may appear if the vertical density profiles deviate from a Gaussian profile and consider an analytical disk prescription that gives a better representation of the vertical temperature structure (e.g. Chiang & Goldreich 1997; Dullemond et al. 2002).

3.3.3 Other tracers

For the MAPS programme targets we are able to trace the vertical profile of HCN, H_2CO , HCO^+ and C_2H in the same way as with the CO isotopologues. In the case of WaOph 6, the lack of spectral and spatial resolution in the data only allowed us to recover the surface of HCO^+ , even though HCN and H_2CO emission data are available too (see Appendix A). The vertical profiles of these molecules are shown, compared to the CO vertical layers, in Fig. 3.9. Elias 2-27 has observations of CN $N = 3 - 2$ hyperfine transitions from which the emitting surface has been recovered (Paneque-Carreño et al. 2022). However, as we are able to recover the emitting surface of CN $N = 1 - 0$ only in HD 163296 (shown in Fig. 3.2), we do not display this molecule in Fig. 3.9.

3.3.3.1 Complete sample

Molecules beyond CO isotopologues seem to mostly reside close to the midplane. Due to this, we are not able to visually separate upper and lower sides of the disk when masking the channel maps to extract the vertical profiles. This implies that

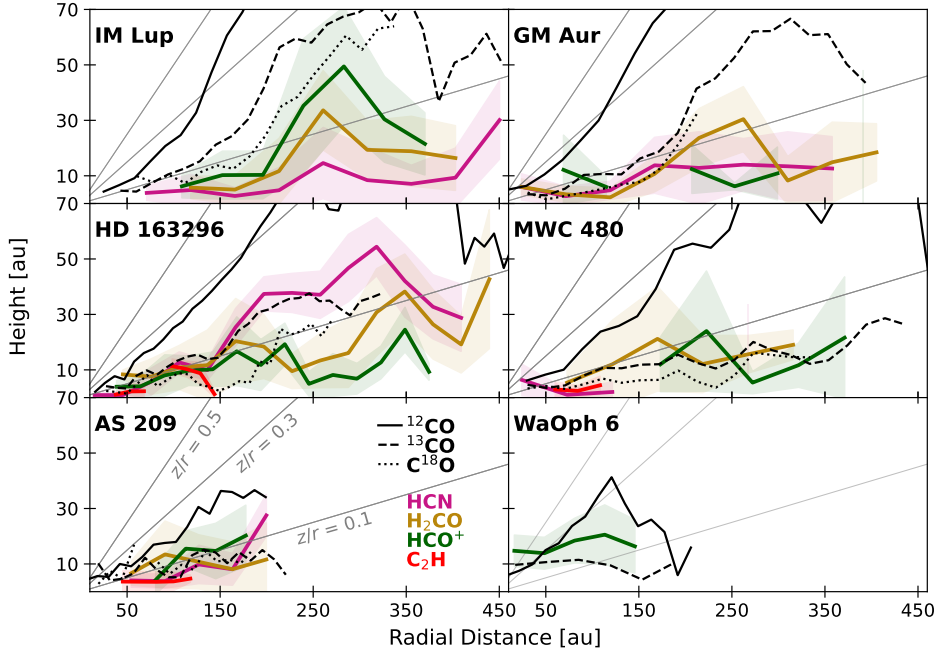


Figure 3.9: Vertical profiles of the emission surface for molecules other than CO isotopologues in the studied disks. Elias 2-27 is not shown due to a lack of data in other tracers. Black curves show the location of the CO isotopologues in the $J = 2 - 1$ transition for reference. The solid line is ^{12}CO , the dashed line ^{13}CO , and the dotted line C^{18}O . Each coloured curve shows a different tracer, where the solid line is the mean value and the shaded region shows the dispersion of the retrieved data points within each radial bin. Grey lines mark a constant z/r of 0.1, 0.3, and 0.5.

there could be some contamination and scatter caused by the lower side of the disk. Additionally, for some tracers the vertical extent of the emission is comparable with the beam size, and therefore the profiles of these molecules are considered tentative results. Higher spatial resolution and better S/N data may allow us to constrain them in more detail in the future. The gaps in the vertical profiles are due to lack of data (under two points) in the radial bin (see Sect. 2). We note that our results are in agreement with those obtained by Law et al. (2021b) for HCN and C_2H in the inner ~ 150 au.

The overall average z/r values of each tracer are shown in Fig. 3.10. As various tracers have different turnover radii and extent, we follow a similar approach to Law et al. (2022) and consider the emission only from within 80% of the ^{13}CO $J = 3 - 2$ r_{taper} . For MWC 480 and AS 209 we use ^{12}CO , as no turnover is detected in ^{13}CO (see Table 3.B.1). The emission from most tracers beyond CO isotopologues has a large scatter, but overall comes from regions with $z/r \leq 0.1$ (see the right panel of Fig. 3.10). This is in agreement with the flat morphology of the channel maps and the assumptions of flat disk used in MAPS for emission

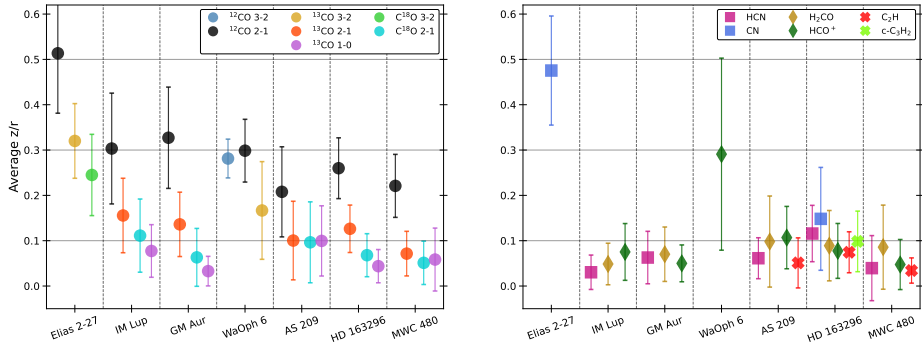


Figure 3.10: Average z/r values of each tracer and disk under study. To avoid the effect of the turnover in the case of vertically extended molecules, only data within 80% of the ^{13}CO (or ^{12}CO for MWC 480 and AS 209) r_{taper} is considered. Note that for Elias 2-27, CN is a higher transition ($N = 3 - 2$) than the CN shown in HD 163296 ($N = 1 - 0$).

other than CO (e.g. Law et al. 2021a; Guzmán et al. 2021; Bergner et al. 2021). HCN rises from an upper layer only in HD 163296 and HCO^+ shows a moderate elevation in IM Lup, AS 209 and WaOph 6. H_2CO has a consistent behaviour across all stellar masses, with $z/r \sim 0.1$. The emitting surface of CN can only be traced in Elias 2-27 and HD 163296. Both disks show CN is the highest emitting molecule, aside from ^{12}CO . However, in Elias 2-27 it traces the same region and in HD 163296 it is in a middle layer closer to the rest of the molecular reservoir.

The stars in Fig. 3.10 are ordered in the horizontal axis by increasing stellar mass; however, the scale is not linear as several of them have almost equal mass value (see Table 5.3). A tentative relation between the z/r values of CO tracers and stellar mass may be recovered from the left panel of Fig. 3.10 such that z/r decreases with increasing stellar mass. This relationship has been tested for ^{12}CO (Law et al. 2021b, 2022) and in this work we tentatively recover it for ^{13}CO $J = 2 - 1$ and C^{18}O $J = 2 - 1$ too (orange and light blue dots in Fig. 3.10). Contrary to the behaviour of its higher transitions, ^{13}CO $J = 1 - 0$ emits from a lower $z/r \leq 0.1$ layer and does not have any correlation to the stellar mass. Considering the mean values we note that ^{13}CO $J = 2 - 1$ lies in a vertical region 2-3 times lower than ^{12}CO $J = 2 - 1$ for all the disks in the MAPS sample. This also applies for WaOph 6 in $J = 3 - 2$ transitions, but for Elias 2-27 ^{13}CO is located closer to ^{12}CO and the ratio between their mean values is 1.5.

3.3.3.2 Structure in HCN and H_2CO

The HCN and H_2CO vertical profiles are well sampled (see all of the extracted data points in Appendix B) and show distinct morphologies, which in most cases do not follow an exponentially tapered power law or a single power-law model. These profiles are presented separately in Fig. 3.11 for all disks in the MAPS sample except MWC 480, which is not included due to the lack of data points for HCN emission. Overlaid on the profiles are the locations of rings and gaps

found in the integrated emission of each corresponding molecule and the edge of the millimetre continuum (Law et al. 2021a).

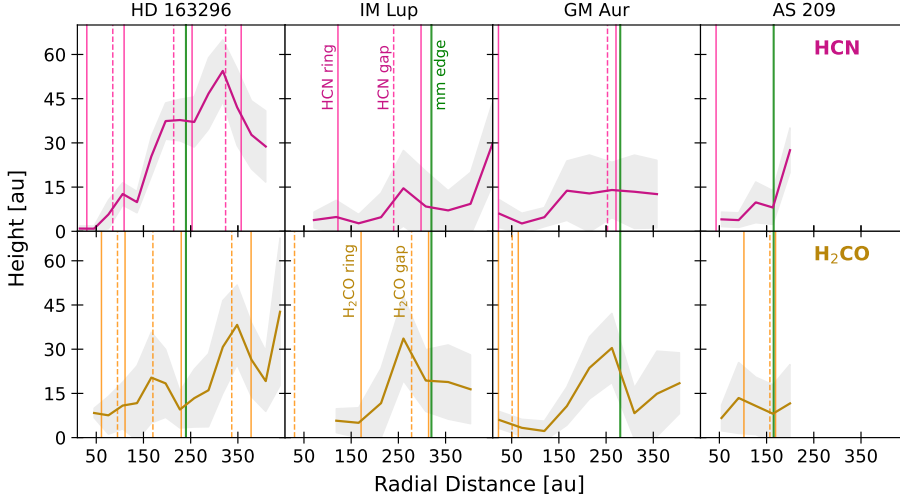


Figure 3.11: Vertical surface profiles for HCN (top row) and H_2CO (bottom row). The green vertical line marks the edge of the dust continuum as reported in Law et al. 2020a. The solid and dashed lines in each panel mark the rings and gaps, respectively, found in the emission maps of each molecule from Law et al. 2020a. In the profiles, the solid line marks the mean value and the grey shaded area the dispersion of the retrieved data points in each radial bin.

HCN shows a step-like profile in HD 163296, with peaks that mostly coincide with gaps in the integrated HCN emission. IM Lup shows a peak in the HCN profile at ~ 270 au, which is in between a gas gap and a ring and also coincides with the single peak seen in the H_2CO vertical profile. GM Aur and AS 209 may have tentative HCN peaks around ~ 150 au; however, the data do not allow us to properly characterize the profiles and there is a large dispersion in the recovered data points from the channel maps. While HCN is expected to trace high layers in the disk atmosphere (Visser et al. 2018; Bergner et al. 2021), it is clear that this is only the case in HD 163296 (see also Fig. 3.10).

The H_2CO vertical profiles can be traced with less scatter in all disks and for HD 163296, IM Lup and GM Aur we see clear peaks. In all cases there seems to be a peak close to and just inwards with respect to the edge of the millimetre continuum. The peaks in the vertical profile of HD 163296 and IM Lup coincide with gas gaps, as was the case for HCN. GM Aur has gas rings and gaps detected only in the molecular emission at small (<100 au) radii; however, it has a strong, well constrained rise in the emitting layer close to the continuum edge.

In HD 163296 and IM Lup there seems to be a correlation between the presence of line emission gaps and the peaks in the vertical structure for both HCN and H_2CO . It could be that the substructure of the molecular emission affects our profiles, as we are tracing the data directly from the channel maps, assuming that

the emission maxima trace an isovelocity curve. However, we do not see this effect in GM Aur, where H_2CO also has a strong vertical perturbation, and we note that most of the gaps in the molecular emission at outer radii in HCN and H_2CO have a very low-contrast (Law et al. 2021a). Therefore, we do not expect them to have such a noticeable impact on the retrieved profile. All vertical profiles show peaked features beyond the continuum emission border, and therefore it is also unlikely that this is an effect of continuum over-subtraction. Overall, if the emission is optically thin, which is expected from the brightness temperature profiles of HD 163296 (Fig. 3.2) and previous studies (Bergner et al. 2021; Guzmán et al. 2021), the vertical profiles seem to be tracing distinct variations of the physical location from where HCN and H_2CO are being emitted.

3.4 Discussion

3.4.1 CO isotopologue vertical layering

There have been dedicated studies to predict the regions from where molecules emit in protoplanetary disks (van Zadelhoff et al. 2001; Aikawa et al. 2002; Walsh et al. 2010; Miotello et al. 2014; Woitke et al. 2016). We trace the location of the emitting region for various CO isotopologues in our seven disks, including different transitions of ^{13}CO in the MAPS sample and ^{12}CO in WaOph 6. Our analysis shows that ^{12}CO emission comes from a wide range of vertical locations, which is in agreement with previous studies (Law et al. 2021b, 2022). This does not correlate directly with the emission location of other CO isotopologues or different molecules, except possibly ^{13}CO (see Sect. 3.3 and Fig. 3.10).

We take as reference the work by van Zadelhoff et al. (2001), where literature disk models are processed using a full 2D Monte Carlo radiative transfer code to determine the vertical location of the emitting surfaces for CO and HCO^+ isotopologues. The locations traced for the CO isotopologues in our work are qualitatively compared with the expected location of CO for a chemical abundance similar to the interstellar medium (ISM), and a more depleted abundance. In both scenarios it is expected to have a layering where ^{12}CO traces the upper layers, followed by ^{13}CO and C^{18}O , considering all transitions (see also Miotello et al. 2014). For the disks in the MAPS sample, we clearly recover that ^{12}CO emission comes from a higher region than ^{13}CO . Also, for ^{13}CO the $J = 2 - 1$ transition emission surface is above the $J = 1 - 0$ transition, as expected. However, we observe that C^{18}O $J = 2 - 1$ is emitting from a layer very close to ^{13}CO $J = 2 - 1$ and in most cases above ^{13}CO $J = 1 - 0$, which is not expected from the models. This overlap in the emission regions of C^{18}O $J = 2 - 1$ and ^{13}CO $J = 1 - 0$ could be explained by both of them emitting from just above the CO freeze-out region, which is also coherent with the measured low brightness temperature (see Fig. 3.6). Indeed, it has been proposed that C^{18}O $J = 2 - 1$ emission in IM Lup traces the freeze out (Pinte et al. 2018a). Our new results showing that ^{13}CO $J = 1 - 0$ emits from the same region or even closer to the midplane may be additional evidence of the freeze-out region location. C^{18}O $J = 1 - 0$ is also detected for the MAPS sample but unfortunately, due to the low S/N of this

transition, it is not possible to trace its emitting surface, which would be useful for additional comparison.

In WaOph 6 $^{12}\text{CO } J = 3 - 2$ and $J = 2 - 1$ trace the same region, which is in agreement with the previously discussed theoretical models. Future work obtaining observations at higher transition such as $^{12}\text{CO } J = 6 - 5$ could help differentiating between a depleted or ISM-like abundance, depending on how similar the emitting region is to that traced by lower transitions (van Zadelhoff et al. 2001). Elias 2-27 shows a highly elevated emission layer, where the $J = 3 - 2$ transitions of ^{13}CO and C^{18}O are very close to the $^{12}\text{CO } J = 2 - 1$. These two disks do not have a detailed description of their surface density or temperature structure, which would be useful for comparing them with the rest of the sample and obtaining the gas pressure scale height. Both disks have spiral structures in the dust continuum emission, which have been proposed to be linked to the effects of the disk self-gravity (Huang et al. 2018c; Paneque-Carreño et al. 2021). Our results show that in the line emission they both have very different structures, both radially and vertically; therefore, it remains unclear how dust continuum features relate with the vertical material distribution.

3.4.2 Vertical distribution of other molecules

Our work presents direct constraints of the emitting location for several molecules, extended to radial distances beyond ~ 150 au. Overall, the results show that most of these molecules emit from regions very close to the midplane ($z/r < 0.1$; see Fig. 3.10), which conflicts with theoretical predictions, in particular when analysing the location of UV sensitive tracers such as HCN and C_2H (Aikawa et al. 2002; Walsh et al. 2010; Bergner et al. 2021; Guzmán et al. 2021).

Various physical-chemical models have predicted that CN and HCN emission should be sensitive to UV flux (Cazzoletti et al. 2018; Bergner et al. 2021). The emitting layer of HCN should be located just below CN, due to the higher photodissociation rate of HCN compared to CN (Bergner et al. 2021). Overall, the emission of both tracers is expected to arise from the upper atmosphere of disks, in regions close to the ^{12}CO emitting layer (see also Walsh et al. 2010). The only system where we are able to extract the emitting surfaces of both tracers is HD 163296. In this disk we find that CN $J = 1 - 0$ emission is located in an intermediate layer, between ^{12}CO and $^{13}\text{CO } J = 2 - 1$ (see Figs. 3.2 and 3.10). In all the other disks, except for Elias 2-27, it is not possible to extract CN surfaces and HCN traces a region close to the midplane ($z/r < 0.1$). Observing emission from regions closer to the midplane may be an indicator of deeply penetrating UV flux either from the central star or from an external source (see models by Flores et al. 2021). Another alternative is that X-ray radiation is responsible for the emission, as suggested for the Flying Saucer system (Ruíz-Rodríguez et al. 2021). Ultraviolet radiation is deeply affected by the location of small dust particles, and therefore the constraints on the emitting surfaces shown in this work may be used for dust growth and settling models in disks through simultaneous modelling of the dust location, UV radiation and molecular excitation. C_2H is also a molecule expected to be a good UV tracer (Miotello et al. 2019; Guzmán et al. 2021) and

even though it is less radially extended, in the inner disk it traces the same region as HCN. Future observations of higher CN transitions may allow us to study the distribution of this molecule for the rest of the sample and compare its location with the retrieved HCN emitting region.

Models suggest that HCO^+ should be emitting from a region similar to the CO emission layer (Aikawa et al. 2002). We find that the average z/r of the molecule is indeed close to C^{18}O . In IM Lup, AS 209 and WaOph 6 the emission comes from above z/r of 0.1. These disks are expected to be the youngest of the sample (Huang et al. 2018c; Öberg et al. 2021b), which could imply they have had less chemical reprocessing and CO abundances similar to the ISM. Disks in which CO has been transferred into other species (expected for older systems) have HCO^+ emission located closer to the midplane, compared to models with ISM-like abundances (van Zadelhoff et al. 2001). Constraints from the measured excitation temperature of H_2CO (Pegues et al. 2020) and chemical models (Walsh et al. 2010) also predict that it should be located in the molecular layer, but above the CO freeze-out region. Indeed, we trace the emission from H_2CO in a very similar region to that of C^{18}O and HCO^+ .

The morphology of the HCN and H_2CO emitting layers show a distinct peaked structure (see Fig. 3.11). A possible relation is observed between the location of radial gaps in the molecular distribution and the peaks in the vertical profile. H_2CO is a molecule that has two formation pathways, it may emit due to desorption processes, from dust grains close to the midplane, or warm gas phase chemistry (Terwisscha van Scheltinga et al. 2021; Carney et al. 2017; Guzmán et al. 2021). The distinct surfaces we trace in H_2CO could be the first direct indication of regions where different emission mechanisms are acting. In particular, modelling of HD 163296 by Carney et al. (2017) predicts that in order to reproduce the radial intensity profile the outer disk (beyond the millimetre edge) must have an increased H_2CO abundance. The model considered a higher abundance compared to that of the inner disk that extends vertically (see Fig. 5 of Carney et al. 2017, for the R-step case), which is coincident with the peak traced in the emission surface of H_2CO in HD 163296 beyond the millimetre edge (see Fig. 3.11). It is important to note that the results of Carney et al. (2017) showed that the H_2CO could not be produced uniquely by gas-phase reactions. Our vertical profile shows that at radius ~ 240 au the emission comes from closer to the midplane, which would be coherent with thermal desorption of the molecule from icy grains.

Previous works focused on H_2CO emission have not recovered the structure we see in this study. However, models for DM Tau that consider gas-phase and grain chemistry recover a bulged H_2CO density structure in the vertical profile (Loomis et al. 2015). This bulged feature is expected at a higher elevation than what we trace in our vertical profiles and may not necessarily be reproduced in the emission surface. Pegues et al. (2020) find that measurements of the H_2CO excitation temperature in various systems show mostly constant radial temperatures; however, clear peaks are detected in LkCa15 and J1604-2130. If the densities are sufficient to assume that the emission is in local thermodynamic equilibrium, then the excitation temperature may be a proxy of the kinetic temperature and thus the vertical emission distribution. For HCN there are no sources in the literature

that show evidence of a structured vertical distribution, and the excitation temperature profiles derived for the MAPS sample do not have any noticeable relation to the features seen in our vertical profiles (Guzmán et al. 2021).

3.4.3 CO modulations: Correlation to millimetre gaps and kinematic features

Vertical structure is found in the CO isotopologue emission for IM Lup, HD163296 and MWC 480, this structure can be modelled as drops from a determined baseline, using Gaussian functions (see Sect. 3.2.1). We name these drops modulations. There seems to be a consistent relation between the locations of the modulations, gaps observed in millimetre continuum and kinematical residuals. As the emission surfaces are traced directly from the channel maps there are several possibilities regarding their origin. It could be that, if the kinematical features are caused by a planetary companion, the vertical modulations are a tracer of the material infalling and possibly accreting on to the planet. The kinematic residuals used in this work have all been related with the presence of planetary companions (Pinte et al. 2018b; Teague et al. 2018a; Izquierdo et al. 2022; Teague et al. 2021a). If there are planets in these disks, it has been shown that meridional flows of material (Fung & Chiang 2016) will be capable of disturbing the vertical density structure (Morbideilli et al. 2014; Szulágyi 2017; Szulágyi et al. 2022). Meridional flows have been detected observationally in HD 163296 (Teague et al. 2018a); however, it is unclear if the modulations we detect in the vertical disk structure are related to the meridional flows, as simulations do not provide clear predictions on the vertical structure, for they are mainly focused on density and velocity perturbations. It is expected that the vertical profiles trace the location where the gas becomes optically thick; therefore, the modulations could also be related to density drops. However, as mentioned in Sect. 3.2.1, the locations of vertical modulations do not coincide with the gaps and rings in the integrated emission map of each molecule (Law et al. 2021a), which should be a direct proxy for density variations.

Another possibility could be that there are no real vertical modulations, but rather we are recovering artefacts as we assume that the emission maxima trace an isovelocity curve in a smooth disk, but in the sample there are perturbed channel maps (MWC 480 and HD 163296; Teague et al. 2021a). Alternatively, it could also be that the emitting layer is indeed perturbed and causing the channel map to appear perturbed due to projection effects. Future detailed studies on the effect of velocity perturbations in the extraction of emission surfaces will aid in breaking this degeneracy and understanding the observational characteristics of each effect. However, as we clearly recover the modulations at a constrained radial distance on both sides of the disk, with respect to the semi-minor axis and in all of the studied channels, we propose that they are real perturbations present in the vertical structure.

If the surface modulations are related to planetary companions in the disks, the feature at ~ 393 au in IM Lup is particularly relevant. It is a coherent, strong and well defined modulation present in ^{12}CO and ^{13}CO emission, with no kinematical feature associated with it. The radial location of this dip is close to where the

gas component of the disk is expected to have a sharp change in the surface density (Panić et al. 2009). Searches for planetary companions in IM Lup have been performed (Mawet et al. 2012; Launhardt et al. 2020) but no object has been detected, considering a detection probability of $\sim 30\%$ for a planet of $13M_J$ at 400 au. For MWC 480 and HD163296 there are coherent inner modulations that are coincident with dust gaps, which for MWC 480 have no kinematical counterpart. However, for HD163296 there is a strong linewidth residual at ~ 38 au and a positive velocity gradient at ~ 45 au (Teague et al. 2018a; Izquierdo et al. 2022). Detailed models studying the effect of planetary companions on the CO emitting layer will be useful to determine if the detection of vertical features may be an indirect measure of the presence of a planet, but this goes beyond the scope of this paper.

3.5 Conclusions

In this work we have presented observational constraints on the vertical location of the molecular emission of seven disks. Using data of high angular and spectral resolution, we directly traced the emission location for up to ten different molecules. Our main findings and conclusions are the following:

1. We have characterized the emission surfaces of multiple molecules through a geometrical analysis of the channel map emission. We have also detected structured emission layers with modulations and spikes. Using an implementation of the Pinte et al. (2018a) method, where we mask the observed emission layer, we traced the emission surfaces at larger radii and for lower S/N molecular emission compared to previous work.
2. The derived emitting surfaces for CO isotopologues show a clear layering, with ^{12}CO being the most vertically extended tracer. ^{13}CO and C^{18}O of the same transition trace similar regions. From our available data, we can also corroborate that lower transitions trace closer to the midplane than higher transitions in the case of ^{13}CO , consistent with thermochemical models.
3. If the emission is optically thick and good approximations for the surface density and CO abundance are available, the ^{12}CO emission surface can be used to obtain the gas pressure scale height of the disk. Our values indicate that the scale height is consistent with values of $H/R = 0.1$. These results were obtained using a simple analytical one-layer disk model, and initial testing with thermochemical DALI models indicates the method is robust, at least if the vertical material in the disk follows a Gaussian distribution.
4. The locations of the detected modulations in the CO isotopologue emitting surfaces are correlated to that of millimetre continuum gaps and kinematic perturbations. These modulations may be related to the presence of planetary companions or other mechanisms that cause variations in the gas density distribution.

5. HD 163296 shows a rich molecular reservoir from which most tracers can be located in distinct vertical regions. Overall, in our sample most of the molecular emission for tracers other than CO originates close to the midplane at $z/r < 0.15$. In the cases of HCO^+ and H_2CO , the observational constraints agree with theoretical predictions and constraints on the excitation temperature. Both molecules seem to be tracing the molecular layer above the CO freeze-out region. The particular morphology of the H_2CO emitting surface may be the first direct indicator of this molecule originating from both ice grain desorption and gas phase chemistry.
6. HD 163296 displays CN and HCN in an intermediate vertical region. Their location is in agreement with theoretical predictions (e.g. Cazzoletti et al. 2018; Bergner et al. 2021) that HCN traces a layer just below CN. The rest of the systems in the MAPS sample show HCN very close to the midplane, and it is not possible to retrieve CN emission surfaces for a comparison. This is not expected from theoretical models. Future observations of higher CN transitions will allow us to compare our results on the location of HCN and better understand the disk radiation conditions.
7. This sample of disks and molecules represents the largest survey to date of the direct characterization of the emitting regions for multiple tracers. Dedicated physical-chemical modelling is crucial for understanding the diversity in the location of each molecule and how to relate the vertical profiles to actual disk properties.

We aim for this work to be used as a reference catalogue for future dedicated models on each of the sources so that the physical-chemical origin of each emission line can be adequately studied. With the sensitivity of instruments such as ALMA, we hope to enlarge the sample of disks where this kind of study is possible.

Acknowledgements

We thank the referee for the constructive comments. This paper makes use of the following ALMA data: #2015.1.00168.S, #2016.1.00484.L, #2016.1.00606.S, #2017.1.00069.S and #2018.1.01055.L. ALMA is a partnership of ESO (representing its member states), NSF (USA), and NINS (Japan), together with NRC (Canada), NSC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO, and NAOJ. Astrochemistry in Leiden is supported by the Netherlands Research School for Astronomy (NOVA), and by funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 101019751 MOLDISK). B. T. is a Laureate of the Paris Region fellowship program, which is supported by the Ile-de-France Region and has received funding under the Horizon 2020 innovation framework program and Marie Skłodowska-Curie grant agreement No. 945298.

Appendix

3.A WaOph 6 data and self-calibration

The emission lines studied in WaOph 6 are mostly observed by ALMA programme #2015.1.00168 (P.I. G. Blake). The data were obtained in two consecutive observations, performed on 28 June 2016, and the total integration time on source was 29 minutes. Table 3.A.1 shows the information for all of the detected lines together with their integrated emission and imaging parameters after self-calibration. Besides the detected species, the spectral setup was also intended to observe H^{13}CN $J = 4 - 3$ and SO_3 $7(8) - 6(9)$. We do not detect either of them even when using a natural weighting of the visibilities, at the achieved sensitivity level of 6mJy beam^{-1} (beam values for these tracers are $\sim 0.4''$). Of the detected lines, not all of them can be used to extract the emitting surfaces, due to low S/N, compact radial extent and lack of spatial resolution. Of this dataset only ^{12}CO , ^{13}CO and HCO^+ have their emission surfaces extracted in the main text.

The data were initially calibrated the ALMA pipeline. Afterwards, phase and amplitude self-calibration were performed to enhance the signal to noise of the emission. To do this we use the tools found in the Common Astronomy Software Applications (CASA; McMullin et al. 2007), version 6.1.1.15. The self-calibration solutions were found using the line-subtracted continuum channels in all available spectral windows. Solutions for phase and amplitude were considered until the S/N improvement of the continuum was less than 2%. Four rounds of phase self-calibration were applied, using a maximum time interval of 965 seconds and dividing by two in each iteration to reach a minimum time interval of 120 seconds. After this, two rounds of amplitude self-calibrations were done, using a solution time interval of 965 and 480 seconds in each iteration. The overall peak signal to noise improvement was of 1300% in the continuum after completing self-calibration.

In the self-calibrated continuum data the centre of emission was found through a Gaussian fit in the image plane. The phase and pointing centres in the whole dataset were adjusted using CASA tasks `FIXVIS` and `FIXPLANETS`, respectively. The self-calibration solutions are then applied to the line emission channels and images of each line are produced using multi-scale `TCLEAN` and varying robust parameters to compromise between S/N and spatial resolution. Details on the robust and final full width half maximum beam values are found in Table 3.A.1. In all cases a stopping threshold of 3σ is used to compute the image. The integrated emission (moment 0) maps and line spectra are shown in Fig. 3.A.1.

Table 3.A.1: Imaging and emission parameters for WaOph6 data.

Molecule	Transition	Freq. [GHz]	Int. Flux [Jy km s ⁻¹]	Robust	Beam		
					b_{min}	b_{max}	PA
¹² CO	$J = 3 - 2$	345.795	21.343 ± 0.069	0.5	0.27''	0.35''	86.77°
¹³ CO	$J = 3 - 2$	330.588	5.073 ± 0.069	0.5	0.28''	0.43''	-85.74°
C ¹⁸ O	$J = 3 - 2$	329.330	1.364 ± 0.087	0.5	0.31''	0.48''	-80.11°
HCO ⁺	$J = 4 - 3$	356.734	3.988 ± 0.077	2.0	0.26''	0.35''	87.05°
CN	$J = 5/2 - 3/2$	340.031	2.329 ± 0.064	2.0	0.3''	0.46''	-80.59°
HCN	$J = 4 - 3$	354.505	0.747 ± 0.071	2.0	0.3''	0.39''	85.77°

Notes. This table shows only the data from programme #2015.1.00168.S (P.I. G. Blake).

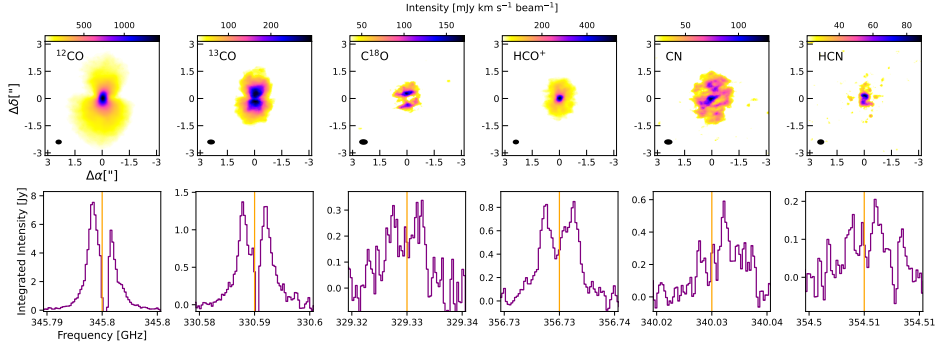


Figure 3.A.1: For each of the detected molecules in WaOph6 from programme #2015.1.00168.S (P.I. G. Blake): the integrated emission maps (moment 0) with an emission cutoff at 3σ (top row) and the emission spectrum of each line (bottom row). The vertical orange line indicates the natural frequency of the molecule.

3.B Data and best-fit parameters for the emitting layers

3.B.1 Data points and averaged vertical profiles

For each molecule and disk in the MAPS sample we present the extracted emission surfaces, showing all of the obtained data points in Figs. 3.B.1, 3.B.2, 3.B.3, 3.B.4, 3.B.5, 3.B.6, 3.B.7, and 3.B.8. The averaged vertical profiles and the best-fit parameters for each CO transition profile are shown in Fig. 3.B.9 compared to those found using DISKSURF (Teague et al. 2021b) in Law et al. (2021b). In general, the surfaces are similar for ¹²CO; however, in ¹³CO and C¹⁸O the previous work underestimates the height of the emission compared to our results. This is particularly apparent beyond 200 au. The best-fit values for the emitting surfaces

of all CO isotopologues, parameterized using an exponentially tapered power law can be found in Table 3.B.1.

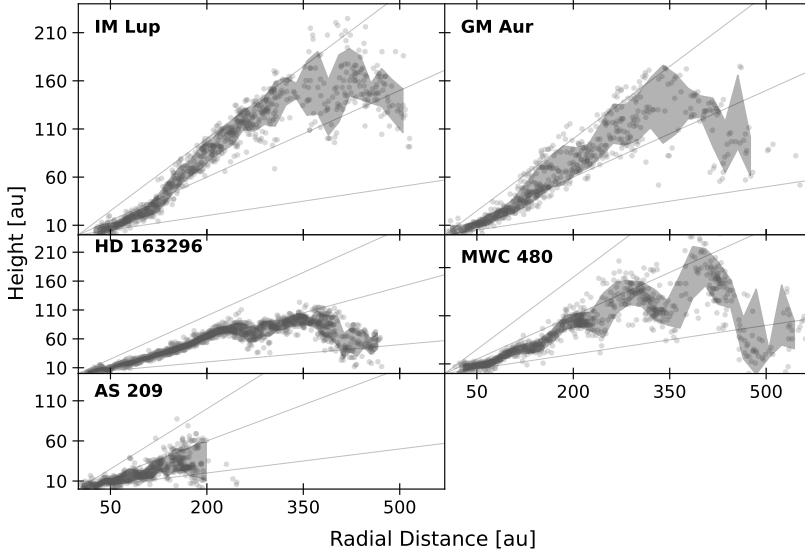


Figure 3.B.1: $^{12}\text{CO } J = 2 - 1$ data points.

3.B.2 Modulations in vertical surface

The modulations detected in the CO isotopologues for IM Lup, HD 163296 and MWC 480 are characterized as detailed in Sect. 3.2.1. Figures 3.B.10, 3.B.11, and 3.B.12 display the baselines, averaged data and location of best-fit Gaussians for each disk and tracer analysed. The values of the best-fit location, width and depth of the vertical Gaussian components for each studied disk and isotopologue are shown in Table 3.B.3.

3.C Tests and comparisons of the gas pressure scale height

3.C.1 Comparison scattering surfaces to CO and gas pressure scale height.

From our simple one-layer model detailed in Sect. 3.2.3 we relate the location of the CO emission layer to that of the gas pressure scale height. This relation has a strong dependence on the surface density profile, CO abundance, and critical density. Figure 3.C.1 shows the relation between these values. We note that the

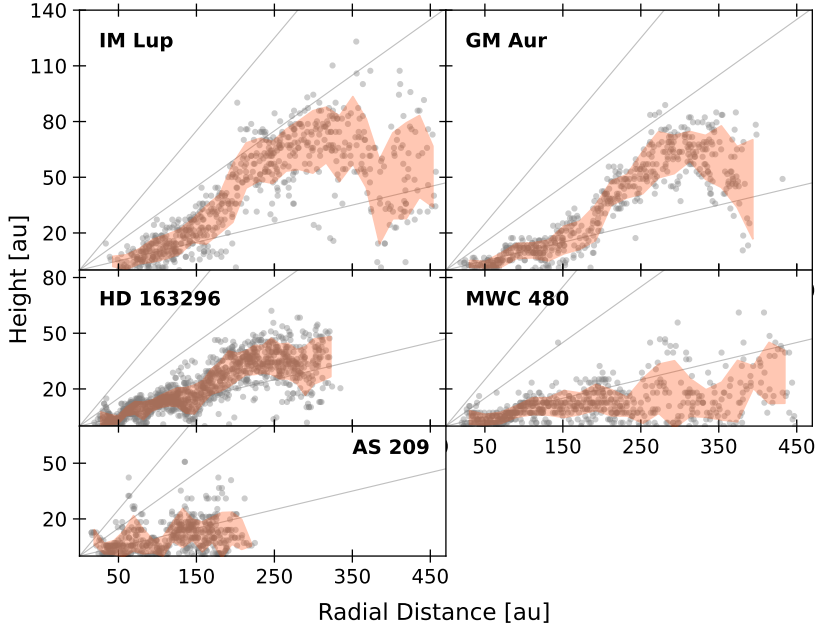


Figure 3.B.2: $^{13}\text{CO } J = 2 - 1$ data points.

critical density value varies according to the optical depth (τ) at the emission location.

Figure 3.C.2 shows the vertical location of the $^{12}\text{CO } J = 2 - 1$ emission layer, the parametrization of the scattering surface (Rich et al. 2021) and the inferred location of the gas pressure scale height obtained in this work. It is seen that for both IM Lup and HD 163296 the ^{12}CO layer traces the most vertically extended region, followed by the scattering surface and closer to the midplane lies the gas pressure scale height.

3.C.2 Conversion factors between z_{CO} and H and an alternative estimate

Another method to estimate the pressure scale height is through the midplane temperature of the disk, calculated considering the luminosity of the star and then related to the scale height through the stellar mass (see Eqs. 3 and 4 from Law et al. 2022). This has been done for several disks with estimates on their CO emission layers, including the MAPS sample in Law et al. (2022). Figure 3.C.3 shows the comparison of the radial conversion factors between z_{CO} and H obtained through our single layer model and what is obtained from the pressure scale height derived through stellar parameters, assuming a flaring angle of 0.02.

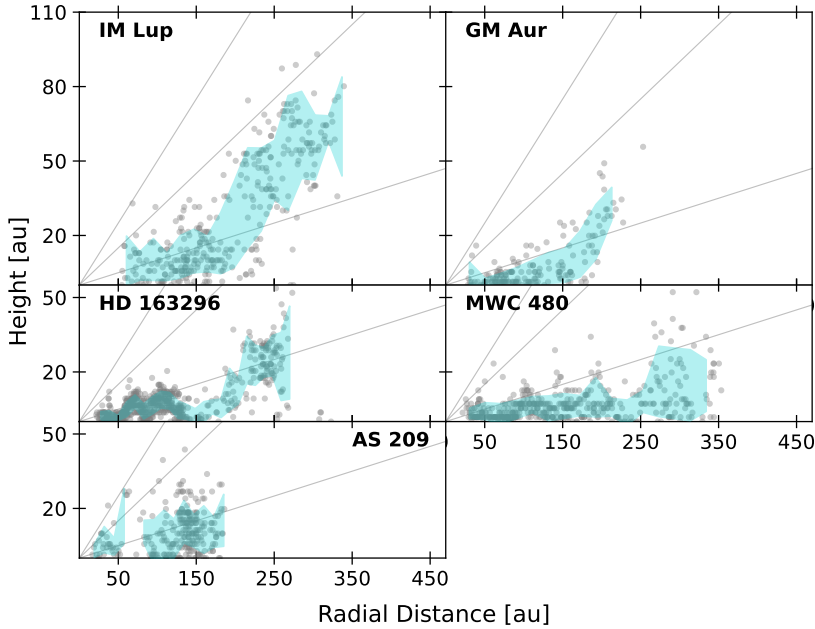


Figure 3.B.3: $\text{C}^{18}\text{O } J = 2 - 1$ data points.

The conversion factors stretch between 3-5 in the inner 300 au and then to lower values in the outer radii for all of our sample. The curves shown in Fig. 3.C.3 are smoother than those derived in Law et al. (2022) because we are using the best-fit parametrization of the CO emitting layer instead of the average height layer values. We note that, with the exception of AS 209, our method obtains a much narrower range for the conversion factor than when considering the stellar parameters. Through our test with thermochemical models we have confirmed the accuracy of our method, which implies that the method using stellar parameters is not a good approximation to the pressure scale height. The narrow range of our result suggests that there may be a direct relation, varying with radius, to convert the location of the CO emitting layer into gas pressure height. The difference in the conversion profile of AS 209 is due to the much lower density it has been reported to have (Zhang et al. 2021). Overall, these high resolution and sensitivity data open new avenues in our understanding of the disk physical structure.

3.C.3 DALI model setups

An initial test on our simple analytical method to estimate the gas pressure scale height is done through thermochemical DALI (Bruderer 2013; Bruderer et al. 2012) models. For details on the code, how the chemical network is set and the calcu-

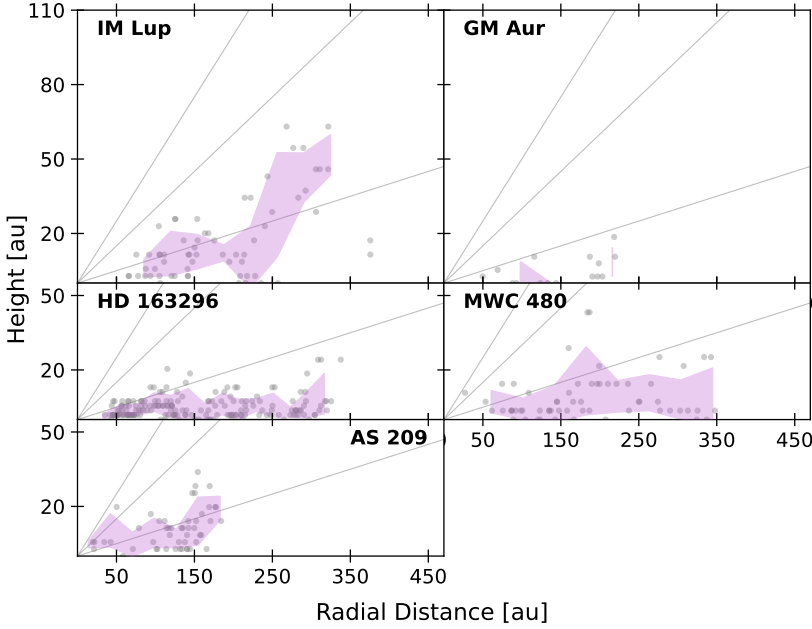


Figure 3.B.4: $^{13}\text{CO } J = 1 - 0$ data points.

lation of the temperature structure, dust populations and flux values we reference to past works using the same code (e.g. Leemker et al. 2022; Miotello et al. 2016; Bruderer et al. 2012; Bruderer 2013). We use the chemical network of Bruderer et al. (2012) and consider a chemical age of 1 Myr for the calculations. Other general parameters common to all simulations are presented in Table 5.1.

The aim of these models is to create a structure using the best-fit gas surface density values reported in Zhang et al. (2021) for each of the MAPS sources (see Table 2 in Zhang et al. 2021). The radial structure of the gas and dust in DALI follows the self-similar solution to a viscously evolving disk (Lynden-Bell & Pringle 1974; Andrews et al. 2011):

$$\Sigma(R) = \Sigma_c \left(\frac{R}{R_c} \right)^{-\gamma} \exp \left[- \left(\frac{R}{R_c} \right)^{2-\gamma} \right], \quad (3.6)$$

where R_c is the characteristic radius and γ the surface density exponent. The vertical structure of the disk follows a Gaussian distribution, which we have modified from the typical DALI prescription (see for example Leemker et al. 2022) to match the prescription of Zhang et al. (2021). The scale height angle (h) is set at each radius following

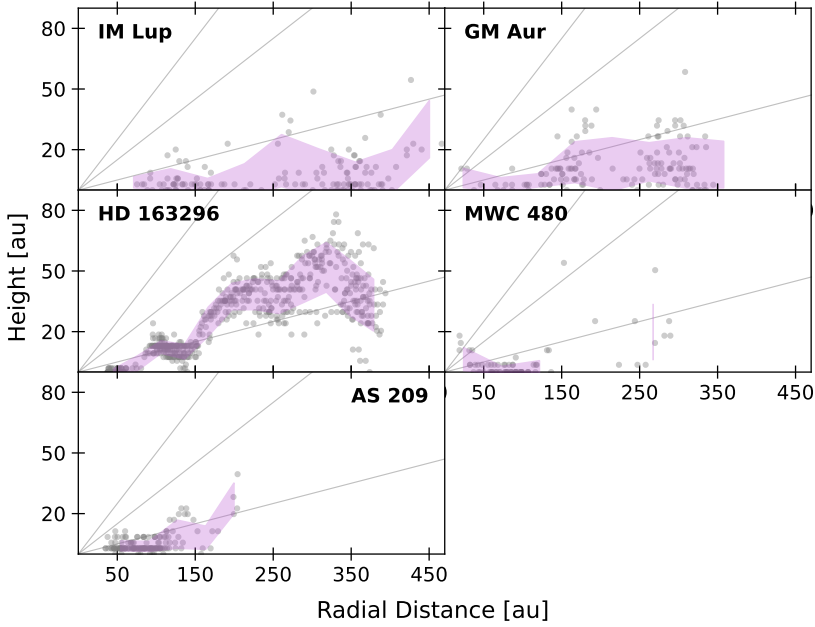


Figure 3.B.5: HCN data points.

$$h = h_{100} \left(\frac{R}{100\text{au}} \right)^\varphi, \quad (3.7)$$

where h_{100} is the scale height angle at 100 au. The scale height angle can be converted to a physical height above the disk midplane, H as $H \sim hR$. We note that as the scale height is defined in angular units, the flaring angle φ will be $1 - \varphi_r$, where φ_r is the flaring angle for a model in physical units (as presented in Zhang et al. 2021). The physical and stellar parameters used for each disk are shown in Table 3.C.2. Using the radiative transfer tools of DALI (Bruderer 2013; Bruderer et al. 2012), we create mock channel maps from each model matching the velocity (0.2 km s^{-1}) and spatial ($0.13''$) resolution of the ^{12}CO observations. These channel maps are analysed using ALFAHOR in the same way as the observations (see Sect. 2.2.1) to extract the emitting layer.

Using the DALI models we additionally test if the inclination of the system may affect on our retrieval of the vertical surface. Figure 3.C.4 shows the retrieved vertical profiles for $^{12}\text{CO } J = 2 - 1$ from the GM Aur model using three different inclinations to compute the channel maps. As can be seen, there is no significant variation between the inclinations, indicating that, at least for optically thick tracers, the orientation of the disk is not a source of concern. What may vary at different inclinations is the radial extent up to which it is possible to confidently

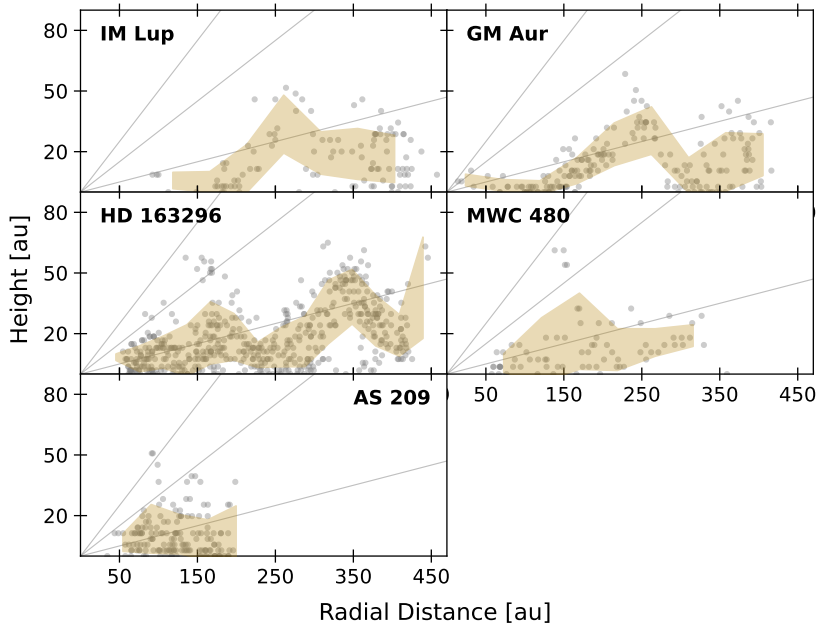


Figure 3.B.6: H₂CO data points.

separate and trace far and near surfaces in the channels. This leads to a difference in the maximum radial region in which we can trace the vertical structure, but, within a radial extent that is sampled by all inclinations, the vertical profiles are in agreement. Further testing with the models of the other studied systems show the same results of coherent values at different inclinations. IM Lup is the disk that shows the largest variations; however, the values are still very similar within the uncertainties. As discussed in Sect. 3.2.3 the surface density model of IM Lup considers the most massive and extended disk of the sample and this could be related to tracing a lower vertical layer and slight differences with varying inclinations. This will be studied in detail in future work focused on thermochemical models.

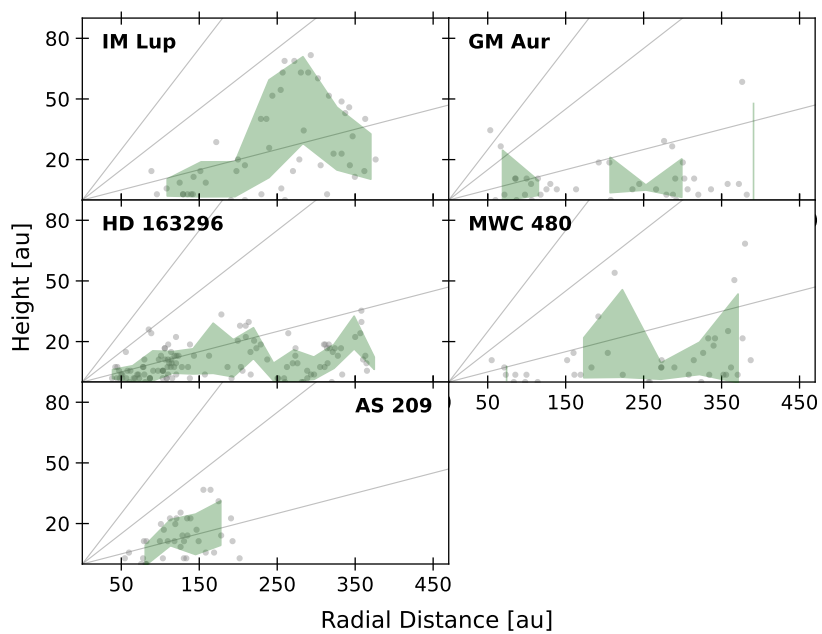


Figure 3.B.7: HCO⁺ data points.

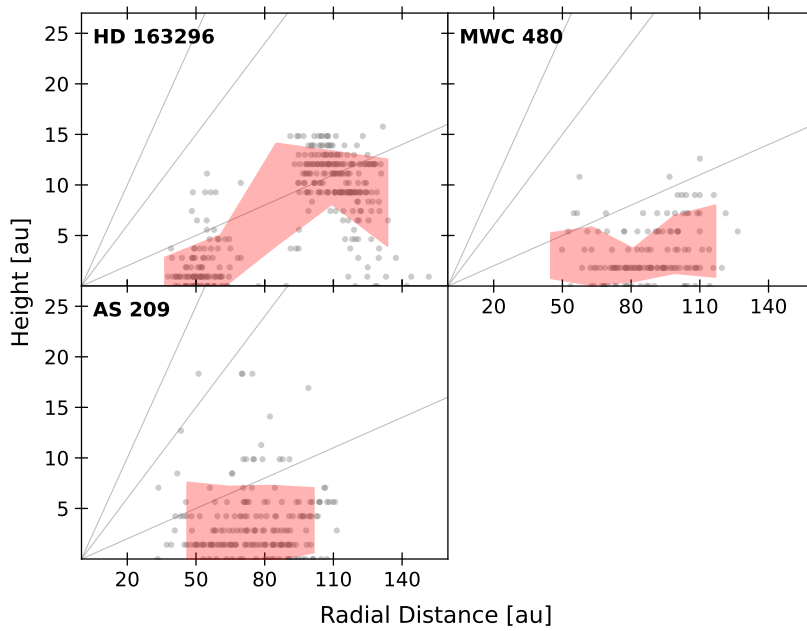


Figure 3.B.8: C₂H data points.

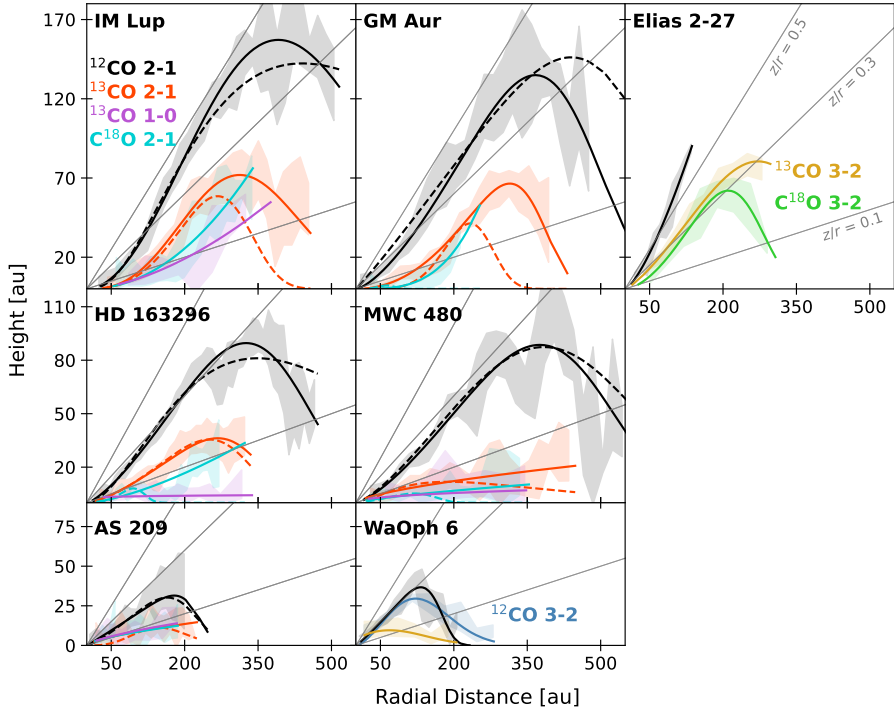


Figure 3.B.9: Best-fit vertical profiles of CO isotopologues (solid coloured lines) compared, when possible, to previously derived emission surfaces by Law et al. 2020b (dashed lines). Shaded background colours show the dispersion of the retrieved data. Solid grey lines indicate the curves of constant z/r for values of 0.1, 0.3, and 0.5.

Table 3.B.1: Best-fit parameters of vertical profiles for CO isotopologues.

Source	Line	z_0 (au)	ϕ	r_{taper} (au)	ψ
IM Lup	^{12}CO 2–1	$25.99^{+0.29}_{-0.25}$	$1.95^{+0.04}_{-0.03}$	$417.65^{+10.26}_{-11.58}$	$2.26^{+0.1}_{-0.11}$
	^{13}CO 2–1	$9.76^{+0.25}_{-0.27}$	$2.65^{+0.12}_{-0.1}$	$310.32^{+12.65}_{-14.28}$	$2.6^{+0.16}_{-0.18}$
	C^{18}O 2–1	$6.07^{+0.18}_{-0.25}$	$2.07^{+0.04}_{-0.03}$	-	-
	^{13}CO 1–0	$5.97^{+0.5}_{-0.48}$	$1.67^{+0.09}_{-0.1}$	-	-
GM Aur	^{12}CO 2–1	$27.54^{+0.18}_{-0.22}$	$1.45^{+0.02}_{-0.01}$	$470.29^{+2.38}_{-2.02}$	$4.94^{+0.24}_{-0.26}$
	^{13}CO 2–1	$7.99^{+0.23}_{-0.22}$	$2.11^{+0.04}_{-0.04}$	$372.93^{+1.49}_{-1.44}$	$7.19^{+0.36}_{-0.38}$
	C^{18}O 2–1	$2.25^{+0.28}_{-0.24}$	$3.4^{+0.16}_{-0.17}$	-	-
	^{13}CO 1–0	$0.08^{+0.5}_{-0.06}$	$6.19^{+1.85}_{-2.52}$	-	-
Elias 2-27	^{12}CO 2–1	$58.65^{+0.39}_{-0.52}$	$1.38^{+0.04}_{-0.03}$	-	-
	^{13}CO 3–2	$31.69^{+0.48}_{-0.34}$	$1.3^{+0.04}_{-0.03}$	$360.79^{+7.7}_{-10.04}$	$3.57^{+0.65}_{-0.54}$
	C^{18}O 3–2	$25.28^{+0.41}_{-0.34}$	$1.68^{+0.06}_{-0.06}$	$262.34^{+3.41}_{-4.16}$	$4.75^{+0.33}_{-0.31}$
HD 163296	^{12}CO 2–1	$25.08^{+0.12}_{-0.11}$	$1.35^{+0.01}_{-0.01}$	$426.44^{+1.35}_{-1.27}$	$4.21^{+0.09}_{-0.1}$
	^{13}CO 2–1	$11.88^{+0.14}_{-0.14}$	$1.4^{+0.03}_{-0.02}$	$343.88^{+4.79}_{-3.86}$	$5.36^{+0.4}_{-0.44}$
	C^{18}O 2–1	$6.02^{+0.2}_{-0.14}$	$1.47^{+0.04}_{-0.03}$	-	-
	^{13}CO 1–0	$3.65^{+0.17}_{-0.23}$	$0.13^{+0.14}_{-0.09}$	-	-
MWC 480	^{12}CO 2–1	$19.82^{+0.17}_{-0.17}$	$1.38^{+0.02}_{-0.02}$	$489.74^{+4.33}_{-4.62}$	$4.25^{+0.24}_{-0.22}$
	^{13}CO 2–1	$7.72^{+0.13}_{-0.13}$	$0.66^{+0.02}_{-0.02}$	-	-
	C^{18}O 2–1	$4.08^{+0.17}_{-0.14}$	$0.73^{+0.05}_{-0.05}$	-	-
	^{13}CO 1–0	$4.04^{+0.46}_{-0.35}$	$0.44^{+0.16}_{-0.22}$	-	-
AS 209	^{12}CO 2–1	$19.49^{+0.26}_{-0.2}$	$1.05^{+0.03}_{-0.03}$	$229.98^{+2.5}_{-2.13}$	$8.12^{+0.76}_{-0.7}$
	^{13}CO 2–1	$8.54^{+0.17}_{-0.18}$	$0.66^{+0.04}_{-0.05}$	-	-
	C^{18}O 2–1	$8.36^{+0.34}_{-0.29}$	$0.64^{+0.1}_{-0.08}$	-	-
	^{13}CO 1–0	$9.17^{+0.57}_{-1.15}$	$0.69^{+0.33}_{-0.15}$	-	-
WaOph 6	^{12}CO 3–2	$44.82^{+9.37}_{-5.39}$	$1.6^{+0.22}_{-0.2}$	$140.52^{+13.07}_{-16.47}$	$2.18^{+0.28}_{-0.27}$
	^{12}CO 2–1	$31.69^{+0.69}_{-0.64}$	$1.12^{+0.03}_{-0.03}$	$173.07^{+2.9}_{-1.58}$	$6.67^{+0.99}_{-1.47}$
	^{13}CO 3–2	$13.24^{+9.46}_{-2.12}$	$0.41^{+0.33}_{-0.2}$	$145.19^{+43.16}_{-33.62}$	$2.34^{+4.64}_{-1.07}$

Table 3.B.2: Best-fit parameters of vertical profiles for other tracers in HD 163296.

Molecule	Transition	z_0 (au)	ϕ	r_{taper} (au)	ψ
CN	$N = 1 - 0$	$10.92^{+0.37}_{-0.41}$	$1.62^{+0.05}_{-0.05}$	$401.11^{+2.81}_{-2.98}$	$7.54^{+0.38}_{-0.36}$
HCN	$J = 3 - 2$	$8.45^{+0.15}_{-0.12}$	$2.14^{+0.07}_{-0.08}$	$342.11^{+8.07}_{-9.06}$	$3.75^{+0.38}_{-0.35}$
H ₂ CO	$J = 3_{03} - 2_{02}$	$19.2^{+1.66}_{-2.41}$	$1.0^{+0.09}_{-0.06}$	$462.85^{+331.83}_{-302.32}$	$0.07^{+0.09}_{-0.05}$
C ₂ H	$N = 3 - 2$	$38.13^{+27.14}_{-12.6}$	$5.41^{+0.74}_{-0.72}$	$95.38^{+9.65}_{-11.73}$	$3.78^{+0.81}_{-0.74}$
HCO ⁺	$J = 1 - 0$	$6.45^{+0.41}_{-0.46}$	$0.59^{+0.07}_{-0.08}$	-	-
c-C ₃ H ₂	$J = 7_{07} - 6_{16}$	$9.56^{+0.57}_{-0.64}$	$2.79^{+0.27}_{-0.28}$	-	-

Notes. These values are used to de-project the emission and extract the brightness temperature profiles presented in Sect. 3.1

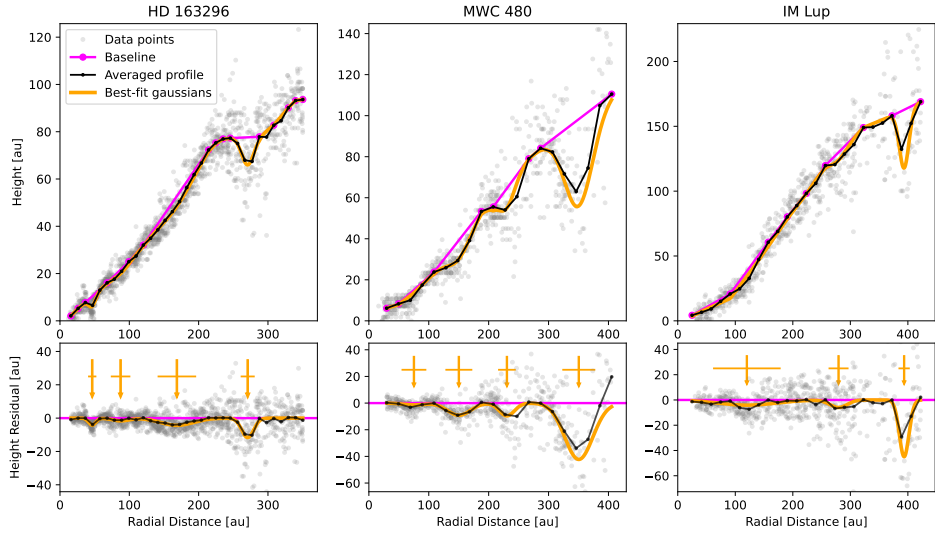


Figure 3.B.10: Data (grey dots), averaged profile (black curve), assumed baseline (pink profile), and best-fit Gaussians (orange line) obtained for each system from the analysis in Sect. 3.2.1 for ¹²CO. The bottom panels show the residuals obtained after subtracting the baseline profile from the data points. The vertical arrows mark the best-fit centre of each Gaussian component considered in each system. The horizontal line marks the width of the Gaussian component.

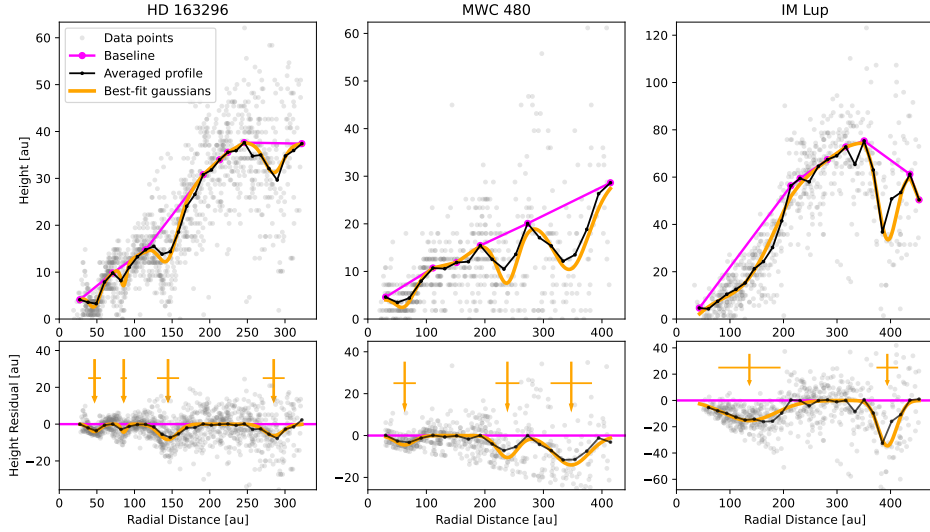


Figure 3.B.11: Same as Fig. 3.B.10 but for ^{13}CO .

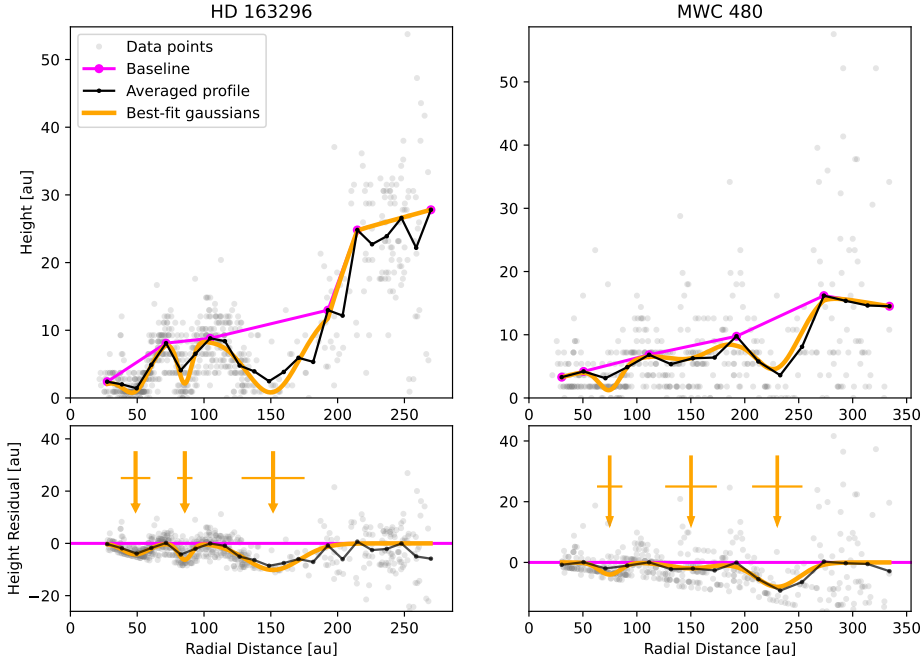


Figure 3.B.12: Same as Fig. 3.B.10 but for C^{18}O .

Table 3.B.3: Modulations in the CO vertical surface for HD 163296, MWC 480, and IMLup.

Source	Line	r_0 (au)	Width (au)	Δz (au)	Depth ($\Delta z/z(r_0)$)
HD 163296	^{12}CO 2–1	46.5 $\pm$ 0.51	11.96 $\pm$ 2.05	4.21	0.41
		87.42 $\pm$ 4.04	28.21 $\pm$ 8.92	1.64	0.08
		168.61 $\pm$ 2.36	55.64 $\pm$ 5.75	4.33	0.08
		270.76 $\pm$ 1.22	20.28 $\pm$ 3.18	11.66	0.15
	^{13}CO 2–1	46.94 $\pm$ 0.67	17.04 $\pm$ 1.53	4.01	0.6
		85.68 $\pm$ 0.9	8.45 $\pm$ 2.03	4.36	0.38
		144.54 $\pm$ 0.81	29.45 $\pm$ 2.12	8.38	0.4
		285.01 $\pm$ 1.89	29.16 $\pm$ 3.6	6.31	0.17
	C^{18}O 2–1	48.77 $\pm$ 0.53	22.13 $\pm$ 1.3	4.19	0.81
		85.63 $\pm$ 0.57	11.5 $\pm$ 1.04	6.22	0.74
		151.7 $\pm$ 2.24	47.17 $\pm$ 3.86	10.17	0.92
MWC 480	^{12}CO 2–1	75.24 $\pm$ 3.71	41.41 $\pm$ 13.82	1.37	0.09
		150.23 $\pm$ 1.7	44.95 $\pm$ 4.1	9.19	0.23
		230.48 $\pm$ 1.63	29.52 $\pm$ 4.45	9.62	0.15
		350.48 $\pm$ 2.18	55.1 $\pm$ 3.06	42.27	0.43
	^{13}CO 2–1	62.89 $\pm$ 1.52	38.34 $\pm$ 3.08	4.46	0.63
		238.47 $\pm$ 1.74	40.88 $\pm$ 4.38	10.51	0.58
		347.62 $\pm$ 2.62	70.83 $\pm$ 5.25	14.05	0.57
	C^{18}O 2–1	74.83 $\pm$ 0.8	23.51 $\pm$ 2.17	3.99	0.76
		150.18 $\pm$ 1.08	47.9 $\pm$ 1.74	1.96	0.24
		230.13 $\pm$ 1.09	46.67 $\pm$ 2.28	8.05	0.63
IMLup	^{12}CO 2–1	120.12 $\pm$ 4.4	117.51 $\pm$ 14.44	4.12	0.11
		279.49 $\pm$ 1.89	34.75 $\pm$ 5.25	5.93	0.05
		393.49 $\pm$ 0.88	19.66 $\pm$ 2.78	44.92	0.28
	^{13}CO 2–1	136.34 $\pm$ 2.1	116.29 $\pm$ 1.58	15.35	0.47
		393.97 $\pm$ 0.9	40.59 $\pm$ 2.24	34.55	0.51

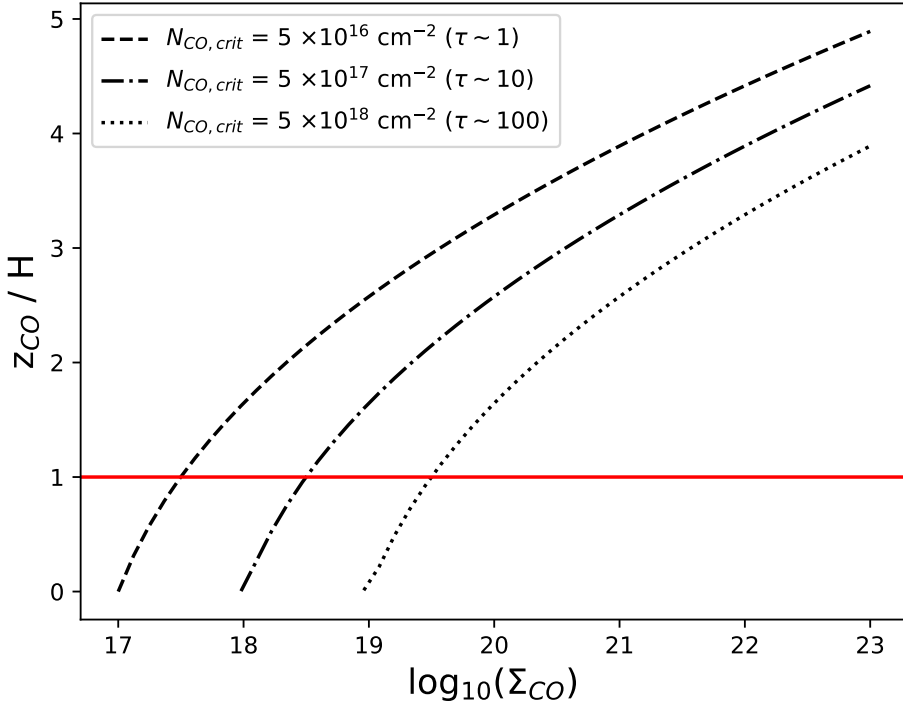


Figure 3.C.1: Conversion factor between the ^{12}CO emitting surface (z_{CO}) and the gas pressure scale height (H) as a function of the assumed CO density profile. This result is obtained by solving Eq. 5 and varying the critical density value for CO as indicated in the legend.

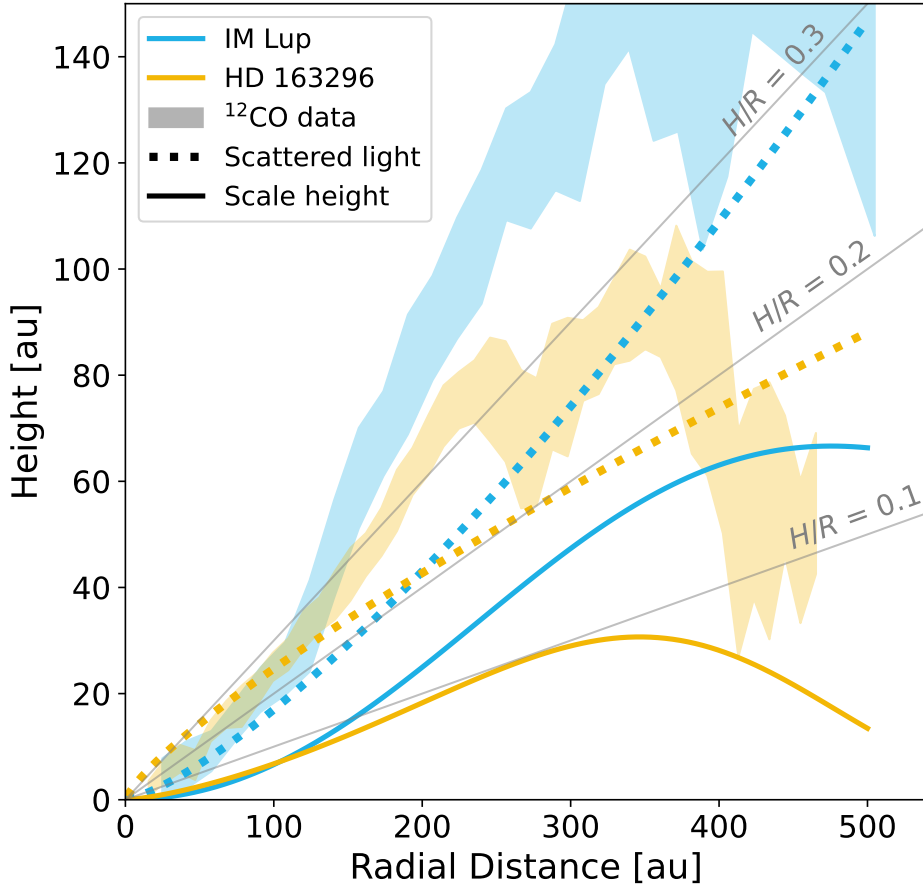


Figure 3.C.2: Location of the emission surface of $^{12}\text{CO } J = 2 - 1$ as extracted in this work, shown by the broad shaded regions for IM Lup (in blue) and HD 163296 (in yellow). Dotted lines indicate the scattering surfaces as parametrized in Rich et al. (2021), and solid coloured lines indicate the parametrization of the gas pressure scale height derived in this work.

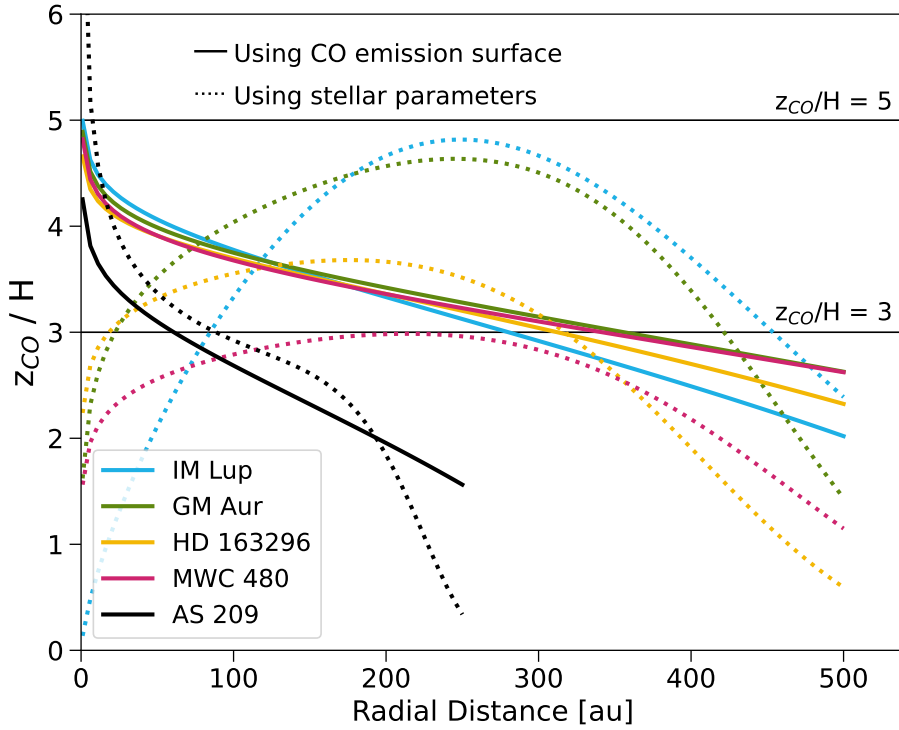


Figure 3.C.3: Comparison of the conversion factor between the ^{12}CO emitting surface (z_{CO}) and the gas pressure scale height (H) obtained through our simple single layer model (solid line) and using an estimate on the midplane temperature from the stellar parameters (dotted line).

Table 3.C.1: Common parameters in DALI models.

Parameter	Value
<i>Chemistry</i>	
Chemical Age	1 Myr
[CO]/[H]	1.35×10^{-4}
[PAH]	10^{-4} ISM abundance
<i>Physical Structure</i>	
gas-to-dust ratio	100
f_{large} (fraction small/large grains)	0.85
χ (Settling of large grains)	0.2
<i>Stellar Parameters</i>	
L_x	$1.0 \times 10^{30} \text{ erg s}^{-1}$
T_x	$7.0 \times 10^7 \text{ K}$
$\zeta_{\text{c.r.}}$ (cosmic ray ionization rate)	$5.0 \times 10^{-17} \text{ s}^{-1}$

Table 3.C.2: Physical parameters for DALI models.

Source	Σ_c (g cm^{-2})	R_c (au)	γ	h_{100} (rad)	φ	r_{in} (au)	r_{out} (au)	T_{eff} (K)	L_* ($L_\odot$)	M_* ($M_\odot$)	$\log_{10}(\dot{M})$ ($M_\odot \text{ yr}^{-1}$)
IM Lup	28.4	100	1.0	0.1	0.17	0.20	1200	4266	2.57	1.1	-7.9
GM Aur	9.4	176	1.0	0.075	0.35	1.00	650	4350	1.2	1.1	-8.1
AS 209	1.0	80	1.0	0.06	0.25	0.5	300	4266	1.41	1.2	-7.3
HD 163296	8.8	165	0.8	0.084	0.08	0.45	600	9332	17.0	2.0	-7.4
MWC 480	5.8	200	1.0	0.1	0.08	0.45	750	8250	21.9	2.1	-6.9

Notes. Values are based on the stellar parameters and best-fit gas surface density results presented in Zhang et al. (2021).

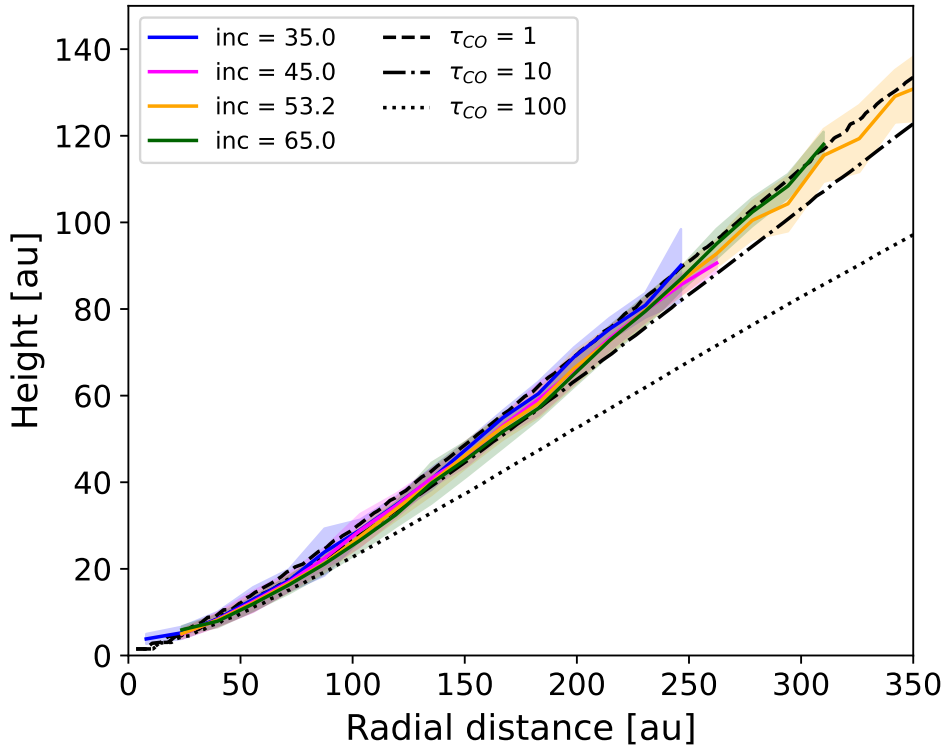


Figure 3.C.4: Extracted vertical profiles for $^{12}\text{CO } J = 2 - 1$ obtained using mock channel maps at different inclinations, from the GMAur DALI model. Different colours trace the various inclinations, and the black lines indicate the ^{12}CO millimetre optical depth values, as done in Fig. 3.8.

Chapter 4

High turbulence in the IM Lup protoplanetary disk: Direct observational constraints from CN and C₂H emission

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Astronomy & Astrophysics, 684, A174 (2024)

Abstract

Context: Constraining turbulence in disks is key to understanding their evolution via the transport of angular momentum. Measurements of high turbulence remain elusive, and methods for estimating turbulence mostly rely on complex radiative transfer models of the data. Using the disk emission from IM Lup, a source proposed to be undergoing magneto-rotational instabilities (MRIs) and to possibly have high turbulence values in the upper disk layers, we present a new way of directly measuring turbulence without the need of radiative transfer or thermochemical models.

Aims: Through the characterization of the CN and C₂H emission in IM Lup, we aim to connect the information on the vertical and thermal structure of a particular disk region to derive the turbulence at that location. By using an optically thin tracer, it is possible to directly measure turbulence from the nonthermal broadening of the line.

Methods: The vertical layers of the CN and C₂H emission were traced directly from the channel maps using ALFAHOR. By comparing their position to that of optically thick CO observations, we were able to characterize the kinetic temperature of the emitting region. Using a simple parametric model of the line intensity with DISCMINER, we accurately measured the emission linewidth and separated the thermal and nonthermal components. Assuming that the nonthermal component is fully turbulent, we were able to directly estimate the turbulent motions at the studied radial and vertical location of CN emission.

Results: IM Lup shows a high turbulence of Mach 0.4-0.6 at $z/r \sim 0.25$. Considering previous estimates of low turbulence near the midplane, this may indicate a vertical gradient in the disk turbulence, which is a key prediction in MRI studies. CN and C₂H are both emitting from a localized upper disk region at $z/r = 0.2-0.3$, in agreement with thermochemical models.

4.1 Introduction

The study of planet formation requires high sensitivity observations that can spatially and spectrally resolve the motions of the material in protoplanetary disks around young stars. In this context, the Atacama Large Millimeter/submillimeter Array (ALMA) is a unique facility, able to characterize these objects and their evolution mechanisms, which depend on the transportation of angular momentum (Lynden-Bell & Pringle 1974). Turbulence is the mechanism proposed to shape the surface density of disks, by transporting angular momentum through velocity fluctuations and providing an effective viscosity at microscopic scales (Shakura & Sunyaev 1973). There are many hydrodynamic processes that could be the origin of turbulent motions (see Lesur et al. 2023, and references therein); however, direct measurements of turbulence in protoplanetary disks have been hard to obtain, with only a few upper limits (e.g., Hughes et al. 2009; Flaherty et al. 2015; Teague et al. 2016) and one candidate with measured turbulence, DM Tau. In this system, high spatial and spectral resolution ALMA observations of CS allowed Guilloteau et al. (2012) to initially measure turbulence values of $0.3\text{--}0.5c_s$ (see also the initial studies by Guilloteau & Dutrey 1998 and Dartois et al. 2003). A later study by Flaherty et al. (2020) obtained lower, but still significant, turbulence values of $0.25\text{--}0.33c_s$ through modeling of CO emission in DM Tau.

Current methods used to constrain turbulence mostly depend on comparing observations to complex parametric and radiative transfer models, which depend on fundamental physical disk properties such as surface density and temperature structure (e.g., Hughes et al. 2009; Guilloteau et al. 2012; Flaherty et al. 2015, 2017, 2020). While these methods constrain their best-fit parameters with state-of-the-art analysis, there are multiple effects that are hard to account for since precisely resolving the gas surface density profile requires knowledge of the dust grain distribution and excitation conditions of the observed molecule (Zhang et al. 2021; Miotello et al. 2023). Furthermore, the presence of substructure in the disk may or may not cause gaps and rings in the surface density, depending on their origin, which is also not trivial to determine (Rosotti et al. 2021; Zhang et al. 2021; Teague et al. 2018a).

Due to their complexity, previous uses of these models to extract disk turbulence have assumed a single turbulence value for the whole protoplanetary disk, neglecting the possibility of a radial or vertical dependence. However, turbulence could have vertical variations, depending on the launching mechanism (Forgan et al. 2012; Simon et al. 2015; Shi & Chiang 2014), and while various molecular tracers are used to probe the vertical structure in searches for vertical turbulence variations (Flaherty et al. 2017), locating the exact position of the molecular emission in the disk is not straightforward in the modeling process and in some cases presents strong discrepancies with observational constraints. A successful case is the best-fit model to extract turbulence in DM Tau, where the CO ($J = 2 - 1$) emission is expected to arise from a layer of $z/r \sim 0.3\text{--}0.4$ (see Figure 2 in Flaherty et al. 2020), in good agreement with observational constraints from Law et al. (2023b). However, analysis of HD 163296, where no significant turbulence was detected, predicts that CO ($J = 2 - 1$) emission is coming from $z/r < 0.1$ (see Figure

16 in Flaherty et al. 2017), which is many times lower than the measured emission surface of CO ($J = 2 - 1$), located at $z/r \sim 0.3$ (Law et al. 2021b; Paneque-Carreño et al. 2023). These differences may be due to the limitations of the method, a lack of spatial resolution, or errors in the assumed density and temperature structure.

To alleviate these issues, this work focuses on directly tracing the vertical location of optically thin CN and C₂H transitions, measuring the radial profile of line broadening due to nonthermal motions, and relating this to vertically and radially resolved turbulence. CN and C₂H are expected to originate from chemical processes requiring energetic UV-photon radiation (Visser et al. 2018; Cazzoletti et al. 2018; Bergin et al. 2016; Teague & Loomis 2020), and therefore their emission should arise from a sweet spot located at high elevation from the midplane (Schreyer et al. 2008; Cazzoletti et al. 2018), in a zone known as the photon-dominated region (Aikawa et al. 2002). As the emission should come from a vertically thin slab, it is possible to accurately determine the location of the emission surfaces of CN and C₂H despite the emission being optically thin (see Paneque-Carreño et al. 2022). In parallel, optically thick CO isotopologs can be used as tracers of the disk structure, with the resolved vertical emission location (Law et al. 2021b; Paneque-Carreño et al. 2022) allowing us to provide a global three-dimensional characterization of the temperature structure, molecular emission, and turbulence in the upper disk layers. This is ultimately achieved by measuring the emission linewidth and separating the thermal from the nonthermal component. As we assume optically thin molecular emission, the nonthermal component is assumed to be mainly turbulent (Hacar et al. 2016). A key tool in our analysis is the use of DISCMINER (Izquierdo et al. 2021, 2023), a disk analysis package that fits the spectra per pixel of our data to precisely extract and parametrize the radial linewidth profile of the data, accounting for the effects of beam convolution and upper and lower emission surfaces.

Our work focuses on the protoplanetary disk around the young K5 star IM Lup, located at a distance of 158 pc (Gaia Collaboration et al. 2023). This system has been extensively studied using multiple tracers. Infrared scattered light shows a large, vertically extended disk, with radial rings and gaps (Avenhaus et al. 2018). Millimeter continuum traces tightly wound spiral arms and an outer ring (Cleeves et al. 2016; Huang et al. 2018b,c), and gas line emission shows a rich molecular reservoir (Pinte et al. 2018a; Öberg et al. 2021b). Recent observational and theoretical works have proposed that IM Lup has an inner turbulent disk (Bosman et al. 2023) and possible turbulent velocities of $\sim 100 \text{ ms}^{-1}$ in the outer disk (Cleeves et al. 2016). Due to its inclination and vertical extent, it is possible to trace the vertical disk structure and molecular layering of various lines; however, previous studies have been unable to extract CN or C₂H vertical profiles due to the low signal-to-noise ratio (S/N) of the lower rotational transitions (Paneque-Carreño et al. 2023). New, higher-energy ALMA Band 7 transitions have sufficient S/N for an adequate characterization of their radial, azimuthal, and vertical features.

This paper is structured as follows. Section 2 presents the data and explains the calibration procedures. Section 3 studies the emission morphology, characterizing the vertical extent of the disk and the brightness temperature of CN and C₂H and comparing them to those of CO isotopologs. Section 4 shows the parametric model

we used to extract the linewidth from CN, and Section 5 presents our results on the radial turbulence profile as traced by CN. Finally, Section 6 discusses the findings of this work in the context of previous constraints, and Section 7 summarizes our main conclusions.

4.2 Observations

This work uses ALMA Band 7 C_2H ($N = 4-3$) and CN ($N = 3-2$) observations of IM Lup (Project code: #2019.1.01357.S, PI: R.Teague) taken during the second semester of 2019 and first semester of 2021. After initial calibration through the ALMA pipeline (Hunter et al. 2023), the data were flux-calibrated and self-calibrated in phase and amplitude using only the line-free spectral windows and channels with the tools of Common Astronomy Software Applications (CASA; version 5.4.0, McMullin et al. 2007) as described in the following.

The observations from each execution block (EB; seven in total) were aligned to a common phase center, considering the peak of the continuum emission of each EB as fitted by CASA task `imfit`. After alignment, an amplitude scaling was applied to correct for the relative flux scale variations between EBs, which were $<10\%$, following the procedures of ALMA large program DSHARP (Andrews et al. 2018). Self-calibration was then applied to the short-baseline observations (two EBs, with a longest baseline of 0.3 km). Five rounds of phase and one round of amplitude calibration were performed, until there was no further improvement of the S/N, starting with a solution interval of 3360s and taking half the time step in each subsequent round. The S/N improvement in the short-baseline data was 726%, from 190 to 1380. Finally, self-calibration was performed on the joint dataset of the previously self-calibrated short baselines, concatenated to the flux-calibrated long baselines (five EBs, with a maximum baseline of 1.5 km). Three rounds of phase and one round of amplitude calibration were performed, the initial time solution interval was 4800s and the final S/N increase was 428%, from 301 to 1289.

Each of the calibration solutions from the continuum analysis was then applied to the whole dataset, to correct spectral windows and channels with line emission. Using the CASA task `uvcontsub`, we produced continuum-subtracted measurement sets for each of our target emission lines. Each C_2H and CN hyperfine group was imaged using `tclean` with Briggs weighting and Keplerian masking¹. Multiple Keplerian masks, one for each of the expected hyperfine components, were used in the cleaning. A stellar mass of $1.1M_\odot$ (Teague et al. 2021a) and a constant z/r value of 0.2 and 0.3 was used for C_2H and CN emission, respectively. To compromise between optimal angular resolution and high S/N, C_2H emission was imaged using a robust parameter of 2.0, resulting in a $0.27'' \times 0.25''$ beam (PA: 64.83°). CN is imaged using a 0.5 robust parameter with a final beam of $0.22'' \times 0.19''$ (PA: 57.56°). JvM correction (Czekala et al. 2021) was applied to our final images to account for the noise caused by having non-Gaussian beams. The epsilon correction factors are 0.24 and 0.52 for C_2H and CN, respectively (for details on

¹https://github.com/richteague/keplerian_mask

this procedure and the epsilon factor, refer to Czekala et al. 2021). The images used in the analysis were obtained using a channel spacing of 200 m s^{-1} for C_2H and 100 m s^{-1} for CN , to optimize spectral resolution and S/N. The final rms of the images for each molecule are 0.6 mJy/beam and 1 mJy/beam for C_2H and CN , respectively.

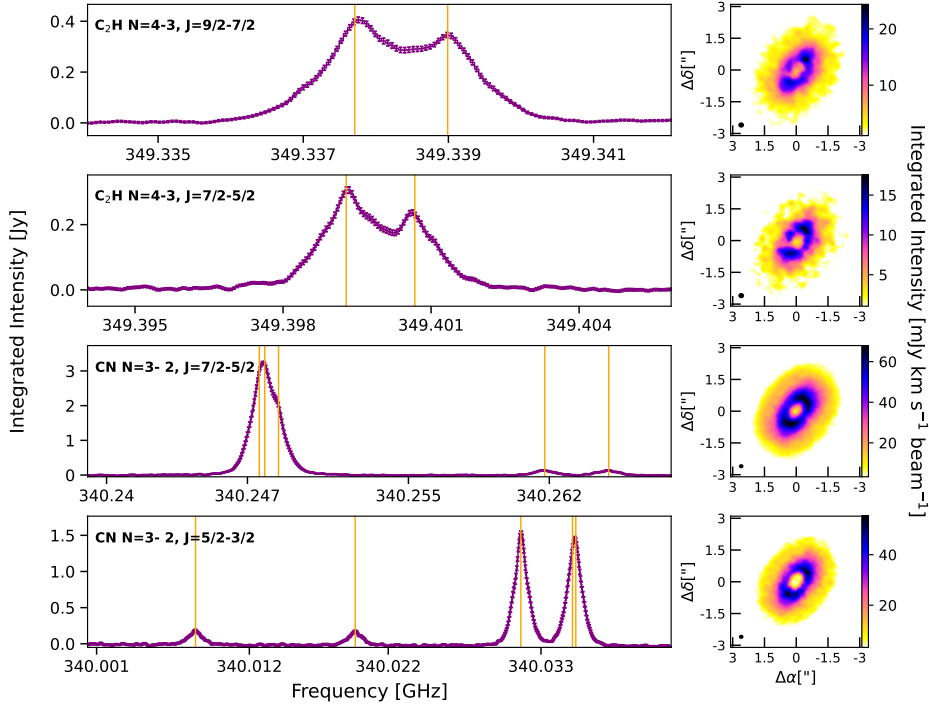


Figure 4.1: ALMA observations of CN and C_2H line emission from IM Lup. Left column: Stacked, integrated spectra extracted from the whole radial extent of the disk, for each transition, obtained using GoFish. The corresponding hyperfine groups are indicated in the top left of each panel. Vertical lines mark the location of the central frequency for each hyperfine component within the spectral range. The channel spacing is 50 m s^{-1} , matching the native spectral resolution of the data. Right column: Integrated intensity maps (moment 0).

Figure 4.1 shows the integrated intensity maps (moment 0) and stacked spectra for the data imaged at the native spectral resolution, 50 m s^{-1} . The spectra were computed using the GoFish (Teague 2019b) function, `integrated_spectrum`, over the whole disk. Each of the detected hyperfine components are marked with an orange vertical line and their properties, together with the integrated fluxes indicated in Table 4.1. A clear ring is observed in both tracers for all hyperfine groups, a detailed analysis of this feature can be found in Appendix A.

Table 4.1: Molecular line data from the LAMBDA database (Schöier et al. 2005).

Species	J Transition	F Transition	Frequency (GHz)	E_u (K)	A_{ul} (s^{-1})	g_u	Int. Flux* (Jy km s $^{-1}$)
CN ($N = 3 - 2$)	$J = 7/2 - 5/2$	$F = 7/2 - 5/2$	340.24759 ^a	32.67	3.797×10^{-4}	8	
		$F = 9/2 - 7/2$	340.24786 ^a	32.67	4.13×10^{-4}	10	4.710 ± 0.029
		$F = 5/2 - 3/2$	340.24854	32.67	3.67×10^{-4}	6	
		$F = 5/2 - 5/2$	340.26177	32.67	0.45×10^{-4}	6	0.133 ± 0.029
	$J = 5/2 - 3/2$	$F = 7/2 - 7/2$	340.26495	32.67	0.34×10^{-4}	8	0.137 ± 0.029
		$F = 5/2 - 5/2$	340.00813	32.63	0.62×10^{-4}	6	0.140 ± 0.001
		$F = 3/2 - 3/2$	340.01963	32.63	0.93×10^{-4}	4	0.091 ± 0.001
		$F = 7/2 - 5/2$	340.03155	32.63	3.84×10^{-4}	8	1.594 ± 0.001
	$J = 9/2 - 7/2$	$F = 3/2 - 1/2$	340.03527 ^b	32.63	2.89×10^{-4}	4	
		$F = 5/2 - 3/2$	340.03551 ^b	32.63	3.23×10^{-4}	6	1.610 ± 0.001
C ₂ H ($N = 4 - 3$)	$J = 9/2 - 7/2$	$F = 5 - 4$	349.33771	41.91	1.31×10^{-4}	11	0.7416 ± 0.0002
		$F = 4 - 3$	349.33899	41.91	1.28×10^{-4}	9	
	$J = 7/2 - 5/2$	$F = 4 - 3$	349.39928	41.93	1.25×10^{-4}	9	
		$F = 3 - 2$	349.40067	41.93	1.20×10^{-4}	7	0.5611 ± 0.0002

Notes. (*) Integrated flux values and the studied lines calculated from the emission spectra in Figure 4.1 ^(a) Value in LAMBDA database is 340.24777 for both; new value from Teague & Loomis (2020) ^(b) Value in LAMBDA database is 340.03541 for both; new value from Teague & Loomis (2020).

4.3 Emission morphology

4.3.1 Vertical profile

From the channel maps it is possible to visually identify the CN and C₂H emission originating from the upper and lower sides of the disk. Tracing the vertical location of each molecule allows us to characterize the disk structure and physical conditions of the emitting gas in defined regions. To extract the vertical profiles, we used the code ALFAHOR (Paneque-Carreño et al. 2023), which traces the maxima of emission within a given masked region. The masks are visually determined and encircle the far and near sides of the disk upper surface (for details on the method and terminology, see Pinte et al. 2018a; Paneque-Carreño et al. 2022, 2023). Only channels where both near and far sides of the upper surface can be confidently identified are used for this analysis. Figures 4.B.1 and 4.B.2 present the masks and location of the emission maxima for each of the occupied transitions.

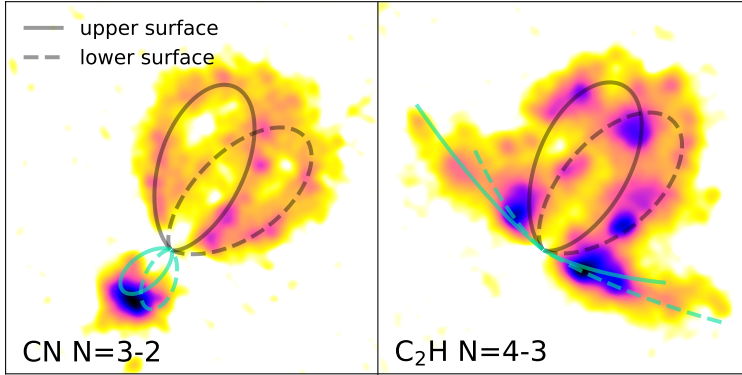


Figure 4.2: Channel map emission for CN (left) and C₂H (right) at equal relative velocity to systemic motion (-1.2 km s^{-1}). Continuous line traces the upper emission surface and dashed line the lower surface. Different colored contours indicate different hyperfine components. Contours are not fit to the data, they represent the visual identification of the emission surfaces and follow constant z/r (0.3 and 0.2 for CN and C₂H, respectively).

A key assumption of this method is that the intensity maxima trace a single isovelocity along each channel. Due to the strong blending of hyperfine components in the CN emission and the low S/N of some detected transitions, we only used the unblended and strongest component CN $N = 3 - 2J = 5/2 - 3/2F = 7/2 - 5/2$. C₂H also has blending in both transitions; however, it has a sufficient separation that we can identify both components in each group (see Fig. 4.2). However, we extracted the surface only using the $J = 9/2 - 7/2$ hyperfine group, as it has a higher S/N. We expect that these transitions are representative of the spatial location of all the detected transitions of the same molecule, as they all have similar upper state energies (see Table 4.1) and thus, originate from the same layer.

The resulting vertical distribution is parametrized with an exponentially tapered power law to capture the inner flared surface, plateau and turnover regions

at larger radii (Teague et al. 2019) following

$$z(r) = z_0 \times \left(\frac{r}{100 \text{ au}} \right)^\phi \times \exp \left[\left(\frac{-r}{r_{\text{taper}}} \right)^\psi \right]. \quad (4.1)$$

The best-fit values for z_0 , ϕ , ψ , and r_{taper} were found using a Markov chain Monte Carlo sampler as implemented by emcee (Foreman-Mackey et al. 2019) and shown in Table 4.2. Figure 4.3 shows the data considering all of the extracted maxima for CN and C₂H, together with the best-fit exponentially tapered power-law model.

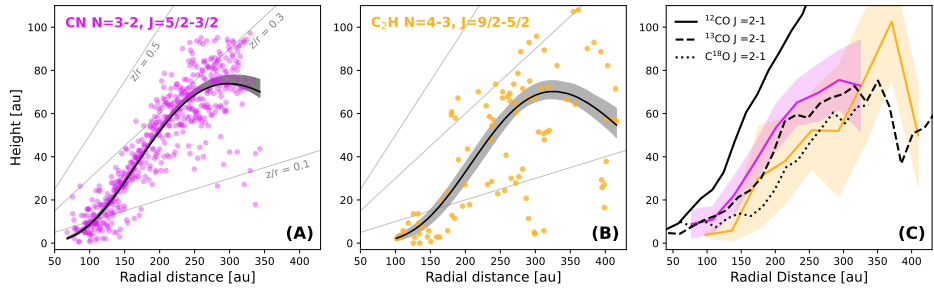


Figure 4.3: Vertical profiles of each tracer. Panels (A) and (B) show the data and best fit model for CN and C₂H, respectively (the molecule and hyperfine group used is shown in the upper left corner). Each colored dot represents the vertical location extracted at a given radius from the maxima of emission traced in the channel maps. Overlaid is an exponentially tapered model with the best-fit parameters and the statistical uncertainty of the profile. Panel (C) presents a comparison between the averaged values and standard deviation within radial bins for CN and C₂H (in colors) compared to the averaged CO isotopolog emission surfaces as presented in Paneque-Carreño et al. (2023).

Table 4.2: Best-fit parameters of vertical profiles.

	CN $N = 3 - 2$	C ₂ H $N = 4 - 3$
z_0 (au)	$40.29^{+12.36}_{-13.87}$	$8.03^{+4.79}_{-3.33}$
ϕ	$4.91^{+0.22}_{-0.38}$	$6.43^{+0.55}_{-0.84}$
r_{taper} (au)	$65.72^{+26.77}_{-11.49}$	$78.16^{+44.18}_{-21.86}$
ψ	$1.03^{+0.13}_{-0.06}$	$1.18^{+0.23}_{-0.12}$

Comparison with previously studied CO isotopolog emission from IM Lup (Paneque-Carreño et al. 2023) is presented in Figure 4.3 demonstrating that the location of CN ($N = 3 - 2$) is comparable to that of ¹³CO ($J = 2 - 1$). The C₂H ($N = 4 - 3$) emission is located slightly below, tracing the same region as C¹⁸O ($J = 2 - 1$). We note that C₂H presents a large scatter, likely due to the lower S/N of the observations; however, our result on the average vertical profile (panel

C of Fig. 4.3) is consistent with $z/r \sim 0.2$ expected from the visual channel map analysis (Fig. 4.2).

4.3.2 Brightness temperature

Considering the best-fit vertical surfaces, the radial peak brightness temperature profiles were extracted from the peak intensity maps (moment 8). The conversion from peak intensity (I) to brightness temperature (T_b) was done using Planck's law,

$$T_b = \frac{h\nu}{k} \ln^{-1} \left(1 + \frac{2h\nu^3}{Ic^2} \right), \quad (4.2)$$

where h is the Planck constant, k the Boltzmann constant, c the speed of light, and ν the frequency of the emission. To compare the brightness temperatures of CN and C₂H to those of the CO isotopologs previously studied in Paneque-Carreño et al. (2023), all brightness temperature profiles were calculated using cubes with an equal spectral resolution of 0.2 km s^{-1} to match the resolution of the Molecules with ALMA at Planet-forming Scales (MAPS) Program data (Öberg et al. 2021b).

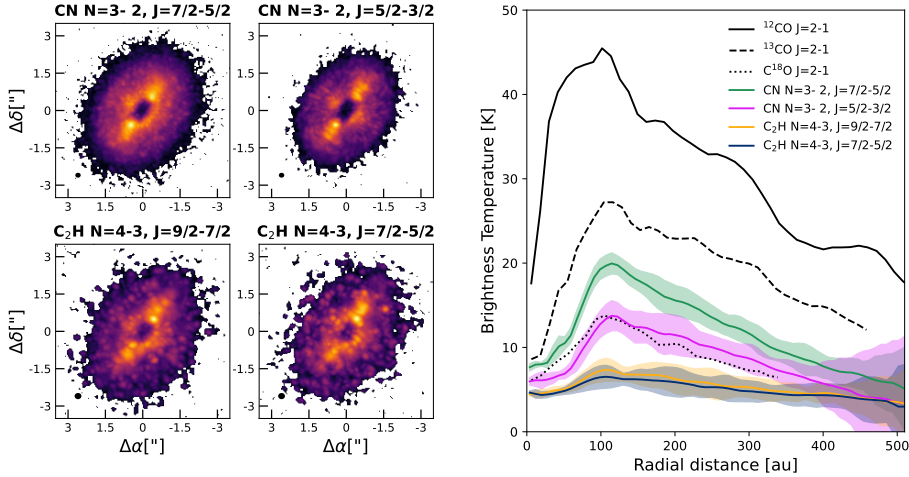


Figure 4.4: Brightness temperature analysis for each tracer. Left panels: Peak intensity (moment 8) maps for each hyperfine group under study. The extended feature toward the semimajor axis results from the radiative transferred effects due to higher velocity density in this region. Right panel: Brightness temperature profiles of each hyperfine group, compared to those of CO ($J = 2 - 1$) isotopologs.

The peak intensity maps and brightness temperature profiles, compared to those of CO isotopologs (Paneque-Carreño et al. 2023), are presented in Figure 4.4. The radially extended bright feature along the major axis seen in the peak intensity maps for all tracers is a radiative transfer effect related to the higher density of isovelocity contours and does not indicate a physical feature. Based on

our previous analysis we know that CN and C₂H emission is spatially colocated with ¹³CO; however, both transitions show lower brightness temperatures than ¹³CO for all hyperfine groups. The drop in temperature at the innermost radii is dominated by beam dilution as the emitting area becomes comparable to or smaller than the spatial resolution; however, this drop extends out to ~ 150 au, which is beyond the beam size. Dust absorption is likely a big contributor to the low temperatures, as several works have shown that the inner disk of IM Lup is optically thick (Cleeves et al. 2016; Sierra et al. 2021).

The brightness temperature may be a tracer of the excitation temperature of the region, but only in the cases where the emission is optically thick ($\tau \gg 1$), as it is proportional to $T_{ex}(1 - e^{-\tau})$. CO is expected to be abundant in IM Lup, in particular ¹²CO and ¹³CO should be optically thick (Cleeves et al. 2016) and therefore their brightness temperature may be taken as a tracer of the kinetic temperature in the region. On the other hand, CN and C₂H are expected to have lower column densities and be optically thin tracers (Cazzoletti et al. 2018; Bergner et al. 2021; Bergin et al. 2016), which is corroborated by the lower brightness temperatures measured in this work. We note that the temperature difference between both CN hyperfine groups is due to the strong blending in the $J = 7/2 - 5/2$ transition (see Fig. 4.1), which means that the peak flux for a given pixel is the sum of multiple hyperfine components. This is the same situation that affects the integrated flux values shown in Table 4.1.

4.4 Parametric emission model: DISCMINER fit

Knowing that the molecular emission is optically thin enables us to directly determine turbulence from the nonthermal contributions to the linewidth (Hacar et al. 2016). This is not possible in optically thick tracers (such as CO isotopologs) due to the additional opacity broadening that affects the linewidth in those cases, which is why in these cases radiative transfer models are needed to account for the opacity effect. Extracting the linewidth is not straightforward, it requires a parametric model that accounts for the vertically elevated emission, the upper and lower sides as well as radial intensity and velocity gradients. To this end, we used DISCMINER (Izquierdo et al. 2021), which allowed us to find the best-fit parametrization of our emission.

4.4.1 Model setup

DISCMINER determines the best orientation, velocity, surface and line profile parameters for the observed emission by creating a model intensity, I_m as a function of the disk cylindrical coordinates (R, z) and the velocity. The emission kernel has two components, one for the upper and another for the lower surface, which are well separated in the case of our studied emission. Contrary to previous works with DISCMINER, which focus on CO isotopolog emission (Izquierdo et al. 2021, 2022, 2023), this work traces optically thin molecules that will be well reproduced by a Gaussian line profile (Hacar et al. 2016). Therefore, we used a Gaussian

kernel for each surface such that

$$I_m(R, z; v_{chan}) = I_p \exp \left[-\frac{(v - v_{chan})^2}{\Delta V^2} \right], \quad (4.3)$$

with I_p being the peak intensity and ΔV the linewidth at a given radial and vertical distance from the star. Since we assumed fully optically thin emission, the final model intensity is given by the direct sum of the upper and lower disk surface intensity contributions and compared against the emission spectra extracted from each pixel of our observational data cube (for specific details, see Izquierdo et al. 2021, 2023). Table 4.3 indicates the equations used to model each of the disk attributes. Each emission surface is modeled independently as an exponentially tapered power law, the intensity is considered to be a power law with a Gaussian component, to account for the ring in the integrated emission maps (see Figure 4.1). The linewidth is assumed to follow a simple radial and vertical power law (as indicated in Table 4.3).

Table 4.3: Parametric model attributes.

Attribute	Prescription
Orientation	i, PA, x_c, y_c
Velocity	$v_{\text{rot}} = \sqrt{\frac{GM_*}{r^3}} R, v_{\text{sys}}$
Upper Surface	$z_{\text{up}} = z_0(R/D_0)^p \exp[-(R/R_t)^q]$
Lower Surface	$z_{\text{low}} = -z_0(R/D_0)^p \exp[-(R/R_t)^q]$
Peak intensity	$I_p = I_0(R/D_0)^p(z/D_0)^q + I_g \exp \left[-\frac{(R-R_g)^2}{2\sigma_g^2} \right]$
Line width	$\Delta V = L_0(R/D_0)^p(z/D_0)^q$

Notes. G is the gravitational constant and $D_0 = 100$ au is a normalization factor. R is the cylindrical radius and z is the height from the midplane, always positive, r is the spherical radius. The other variables are free parameters, even if named alike they are modeled independently for each attribute.

DISCMINER is not built to fit emission with multiple hyperfine components; therefore, we created a cube that only covers the emission of the strongest unblended hyperfine component of CN 3-2, $J = 5/2 - 3/2$ F= 7/2-5/2 (see Figure 4.1). It is not possible to analyze the other CN hyperfine components, due to the strong blending of the high S/N lines, and the low signal of the other detections. C_2H is also excluded from this analysis due to its low S/N and the close blending of the lines, which does not allow us to isolate them as we can for CN (see Figure 3

for a comparison on how close the CN hyperfine components are compared to C_2H in the channel map emission). Future work incorporating hyperfine components to the DISCMINER kernel could allow us to optimize our model using the whole dataset, but it is beyond the scope of this study.

4.4.2 Comparison to CN observations

The best-fit model parameters are found in Appendix C. Figure 4.5 shows the resulting model channel maps, convolved with a Gaussian beam to be at the same spatial resolution as the observations. The 5σ residuals are presented in the bottom row, no coherent or systematic pattern is identified. Figure 4.6 shows further comparison between the model and data. There is good agreement between the derived vertical and azimuthally averaged intensity profiles and the DISCMINER parametric forms. The rotation curve shows a $\sim 200\text{ms}^{-1}$ residual between 200 and 250 au, which coincides with a $\sim 50\text{ms}^{-1}$ negative residual in the linewidth. This velocity variation is also observed in ^{12}CO (see Figure B.18 in Izquierdo et al. 2023) and the location of the feature is close to a dust gap at 209 au and a dust ring at 220 au (Huang et al. 2018b), which may be related to these variations.

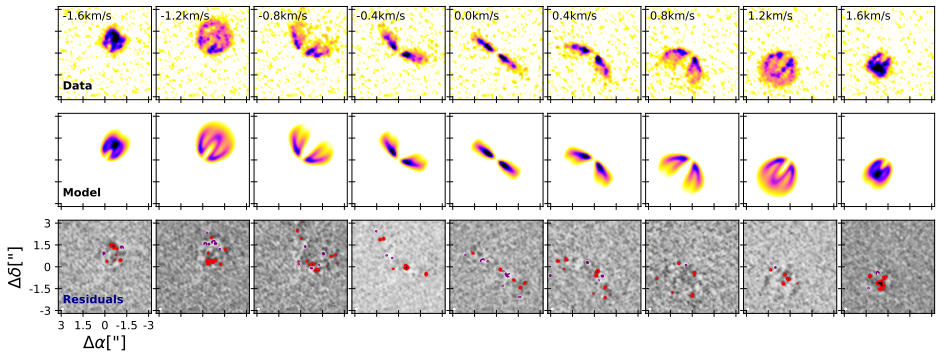


Figure 4.5: DISCMINER results and comparison to CN data. First row: Selection of channel maps from the CN datacube. Velocities are relative to the systemic velocity, and the spectral resolution of each channel is 0.1 km s^{-1} . Middle row: Channel maps from the best-fit DISCMINER model, at the same spatial resolution and intensity scale as the observations. Bottom row: Residual (observations minus model) emission. Contours indicate 5σ positive (red) and negative (purple) residuals, where σ is the data rms (1 mJy/beam).

We note that the linewidth values extracted from the channel map images (red and gray curves, with uncertainty regions in lower right panel) are higher than the best-fit DISCMINER parametric form (traced by dashed black line). This is because the profiles extracted from the image correspond to direct measurements of the linewidth from the spectra extracted at each pixel in the image plane. These measurements will always be broader (have higher values) than the underlying molecular emission linewidth due to the linewidth broadening caused by the finite spatial resolution of the observations (usually called beam broadening and

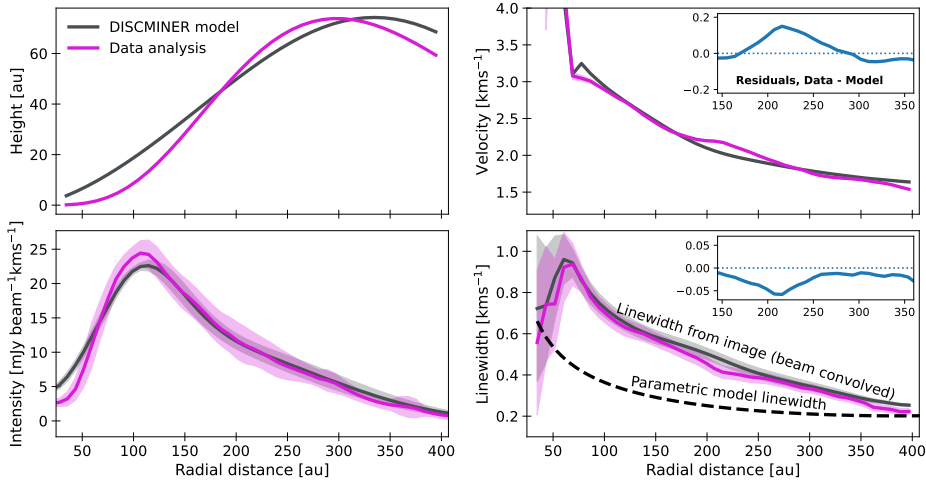


Figure 4.6: Comparison between various radial profiles between the data (magenta curves) and the DISCMINER model (gray curves). All panels except the height profile indicate the profile dispersion as a shaded region. Velocity and linewidth panels have a noticeable difference located at ~ 220 au, a blue residual curve characterizes this feature in the upper right corner of each panel. The linewidth panel shows the measured linewidth extracted from the data and the beam-convolved model by fitting the spectra. Additionally, the dashed black line indicates the intrinsic parametric form of the linewidth, as fitted by DISCMINER. The beam-convolved model will always have a broader linewidth than the parametric form and is used to directly compare our model to the data, which has a finite spital resolution. However, the intrinsic linewidth is what we used in our calculations, as this is expected to be the actual line broadening due to thermal and nonthermal motions.

discussed also in Teague & Loomis 2020). When we refer to the DISCMINER parametric form, we are describing what is expected to be the native molecular linewidth that, convolved with a Gaussian beam equal to the spatial resolution of the ALMA images ($\sim 0.22''$), will match the broader values extracted directly from the data.

4.5 Turbulence as traced by CN

The measured linewidth of an optically thin tracer will be dominated by doppler broadening caused by thermal and nonthermal motions (Hacar et al. 2016). As we used a Gaussian kernel (see Eq. 3), our measured linewidth ΔV corresponds to the velocity dispersion such that the full width at half maximum (FWHM) of the kernel is $2\sqrt{\log 2} \Delta V$. The linewidth can then be written as

$$\Delta V^2 = V_{\text{th}}^2 + V_{\text{non-th}}^2. \quad (4.4)$$

The thermal component is well characterized and proportional to the ratio

between the kinetic temperature and the molecular mass of the observed tracer (Myers et al. 1991). The nonthermal component can originate from non-Keplerian motion such as photo-evaporative winds, planet–disk interactions, or turbulence (e.g., Fuller & Myers 1992; Hacar et al. 2016; Izquierdo et al. 2023). For this analysis we considered the case where nonthermal motion is fully due to turbulence; the implications and possibilities of other origins are reviewed in the discussion section. Therefore, the two components of the measured linewidth can be decomposed as

$$\Delta V^2 = \frac{2kT_{kin}}{m_X} + v_{turb}^2. \quad (4.5)$$

Here k is the Boltzmann constant and m_X the molecular mass, in this case, for CN, $m_X = 26.0$ (Klisch et al. 1995; Schöier et al. 2005). The nonthermal broadening is assumed to be completely due to turbulence, v_{turb} . Turbulence can then be expressed in terms of the Mach number, $\mathcal{M}$, such that

$$\mathcal{M} = \frac{v_{turb}}{\sqrt{2}c_s}, \quad (4.6)$$

where c_s is the local sound speed in the studied layer $c_s^2 = \frac{kT_{kin}}{\mu m_H}$ (Balbus & Hawley 1998; Flaherty et al. 2015). We generally refer to turbulence in terms of the Mach number so it may be directly compared to previous works and estimations (Flaherty et al. 2015, 2017, 2020; Teague et al. 2016, 2018b).

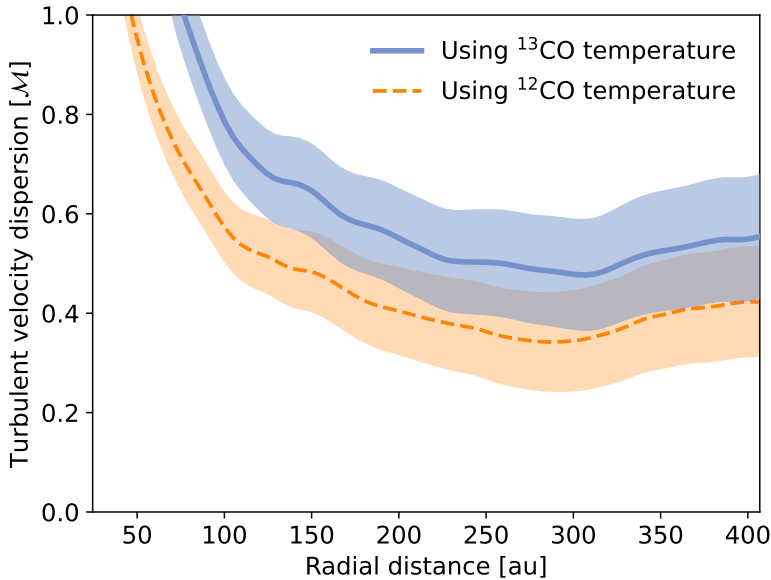


Figure 4.7: Turbulence extracted from the nonthermal component of the CN ($N = 3-2$) linewidth. The blue curve indicates results when considering the brightness temperature of ^{13}CO . The orange curve traces results using the brightness temperature of ^{12}CO . Shaded regions represent the dispersion when considering an error of 50 ms^{-1} on the measured linewidth.

By spatially localizing the CN emission vertically and radially close to the optically thick CO isotopes, we have a tool to directly access the kinetic temperature without need to use parametric models or additional molecular transitions. Using the linewidth parametrization found by DISCMINER we can immediately calculate the turbulence radial profile, presented in Figure 4.7. Our results indicate turbulent motions of $\mathcal{M} = 0.4\text{--}0.6$ at radii beyond ~ 150 au. The shaded regions of the plot represent the variation of our results considering a 50 m s^{-1} error in the linewidth measurement. While the statistical error of our fit is $< 5 \text{ m s}^{-1}$, we took the native resolution of our data as the largest possible deviation, in case effects such as Hanning smoothing are significantly affecting our linewidth extraction (Cortes et al. 2023). Under the α -prescription for turbulent viscosity ($\nu = \alpha c_s H$, Shakura & Sunyaev 1973) it is possible to relate the turbulence Mach number $\mathcal{M}$ to α following, $\alpha \sim \mathcal{M}^2$ (Rosotti 2023). Our measurements indicate $\alpha \sim 10^{-1}$.

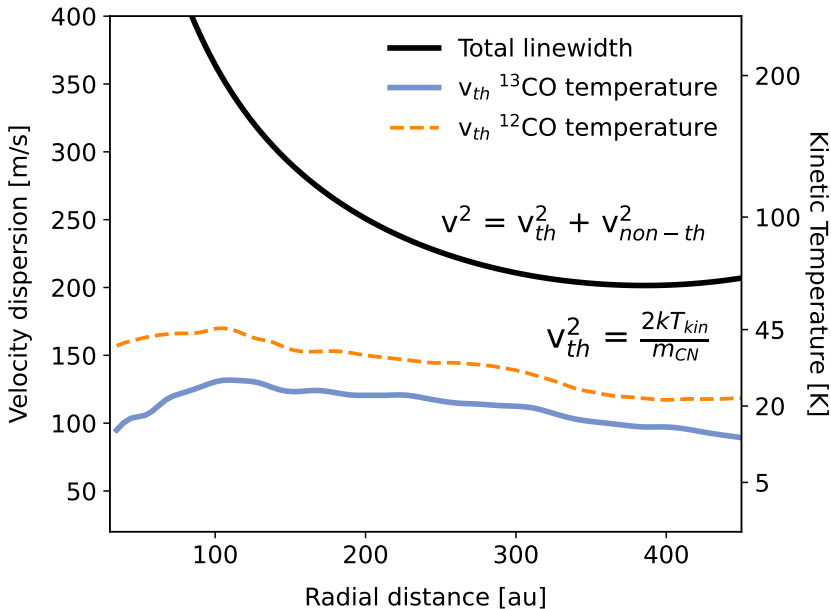


Figure 4.8: Total intrinsic linewidth determined from the best-fit DISCMINER model (solid black line; this is the same as the dashed black line in the bottom-right panel of Figure 4.6). It is compared to the thermal component obtained using the ^{13}CO (blue) or ^{12}CO (orange) brightness temperatures.

The total measured linewidth (ΔV) and turbulence values increase steeply in the inner ~ 150 au. While IM Lup has been proposed to be extremely turbulent in the inner disk (Cleeves et al. 2016; Bosman et al. 2023) it is unclear if our analysis is sensitive to this effect, or if the high turbulence should extend beyond the innermost 20 au, given the lower estimated scale height for millimeter dust in this system (Bosman et al. 2023). Linewidth measurements are strongly affected by overlapping velocities in the inner disk (Teague & Loomis 2020; Izquierdo et al.

2022); therefore, we only considered the values beyond 150 au as accurate measurements and do not refer to the high values inward of 150 au.

The average total linewidth measured outward of 150 au is $\sim 221 \text{ m s}^{-1}$. Thermal broadening only accounts for $105\text{--}132 \text{ m s}^{-1}$, using the ^{13}CO and ^{12}CO brightness temperatures, respectively. Therefore, the nonthermal broadening ranges between 177 and 194 m s^{-1} and would require temperatures $\sim 40 \text{ K}$ higher than measured to account for it as thermal motion. Figures 4.8 and 4.9 illustrate the need of a high nonthermal component in order to explain the measured total linewidth (see Fig. 4.8) and the data spectra (see Fig. 4.9).

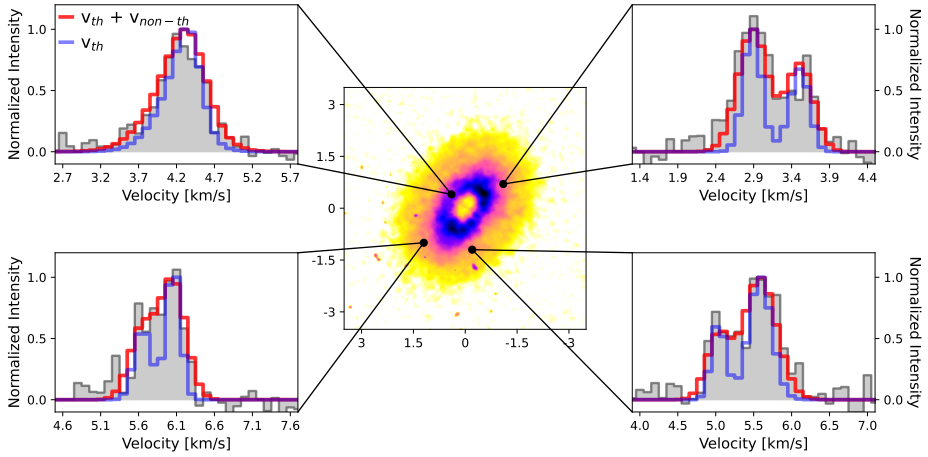


Figure 4.9: Spectra of four different pixels in the CN disk emission (in gray), indicated on the central integrated moment map. Overlaid are the DISCMINER model spectra from the best-fit parameter fit, considering the total measured linewidth (thermal and nonthermal components) in red. For comparison, the best-fit DISCMINER model considering a linewidth from only the thermal component calculated using the ^{13}CO temperature is overlaid* in blue.

4.6 Discussion

4.6.1 Vertical location of CN and C_2H

Our work traces the CN and C_2H emission originating from a vertical region similar to ^{13}CO , at $z/r = 0.2\text{--}0.3$ constrained radially between 50 and 350 au. These results are in agreement with chemical models of IM Lup that locate the tracer at $z/r = 0.2$ (Cleeves et al. 2018). However, while in agreement with theoretical models, this is the first direct observational evidence of C_2H coming from vertically elevated layer in the outer disk, as previous works studying other protoplanetary disks had only traced C_2H inward of 150 au and closer to the midplane (Law et al. 2021b; Paneque-Carreño et al. 2023).

Both CN and C₂H are formed via UV-driven chemistry (Nagy et al. 2015; Bergin et al. 2016; Visser et al. 2018; Cazzoletti et al. 2018; Miotello et al. 2019; Guzmán et al. 2021; Bergner et al. 2021) and tracing their vertical distribution in various transitions will allow us to further understand the range of penetration that these energetic photons have toward the midplane, or the mixing processes that may result in some transitions tracing different vertical zones. The distribution of the small grains may have a particularly strong effect on how the UV field affects the disk (Bergin et al. 2016; Bosman et al. 2021). Combining scattered light observations with high resolution ALMA data of UV-sensitive molecular lines will give insight into these effects. Overall, future work should focus on characterizing differences in the vertical location of various transitions for a single system, particularly of CN and C₂H. IM Lup is the perfect laboratory for these studies.

4.6.2 Origin of high turbulence in IM Lup

The physical structure of IM Lup has been thoroughly studied with models (e.g., Cleeves et al. 2016) that propose the existence of a turbulent inner disk (<20 au Cleeves et al. 2018; Bosman et al. 2023) with high dust optical depth (Huang et al. 2018b; Sierra et al. 2021) that may be causing the cavity seen in molecular emission. Additionally, a series of instabilities may be ongoing in IM Lup. Bosman et al. (2023) proposed that the turbulent inner disk could be related to vertical shear instability (Urpin & Brandenburg 1998). The high disk-to-star mass ratio measured in multiple works (0.1-0.2, Lodato et al. 2023; Cleeves et al. 2018; Zhang et al. 2021; Sierra et al. 2021) suggests gravitational instabilities (Kratter & Lodato 2016) throughout some portion of the system. Finally, analysis of the ionization structure suggests a radial gradient in the cosmic ray ionization rate and adequate conditions for magneto-rotational instabilities (MRIs; Balbus & Hawley 1991) in disk regions beyond the millimeter continuum disk edge (~ 313 au) or above 20 au or $z/r \sim 0.25$ from the midplane (Seifert et al. 2021).

Indeed, high turbulence in this system is not surprising. Any of these instabilities, or their combined effect, could be causing turbulent motions. There have already been suggestions of nonthermal broadening from low-resolution CO data, as thermochemical models are able to explain the CO morphology using 100 m s^{-1} turbulent velocities (Cleeves et al. 2016) a value within the order of our derived range of $177\text{--}194 \text{ m s}^{-1}$. In contrast with this, low turbulence values ($\alpha \sim 10^{-3}$) are derived from simultaneous modeling of millimeter (ALMA) and micrometer (SPHERE) dust observations (Franceschi et al. 2023; Jiang et al. 2023). This low turbulence is mainly driven by the millimeter dust distribution, which traces the cold midplane. Through our analysis, we constrain high turbulence values ($\alpha \sim 10^{-1}$) traced by CN at $R > 150$ au and in the vertically elevated disk layers (above the midplane) at $z/r = 0.25 - 0.3$, which would suggest a vertical gradient in the turbulence, with higher values in the upper disk and lower values toward the midplane. Theoretical MRI studies have shown that high α values may correlate with higher accretion rates (Simon et al. 2015). IM Lup has a measured disk accretion rate of $10^{-8} \text{ M}_{\odot} \text{ yr}^{-1}$ (Alcalá et al. 2017), which is typical of lower α . This is reminiscent of DM Tau, where the system showed measurable turbulence,

but a low accretion rate (Flaherty et al. 2020). It is important to note that the measured accretion rate is taken from the instantaneous accretion rate onto the star; however, the α values represent disk motions throughout the outer, and in the case of IM Lup the elevated, regions of the disk. Future work should look into this with dedicated models.

A vertical gradient in the turbulence, with high values approaching the sound speed above $2H$, with H being the disk hydrodynamical scale height, is a key prediction of MRIs (Simon et al. 2015; Flock et al. 2015). The scale height in IM Lup is expected to be $H \sim 0.1$ (Zhang et al. 2021; Paneque-Carreño et al. 2023); therefore, CN emission is originating above $2H$. To fully confirm a vertical gradient in turbulence, studying molecules in the intermediate layers is necessary, such as HCO^+ , H_2CO , and HCN , which have their vertical heights characterized and emit from in-between the midplane and ^{13}CO (Paneque-Carreño et al. 2023). Unfortunately, the sensitivity and spectral resolution of the available data for these tracers ($\leq 200 \text{ m s}^{-1}$, Öberg et al. 2021b) is not sufficient to detect nonthermal broadening of $\leq 90 \text{ m s}^{-1}$, such as detected for CN. Follow up observations at higher spectral resolution would allow us to replicate this analysis and confirm the existence of a vertical gradient.

As a first attempt to compare our results with other less abundant tracers, we repeated our analysis on $\text{C}^{18}\text{O } J = 2 - 1$ data from the MAPS program (Öberg et al. 2021b). Figure 4.3 shows that $\text{C}^{18}\text{O } J = 2 - 1$ comes from an elevated layer, comparable to that of CN, but slightly below. This emission is expected to come close to the CO freeze-out region and previous works have assumed an excitation temperature of 21 K for the C^{18}O gas (Pinte et al. 2018a; Paneque-Carreño et al. 2022). Assuming that the nonthermal contribution is fully turbulent, the extracted turbulent dispersion profile of C^{18}O are slightly higher, but comparable within the uncertainty to the results obtained from CN assuming the temperature profile of ^{13}CO . We note that while the brightness temperature of C^{18}O is below the assumed excitation temperature (see Figure 4.4), the column density of CO in IM Lup (Zhang et al. 2021) and estimates from Elias 2-27 of C^{18}O under similar conditions (Paneque-Carreño et al. 2022), show that this isotopolog may have optical depths of 1-2. In this case, opacity broadening could account for up to 25% of the measured linewidth value (Hacar et al. 2016), biasing our result to higher turbulence profiles. Figure 4.10 shows the comparison between the CN results and the turbulent dispersion profiles of C^{18}O assuming a fully turbulent nonthermal contribution in the same way as our CN analysis (solid line) and considering an opacity broadening of 25% to the measured linewidth (dotted line). While the analysis of C^{18}O considering opacity broadening gives a turbulent dispersion profile below that of CN (using the ^{13}CO temperature), all profiles are comparable within their uncertainty. This is likely due to the similarity in the emitting region, which overlap within the dispersion (for details, see Paneque-Carreño et al. 2023) and highlights the need for a follow up study using other optically thin tracers that clearly probe different innermost disk layers.

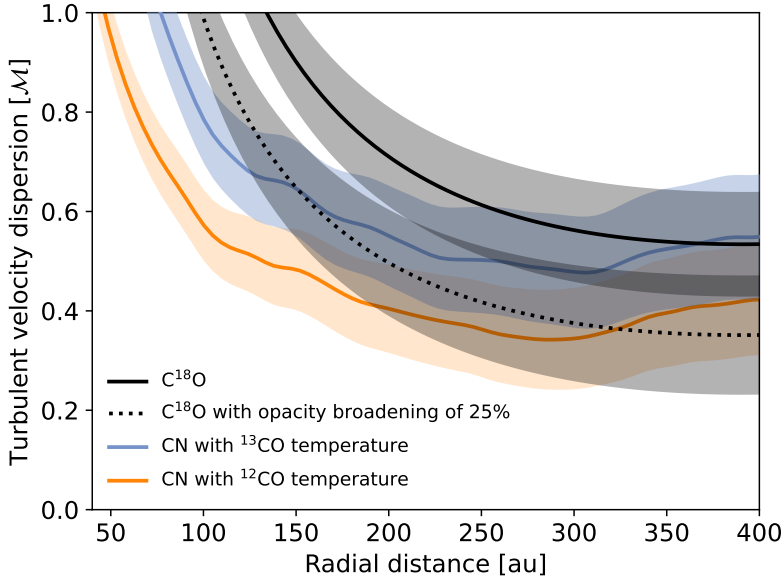


Figure 4.10: Same as Figure 7, but including an analysis of the nonthermal component of $\text{C}^{18}\text{O } J = 2 - 1$ data. The solid black line traces the results when applying the same methodology as previously used in CN to C^{18}O . The dashed black line is the turbulence profile obtained after assuming a 25% opacity broadening in the measured linewidth, which may be the case if C^{18}O has optical depths of 1-2.

4.6.3 Possible overestimation of the nonthermal component

We considered the possibility that we overestimated the turbulence in our analysis, for example by underestimating the temperatures in the CN emitting region or not taking into account alternative origins of the nonthermal broadening. Regarding the temperature profiles, we are confident that CO traces optically thick gas, even toward the outer disk regions. We confirmed this by comparing our temperature profiles to the gas temperature from dedicated thermochemical models of IM Lup (see Figs. 8 and 9 of Cleeves et al. 2016), which coincide with the values used in this work; therefore, we have not underestimated the temperature. Determining other contributors to nonthermal broadening is harder: it could be that CN emission is not as optically thin as expected, that it is vertically extended and the velocity dispersion along the line of sight is considerable, or that some strong non-Keplerian motion is affecting the system. Below, we analyze each of these scenarios.

At optical depths of $\tau \sim 0.1$ the opacity contribution to the linewidth is negligible, but at slightly higher values, even while $\tau < 1$ as expected for CN in IM Lup (Bergner et al. 2021), opacity broadening could contribute up to $\sim 15\%$ of the measured linewidth (Hacar et al. 2016). For our measured linewidth of $\sim 221 \text{ m s}^{-1}$ outside of 150 au we considered a systematic error of 50 m s^{-1} to account for Haning smoothing effects, which corresponds to a 23% error in the linewidth measurement and also accounts for the possibility of having CN emission with an optical

depth up to $\tau \sim 2$. Our results would still be consistent with high turbulence, even if the emission were marginally optically thick and opacity was contributing to the nonthermal broadening.

CN emission is expected to arise from a geometrically thin layer (Cazzoletti et al. 2018; Paneque-Carreño et al. 2022); however, at the peak of emission this layer may extend vertically up to ~ 40 au (see Figure 3 from Cazzoletti et al. 2018). It is not possible to estimate the vertical width of the CN emission with our current analysis, but we can test the impact on our measured linewidth caused by Keplerian shear along the line of sight for IM Lup. By considering the inclination of the system and taking the best-fit CN emission layer as the position of the lowest parcel of material, we measured the linewidth broadening caused by having different vertical widths. The detail of this analysis can be found in Appendix D. Figure 4.11 comprises the results, showing that at radial distances beyond 150 au the variation in the linewidth caused by vertical widths of up to 50 au is always $\leq 25 \text{ ms}^{-1}$. The width would have to be broader than ~ 60 au to cause significant variations out to further radii, which is not expected for CN (Cazzoletti et al. 2018). This indicates that even in the case of CN being vertically extended, our results beyond 150 au will not vary beyond our assumed uncertainty of 50 ms^{-1} (Fig. 4.7).

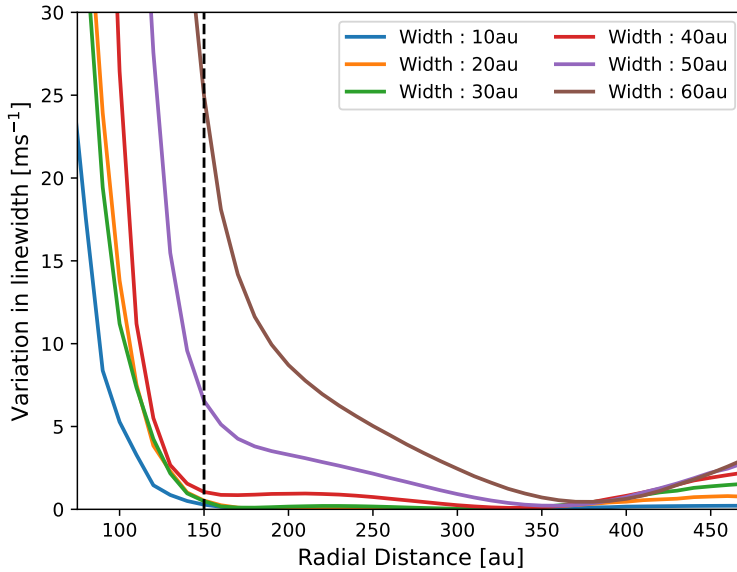


Figure 4.11: Linewidth broadening due to the vertical Keplerian shear, for different vertical widths. Each colored line indicates a specific emission width. The vertical dashed line at 150 au indicates the radial distance beyond which we consider our nonthermal linewidth component measurements robust. Details on the method are found in Appendix D.

There are no immediate signs of non-Keplerian motion (as seen in other systems, for example HD 163296; Pinte et al. 2018b; Teague et al. 2018a; Izquierdo

et al. 2022) beyond the strong residual at ~ 220 au (Figure 4.6), which is in any case radially localized and would not change our main results across the complete radial extent. However, IM Lup has been found to be prone to strong photo-evaporative winds, even in the presence of a weak external radiation field. Theoretical work by Haworth et al. (2017) shows that, if present, these winds would originate in the upper disk layers and possibly cause mass loss rates comparable to the disk accretion rate ($10^{-8} M_{\odot} \text{ yr}^{-1}$, Alcalá et al. 2017), due to the large vertical extent of the disk, which makes the surface material weakly gravitationally bound. Winds are expected to broaden the line (Fuller & Myers 1992); however, as we do not detect any indication of them in the spectra or image plane, we did not include this uncertainty in our analysis.

4.6.4 Comparison with other methods and results

We have presented a new methodology to directly extract turbulence, a fundamental disk property, from molecular line emission. By tracing the vertical location of an optically thin tracer and comparing it to that of optically thick CO lines we can immediately access the kinetic temperature of the region (Law et al. 2021b, 2023b; Paneque-Carreño et al. 2022) and from the measured linewidth calculate the nonthermal contribution attributed to turbulent motions. This requires a precise parametric model of the spectra to extract the linewidth accounting for the upper and lower disk emission layers and the broadening caused by beam convolution, which is why we use DISCMINER (Izquierdo et al. 2021).

Previous works have mostly put upper limits on turbulence by modeling the emission using physical disk models (Hughes et al. 2009; Guilloteau et al. 2012; Flaherty et al. 2015, 2017, 2020). This approach is required when the observed tracer is optically thick, as the linewidth will be affected by an opacity broadening due to the column density of the molecule (Hacar et al. 2016) and the comparison between model and data must be done taking into consideration radiative transfer calculations (Flaherty et al. 2015). However, this has the additional difficulty of determining surface density and temperature structure parameters (e.g., Hughes et al. 2009; Guilloteau et al. 2012), which are hard to constrain (see Miotello et al. 2023, and references within). Models of CO emission must also account for freeze-out and desorption processes that may be relevant (Öberg et al. 2015), adding further complexity in this kind of analysis to obtain turbulence (Flaherty et al. 2020).

Analyzing CO isotopolog data in IM Lup using these complex models also results in high nonthermal motions associated with turbulence of $\mathcal{M} = 0.18\text{-}0.3$ (Flaherty et al. in prep). Within our errors (see Figure 7) these values are consistent with our determination of $\mathcal{M} = 0.4\text{-}0.6$; however, they are a factor of 2 lower. With only one system where it is possible compare both methods, we are not able to conclude if this is a systematic difference or how it would affect the determination of nonthermal motions in other disks. We note that previous best-fit disk radiative transfer models used for studying turbulence in HD 163296 show strong differences with the disk vertical structure that is more recently constrained by Paneque-Carreño et al. (2023). Flaherty et al. (2017) predict that the expected

location for CO ($J = 2 - 1$) in HD 163296, based on their models used for setting upper limits on the turbulence, is $z/r < 0.1$ (see Fig. 16 of Flaherty et al. 2017). Direct observational measurements, however, trace the CO ($J = 2 - 1$) emission surface in HD 163296 at $z/r \sim 0.3$ (Law et al. 2021b; Paneque-Carreño et al. 2023), indicating that some of the underlying model assumptions may be incorrect and highlighting the need for high resolution data as well as the difficulty and possible errors of such methods.

Another approach of directly determining the thermal structure and turbulence is to obtain the temperature using multiple transitions, which is particularly useful for face-on disks where the vertical dimension is not accessible. This has been applied to the TW Hya disk to constrain an upper limit on turbulence of $\mathcal{M} \sim 0.1$ (Teague et al. 2016, 2018b). This method is complementary to our approach, as it relies on direct observational constraints rather than physical models; however, it carries the uncertainty on the exact emission height of different transitions.

4.7 Conclusions

We have presented new Band 7 observations at high spectral and spatial resolution of CN $N = 3 - 2$ and C₂H $N = 4 - 3$ in IM Lup. The emission from both tracers seems to be optically thin and comes from a vertically elevated layer colocated with ¹³CO $J = 2 - 1$. This is the first time C₂H is seen to be vertically elevated as predicted by thermochemical models.

Through the use of a parametric model, we traced the emission morphology and constrained the linewidth of CN, which we then decomposed into its thermal and nonthermal components. Assuming that the nonthermal component corresponds to turbulent broadening, we conclude the following:

1. IM Lup presents strong turbulence in the upper layers ($z/r \sim 0.25$), as traced by CN emission. In this layer and beyond radial distances of 150 au, turbulent velocities are between $\mathcal{M} = 0.4$ and 0.6 ($\alpha \sim 10^{-1}$).
2. Combined with constraints of low turbulence in the midplane (Franceschi et al. 2023; Jiang et al. 2023), IM Lup shows evidence for a vertical gradient of turbulence, with higher values in the upper layers. This is a key prediction of MRI (Simon et al. 2015), which has been proposed to be ongoing in IM Lup due to its ionization structure (Seifert et al. 2021).
3. The use of optically thin tracers, with emission constrained to a localized vertical region, together with the temperature profiles extracted from CO isotopologs can be leveraged to directly measure turbulence through simple parametric models of the line intensity, without the uncertainties imposed by the density and temperature structure of protoplanetary disks.

Further use of ALMA’s exquisite spectral and spatial resolution will allow us to expand this study to other sources and directly confirm if IM Lup is an exception, or if other disks have turbulent motions comparable to the sound speed in the upper layers.

Acknowledgements

This paper makes use of ALMA data from project #2019.1.01357.S. ALMA is a partnership of ESO (representing its member states), NSF (USA), and NINS (Japan), together with NRC (Canada), NSC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO, and NAOJ. Astrochemistry in Leiden is supported by the Netherlands Research School for Astronomy (NOVA), and by funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 101019751 MOLDISK). This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 823823 (DUSTBUSTERS).

Appendix

4.A Radial features

The integrated intensity emission maps (moment 0) show a distinct radial feature for all the studied hyperfine groups (Fig. 4.1). We compute the azimuthally averaged intensity profiles from these maps by accurately deprojecting using the best-fit vertical surfaces and the function `radial_profile` from GoFish (Teague 2019b). Only emission from within a 60° wedge along the semimajor axis is considered, to avoid deprojection effects from emission close to the minor axis (Law et al. 2021a). Our results are shown in Figure 4.A.1, where all tracers display a ringed structure peaking at ~ 106 au.

To characterize the width and any azimuthal variations of the ring feature, a set of two Gaussians are fitted to the radial profiles as done in Law et al. (2021a). A broad component Gaussian is used to trace the emission at further out radii and a second Gaussian traces the ring structure. Figure 4.A.2 shows the fitted Gaussians and FWHM value of the ring-component Gaussian. We used a Gaussian function such that

$$I = I_0 \exp \left[-\frac{1}{2} \frac{(R - R_0)^2}{\sigma^2} \right], \quad (4.7)$$

where I is the measured intensity, R the radial distance, I_0 , R_0 and σ are the fitted parameters and the $\text{FWHM} = 2\sqrt{2\log(2)}\sigma$. While the peak of emission was coherent across different hyperfine groups, the ring width has slight variations. Overall the feature shows an average width of ~ 89 au in CN and ~ 109 au in C₂H.

Considering the broadest value of ~ 115 au we calculate the averaged intensity throughout the angular extent of the ring, using azimuthal bins of 5° . Figure 4.A.3 shows the results. CN displays a symmetric ring across azimuth, with slight variations along the semiminor axis likely due to projection effects. C₂H has a lower S/N and may show tentative asymmetries; however, the quality of the data is not sufficient to characterize them in detail.

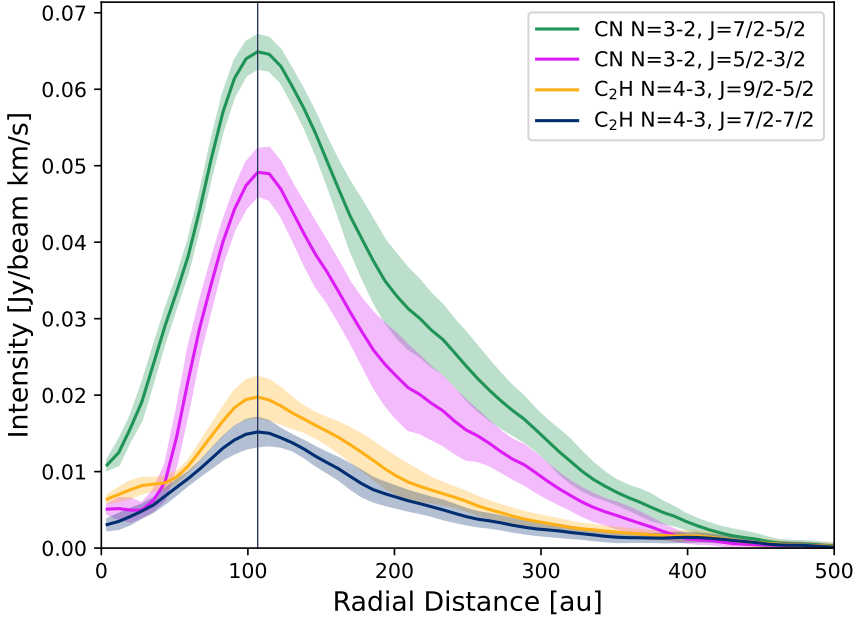


Figure 4.A.1: Azimuthally averaged radial intensity profiles for each of the observed hyperfine groups. The solid line traces the average value and the shaded region the dispersion within each radial bin. The vertical black line indicates the peak of emission, which coincides for all transitions at ~ 106 au.

4.B Channel map analysis

To extract the vertical location of the emission layer, we traced the emission maxima from the channel map emission as explained in section 3.1. The channels, masks, and extracted emission maxima are presented in Figures 4.B.1 and 4.B.2 for CN and C₂H, respectively.

4.C DISCMINER best-fit parameters

Table 4.C.1 indicates the best-fit parameters obtained by DISCMINER for the CN emission model.

4.D Effect of vertical layer width

To estimate the effect of the Keplerian shear due to a nonzero vertical width of the CN emitting layer, we considered the best-fit CN emitting surface as a lower limit

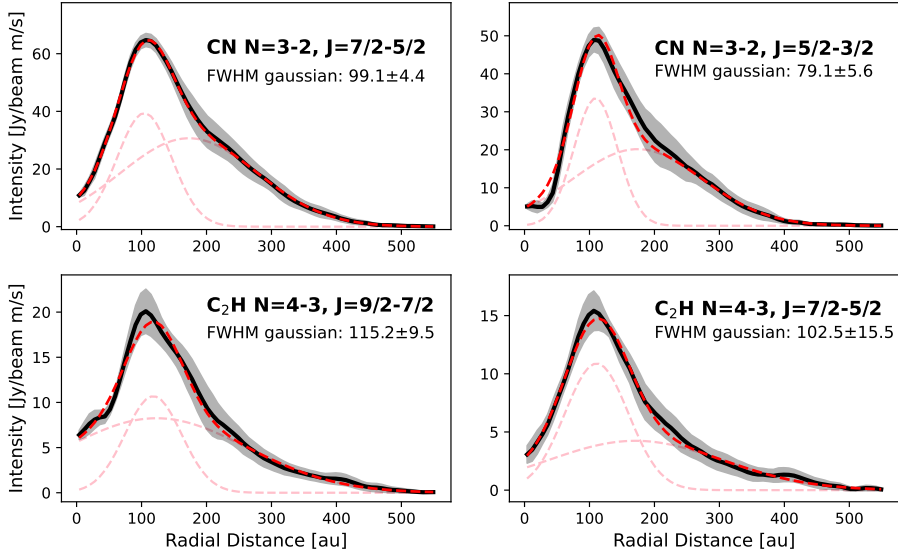


Figure 4.A.2: Gaussian fits to the radial intensity profiles of each transition. The data are shown in black, pink dashed lines trace the two individual Gaussian components, and the dashed red line presents the model curve, obtained by summing both Gaussians. The FWHM of the inner Gaussian, which traces the ring component, is indicated for each panel.

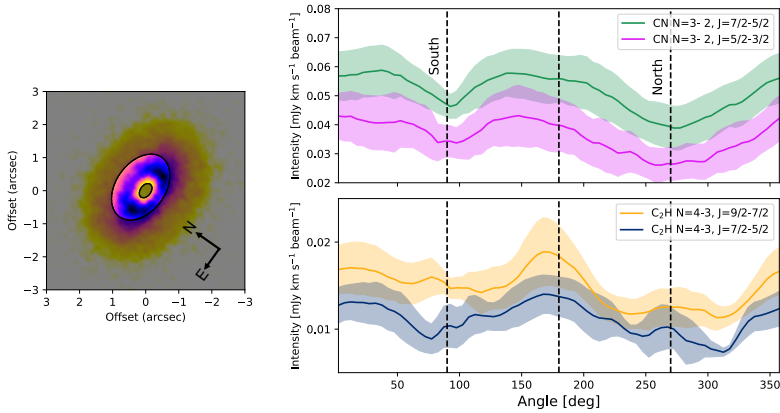


Figure 4.A.3: Azimuthal emission curves along the ring for each transition. The solid line indicates the mean values within each azimuthal bin and the shaded region the dispersion. The panel to the left shows the radial limits used to extract the ring emission.

and used the geometry of the disk to calculate the line-of-sight path for different

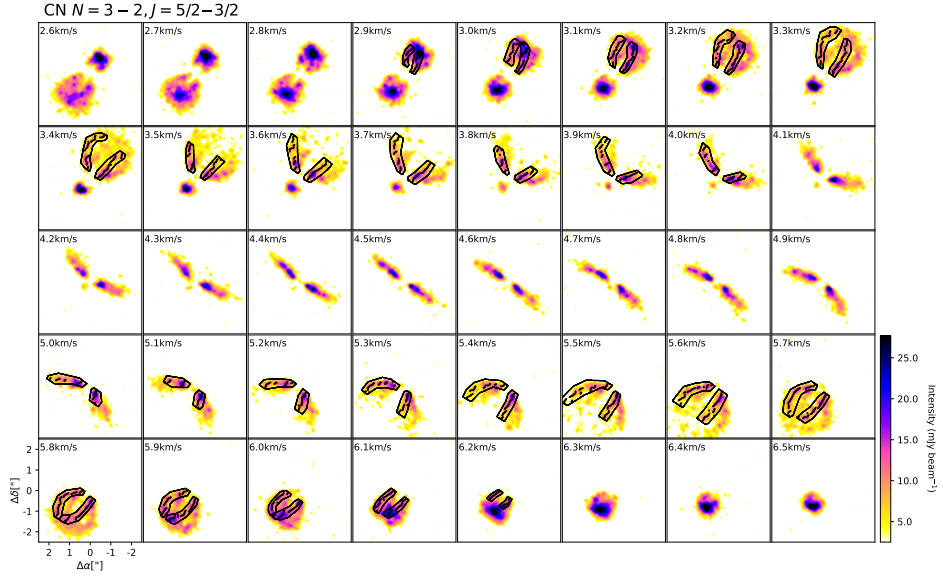


Figure 4.B.1: CN $N = 3 - 2$ emission, showing the channel maps used to extract the vertical emission layer with ALFAHOR. The masked regions are indicated in the black contours and black dots within the masks trace the emission maxima.

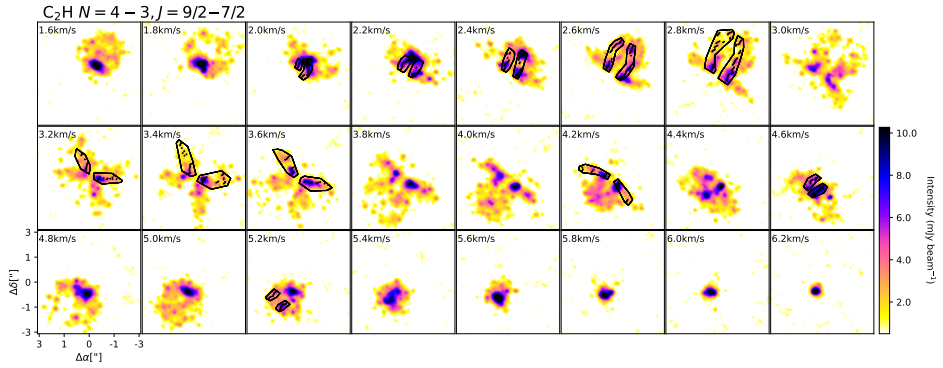


Figure 4.B.2: Same as Fig. 4.B.1 but for $\text{C}_2\text{H } N = 4 - 3$ emission.

vertical widths (see panel A in Figure 4.D.1). The rotation velocity of a parcel of gas located at a position (r, z) , in cylindrical coordinates, from the star is given by

$$V_{\text{rot}}^2 = \frac{GM_* r^2}{(r^2 + z^2)^{3/2}}, \quad (4.8)$$

where G is the gravitational constant and M_* the stellar mass. Using this formula, we calculated the velocity for a parcel of material along the line-of-sight path,

between the initial (r_1, z_1) and final (r_2, z_2) positions, as shown in Figure 4.D.1. The velocity variation is not linear, as it depends on both radial and vertical differences; to be sensitive to these variations, we sampled the line-of-sight path every 1 au. Using a series of Gaussian profiles with line centers at each of the sampled velocities, we computed the resulting average profile, which is of Gaussian form, and estimated the measured linewidth from it (panel B in Figure 4.D.1). As the temperature is not expected to change significantly in these upper disk layers for IM Lup (Cleeves et al. 2016), we assumed a constant intrinsic thermal linewidth in the Gaussian profiles for our estimation. The final linewidth broadening caused by a nonzero emission surface is then calculated by subtracting the intrinsic and measured linewidth values.

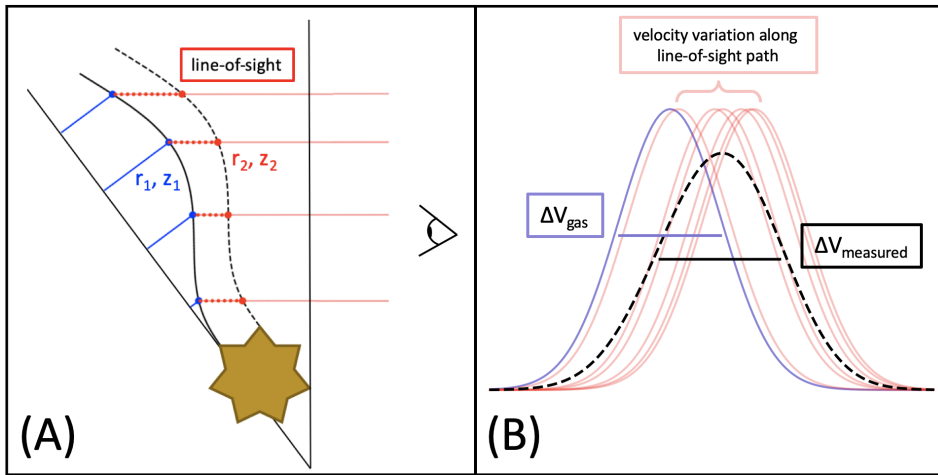


Figure 4.D.1: Sketch of the method used to estimate the effect of a nonzero vertical emitting width for CN. Panel (A) shows the geometry of CN emission in IM Lup, considering an inclination of 47.8° with respect to the observer. For the vertical structure, the solid curve indicates the best-fit vertical profile of CN emission and the dashed curve the extent considering a fixed vertical width. In each case, the blue dot is the observed parcel of gas at position (r_1, z_1) that has to cross the line-of-sight path as indicated by the red line, leaving the zone of CN emission at the red dot location (r_2, z_2) . For different radial distances, the path varies. Panel (B) shows the velocity variation between the blue dot and the final red dot positions. Each solid-line Gaussian is centered at a determined velocity, depending on their (r, z) position along the line-of-sight path. The measured linewidth ($\Delta V_{\text{measured}}$) is taken from the resulting average Gaussian, shown as a dashed black curve and compared to the intrinsic value (ΔV_{gas}).

Table 4.C.1: DISCMINER best-fit parameter values.

Attribute	Parameter	Unit	Value
Orientation	i	[°]	50.53
	PA	[°]	143.76
	x_c	[au]	-1.9
	y_c	[au]	1.3
Velocity	M_*	[M _☉]	1.22
	v_{sys}	[km s ⁻¹]	4.49
Upper surface	z_0	[au]	18.98
	p	[-]	1.50
	R_t	[au]	427.50
	q	[-]	3.34
Lower surface	z_0	[au]	8.35
	p	[-]	1.47
	R_t	[au]	423.38
	q	[-]	3.91
Peak intensity	I_0	[Jy px ⁻¹]	0.69
	p	[-]	-4.30
	q	[-]	3.60
	I_g	[Jy px ⁻¹]	2.42
	R_g	[au]	32.74
	σ_g	[au]	45.97
Linewidth	L_0	[km s ⁻¹]	0.415
	p	[-]	-0.205
	q	[-]	-0.238

Chapter 5

Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion

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submitted to Astronomy & Astrophysics

Abstract

Context: As the sample of mid-inclination disks with measured CO emission surfaces grows, a fundamental unanswered question is how these vertical profiles connect to their host properties.

Aims: This project aims to relate the vertical extent of protoplanetary disks as traced by $^{12}\text{CO } 2-1$ to key stellar and physical parameters. In order to produce a result that is applicable towards an observational analysis, we benchmark our results with ALMA observations of CO emission from nineteen disks.

Methods: We produce a grid of disk models using the physical-chemical code DALI, for a template T Tauri and Herbig star. Our models use an iterative solver to calculate the hydrostatic equilibrium equations and determine a physically-motivated density structure. Key stellar and disk parameters such as stellar luminosity and temperature, total disk mass, carbon abundance and critical radius are varied to determine their effect on the CO emitting surface. Each vertical profile is fitted by an exponentially tapered power-law and characterized by the z/r value that represents the structure inwards of 80% of the tapering radius.

Results: The CO emission surface location is determined by the disk mass (M_d) and the level of carbon depletion. T Tauri and Herbig systems show different vertical profiles, with disks around T Tauri stars being more vertically extended. We derive a z/r - M_d relationship, which for each stellar type has a degeneracy with the volatile carbon abundance. In order to reconcile total disk mass estimates from the characteristic z/r and the values obtained based on dust continuum analysis, a volatile carbon depletion of 10-100 (with respect to the ISM) is needed for the majority of our sources. Our carbon depletion values are in agreement with previous literature estimates, highlighting the potential of this method to rapidly calculate key disk parameters.

5.1 Introduction

Planets form and grow within protoplanetary disks made of dust and gas which orbit around young stellar objects. Through high spatial and spectral resolutions of the Atacama Large Millimeter/submillimeter Array (ALMA) we have been able to trace the extent and structure of these disks in dust and gas across all three dimensions; azimuthal, radial and vertical (e.g. Huang et al. 2018b; Andrews 2020; Law et al. 2021a,b; Paneque-Carreño et al. 2023). To date, most studies have focused on the information offered by the radial and azimuthal structure (for a review see Bae et al. 2023). Radial extent compared to the stellar age is used as an indicator on the governing evolution processes (Rosotti et al. 2019; Tazzari et al. 2021a; Long et al. 2022; Trapman et al. 2023) and radial substructures characterize a number of chemical and physical scenarios (Andrews 2020; Öberg et al. 2021b, 2023). Azimuthal enhancements can signal towards the presence of planetary companions (Ragusa et al. 2017; Pérez et al. 2020; Booth et al. 2023) and some azimuthal asymmetries can be linked to inner warps or other disk processes (Pérez et al. 2018a; Paneque-Carreño et al. 2022). Vertical structure, however, has been less accessible from an observational point of view and therefore less studied in comparison to the other two dimensions.

Directly probing the vertical structure and molecular layering of disks through observations of edge-on disks has offered valuable insight on the thermal and density conditions (Dutrey et al. 2017; Ruíz-Rodríguez et al. 2021), as well as dust-settling processes (Villenave et al. 2020, 2023). In the recent years, novel methodologies (Pinte et al. 2018a) have proven that the vertical structure can also be traced from mid-inclination ($40\text{--}60^\circ$) disks, opening an exciting avenue to explore this dimension in larger samples (Teague et al. 2021b; Rich et al. 2021; Law et al. 2021b, 2022; Paneque-Carreño et al. 2023; Pinte et al. 2023). From a theoretical point of view, the vertical distribution of the gaseous disk material will follow hydrostatic equilibrium between the stellar gravitational potential and thermal pressure support (Armitage 2015). This implies that a number of properties such as stellar mass and radiation field, but also disk temperature structure and density distribution are expected to affect the vertical extent (D'Alessio et al. 1998; Aikawa et al. 2002). While the bulk of the disk material is composed of molecular hydrogen (H_2), we are not able to trace the disk structure through its emission, as it is extremely hard to detect throughout the cold outer ($r > 50$ au) disk region. Due to this difficulty, less abundant, but bright tracers, such as carbon monoxide (CO) are preferred to characterize the disk structure and conditions (for a review see Miotello et al. 2023).

This work focuses on the protoplanetary disk properties that affect the vertical structure as traced by bright CO ($2-1$) emission. CO is the main carrier of gas-phase carbon in the interstellar medium and its chemistry is relatively simple and reliably implemented in various physical-chemical models (e.g. Aikawa et al. 2002; Gorti & Hollenbach 2008; Bruderer 2013; Miotello et al. 2014; Woitke et al. 2016; Yu et al. 2016; Molyarova et al. 2017). For this reason CO is a preferred molecule to study the disk extent (radially and vertically, Ansdell et al. 2018; Sanchis et al. 2021; Law et al. 2021a, 2022; Rich et al. 2021), kinematical processes (Pinte et al.

2023), temperature structure (Law et al. 2021b; Paneque-Carreño et al. 2023; Stapper et al. 2023) and disk mass (which usually requires analysis of rarer CO isotopologues, Miotello et al. 2014, 2016; Booth et al. 2019; Stapper et al. 2024). Vertically, CO gas emission originates from the warm molecular layer defined by the boundary of UV photo-dissociation in the upper regions and low temperatures that cause CO freeze-out (~ 20 K) closer to the midplane (Aikawa et al. 2002). At typical temperatures (40–60 K) and CO column densities ($\geq 5 \times 10^{16} \text{ cm}^{-2}$) of the molecular layer in protoplanetary disks, the CO millimeter emission will be optically thick ($\tau \geq 1$, van der Tak et al. 2007). Indeed, previous works have shown that the emitting surface traced by CO, as extracted from emission channel maps, follows the CO $\tau \sim 1$ region of the disk structure (Paneque-Carreño et al. 2023). Efforts in linking the observationally derived CO surfaces to system or emission properties such as stellar mass, brightness temperature or disk radius have only provided tentative trends (Law et al. 2022, 2023b) and it is not yet well understood how the wide morphology of CO vertical profiles relates to the host disk.

A crucial assumption that most studies related to CO emission make is that its abundance with respect to H_2 , as set by the volatile carbon abundance, follows the canonical interstellar medium (ISM) value of $\sim 10^{-4}$ (e.g. Andrews et al. 2011; Ansdell et al. 2016; Flaherty et al. 2015; Stapper et al. 2024). This is in tension with observational results that show that between 1-2 orders of magnitude of volatile carbon depletion must be present to account for disk masses derived from HD observations (Favre et al. 2013; McClure et al. 2016; Schwarz et al. 2016; Calahan et al. 2021) and derivations of CO depletion, with respect to ISM abundance, from optically thin CO isotopologue emission profiles (Zhang et al. 2019, 2021). Lower-than-ISM CO abundances may be caused by chemical reprocessing of CO into other molecules (Bergin et al. 2014; Bosman et al. 2018; Diop et al. 2024) or physical processing through which carbon is removed from the disk atmosphere by icy dust grains that grow and settle towards the disk midplane (Krijt et al. 2016, 2018, 2020). These processes are in addition to photodissociation and freeze-out, which will also lower the CO abundance throughout the disk and are included in standard thermochemical models (e.g., Bruderer 2013; Woitke et al. 2016). Overall, it is expected that the CO abundance may change as the disk evolves and therefore it is not inherited from the natal cloud environment (Visser et al. 2009; Bergner et al. 2020; Zhang et al. 2021). To the best of our knowledge, there are no previous studies that model or observationally analyze the effect of volatile carbon depletion on the vertical emitting surface of disks.

The remainder of this paper is organized as follows. Section 2 details the setup of thermochemical models used in our analysis, indicating the relevance of accounting for hydrostatic equilibrium for a more realistic approach. Section 3 shows our main results, an overview of the sampled parameter space and the effect of various disk and stellar properties on the location of the $\tau = 1$ CO emission layer. We present a z/r –Disk mass relation for both T Tauri and Herbig disk systems and apply it to a sample of archival protoplanetary disk observations. Our results showcase the necessity of considering carbon depletion in order to obtain disk masses that are in agreement with literature values. Section 4 has a detailed

discussion of our results, comparing them to previous studies and literature values of carbon depletion. Finally, Section 5 indicates the main conclusions of this work.

5.2 Modelling

The results shown in this paper are based on an extensive grid of models run with the thermochemical code DALI (Bruderer 2013). For details on the code, how the chemical network is setup and the calculation of the temperature structure, dust populations and flux values we reference to past works using the same code (e.g. Bruderer et al. 2012; Bruderer 2013; Miotello et al. 2016; Leemker et al. 2022; Stapper et al. 2024). Our models are run using the chemical network from Miotello et al. (2014), that accounts for CO isotope-selective effects, considering selective photodissociation, fractionation reactions, self-shielding, and freeze-out (for more details see Miotello et al. 2014, 2016).

5.2.1 Initial DALI setup

The initial setup of the radial structure for the gas and dust in DALI follows the self-similar solution to a viscously evolving disk (Lynden-Bell & Pringle 1974; Andrews et al. 2011).

$$\Sigma(R) = \Sigma_c \left(\frac{R}{R_c} \right)^{-\gamma} \exp \left[- \left(\frac{R}{R_c} \right)^{2-\gamma} \right] \quad (5.1)$$

where R_c is the characteristic radius and γ the surface density exponent. The initial vertical structure of the disk follows a Gaussian distribution, where the gas density (ρ) corresponds to,

$$\rho(z) = \rho_c(r) \exp \left[- \frac{z^2}{(2H^2)} \right] \quad (5.2)$$

and H is the disk scale height. To set the scale height aspect ratio (H/r), we have modified the usual DALI prescription (where the aspect ratio is typically noted as h , see for example Leemker et al. 2022) to match the parametrization of Zhang et al. (2021). In our model the scale height aspect ratio as a function of radius follows,

$$H/r = h_{100} \left(\frac{R}{100 \text{ au}} \right)^\varphi \quad (5.3)$$

where h_{100} is the scale height aspect ratio at 100 au. The main results in this study are based on the fiducial models for a T Tauri and Herbig system following the values presented in Table 5.1. For the T Tauri, excess UV radiation due to a mass accretion rate of $10^{-8} \text{ M}_\odot \text{ yr}^{-1}$ was taken into account. It was assumed that the gravitational potential energy of the accreted mass is released with 100% efficiency as blackbody emission with $T = 10^4 \text{ K}$ (Miotello et al. 2014, 2016). For our parameters, these assumptions result in $L_{\text{FUV}}/L_{\text{bol}} = 1.46 \times 10^{-1}$. Beyond

Table 5.1: Initial parameters in fiducial DALI model

Parameter	Value
<i>Chemistry</i>	
Chemical Age	1 Myr
Volatile [C]/[H]	1.35×10^{-4} , 10^{-5} , 10^{-6}
Volatile [O]/[H]	2.88×10^{-4} , 10^{-5} , 10^{-6}
[PAH]	10^{-4} ISM abundance
<i>Physical Structure</i>	
gas-to-dust ratio	100
f_{large} (small/large grains)	0.95
χ (settling of large grains)	0.2
φ (flaring index)	0.1
h_{100} (scale height aspect ratio)	0.1
R_c (characteristic radii)	100 au
M_d (total disk mass)	10^{-1} , 10^{-2} , 10^{-3} , $10^{-4} M_{\odot}$
<i>Stellar Parameters</i>	
L_x	$1.0 \times 10^{30} \text{ erg s}^{-1}$
T_x	$7.0 \times 10^7 \text{ K}$
<i>T Tauri model</i>	
M_*	$1.0 M_{\odot}$
$\dot{M}_{\text{acc}}$	$10^{-8} M_{\odot} \text{ yr}^{-1}$
L_{bol}	$1.0 L_{\odot}$
T_{eff}	4000 K
<i>Herbig model</i>	
M_*	$2.0 M_{\odot}$
L_{bol}	$17.0 L_{\odot}$
T_{eff}	9000 K

Table 5.2: Variation of DALI model parameters. Bold numbers indicate the fiducial model values.

Parameter	Sampled values
<i>T Tauri model</i>	
φ (flaring index)	0.1 , 0.2, 0.5
f_{large} (small/large grains)	0.9, 0.95 , 0.99
T_{eff}	3500, 4000 , 4500 K
L_{bol}	0.2, 1.0 , $3 L_{\odot}$
$\dot{M}_{\text{acc}}$	10^{-9} , 10^{-8} , $10^{-7} M_{\odot} \text{ yr}^{-1}$
R_c (characteristic radii)	15, 50, 100 au
<i>Herbig model</i>	
[PAH]	10^{-4} , 10^{-2} , 10^{-1} ISM abundance
T_{eff}	7500, 9000 , 10000 K
L_{bol}	10, 17 , $30 L_{\odot}$
R_c (characteristic radii)	15, 50, 100 au

the fiducial models, we study a wider parameter space to determine the effect of key disk properties on the location of the vertical structure as traced by ^{12}CO , Table 5.2 indicates the sampled values.

5.2.2 Hydrostatic equilibrium

The initial setup presented in the previous section is a useful approximation, but is not realistic, as it is known that the disk vertical structure does not follow a gaussian distribution, rather it is set by hydrostatic equilibrium between the stellar gravity and pressure support of the disk (given by the thermal structure). To produce more realistic models, DALI has a hydrostatic equilibrium solver implemented, which self-consistently iterates over consecutive models, starting from the initial parametrization, to compute the disk structure. We use this approach for all of our analysis. To this end, the hydrostatic equilibrium equation that must be solved in the vertical direction, using cylindrical coordinates, is:

$$\frac{1}{\rho} \frac{dP}{dz} = -\frac{d\phi}{dz} \quad (5.4)$$

where ρ is the gas density, P the gas pressure and ϕ the gravitational potential. Without considering self-gravity, ϕ corresponds to the stellar gravitational potential and follows,

$$\phi = -\frac{GM_*}{(r^2 + z^2)^{1/2}} \quad (5.5)$$

Pressure and density can be connected such that $P/\rho = c_s^2 = kT/(\mu m_p)$. Disks are not isothermal in their vertical direction, therefore, the sound speed (c_s) will vary as function of height, depending on the density and thermal conditions. The differential equation for P is

$$\frac{1}{P} \frac{dP}{dz} = -\frac{z GM_*}{c_s^2 (r^2 + z^2)^{3/2}} \quad (5.6)$$

and can be solved through

$$P(z) = c_s(z)^2 \rho(z) = C \exp \left(- \int \frac{z GM_*}{c_s^2 (r^2 + z^2)^{3/2}} dz \right) \quad (5.7)$$

which will obtain the vertical distribution for the gas density ($\rho(z)$). In DALI, the disk temperature structure is first obtained from the initial model, which computes the thermal conditions of the material considering all relevant cooling and heating processes, and then used to update the gas density distribution accounting for thermal support. The updated density is consecutively used to recalculate the temperature for the next iteration and start over until reasonable convergence of the disk structure is achieved. The integration constant C is adjusted such that $\int \rho(z) dz$ is preserved with each iteration. In the isothermal approximation c_s^2 does not have a vertical dependence and we recover the gaussian distribution indicated in equation 2.

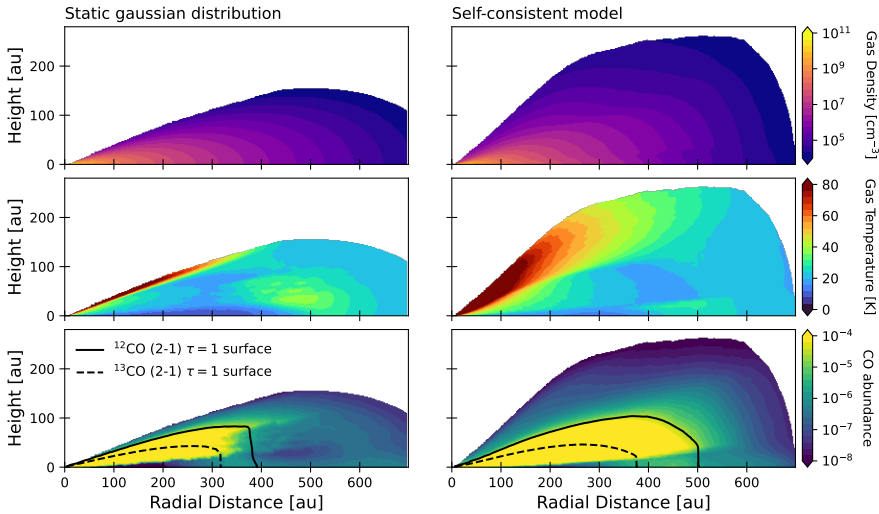


Figure 5.1: Comparison between the outputs of a vertically static gaussian distribution and a model after solving self-consistently for the vertical material distribution. Each row shows the 2D distribution of key parameters, displayed using the same colorbar. From top to bottom the volumetric gas density, gas temperature and CO abundance (relative to H_2) are shown. In the bottom row the solid line traces the ^{12}CO $\tau = 1$ surface and the dashed line the ^{13}CO $\tau = 1$ surface.

Figure 5.1 shows the 2D maps for the gas density, temperature and CO abundance (with respect to H_2) of a converged DALI model for a $10^{-2}M_\odot$ disk around a $1M_\odot$ and $1L_\odot$ stellar system. The static gaussian distribution corresponds to the initial DALI output, computed from the setup equations outlined in section 2.1. The self-consistent model solution is the result of six iterations solving the hydrostatic equilibrium equations, considering the previously computed thermal structure. The material appears to be more vertically extended in the self-consistent model, which is expected due to the increased pressure support of the heated atmosphere calculated from the vertical temperature gradient. Our study focuses on the ^{12}CO 2 – 1 emission surface, which is directly computed from the models as the location where the integrated column density of material results in an optical depth (τ) of 1 for ^{12}CO 2 – 1. Indeed, the $\tau=1$ layer of DALI models is consistent with the emission surfaces extracted from ALMA gas emission maps of ^{12}CO 2 – 1 (Paneque-Carreño et al. 2023).

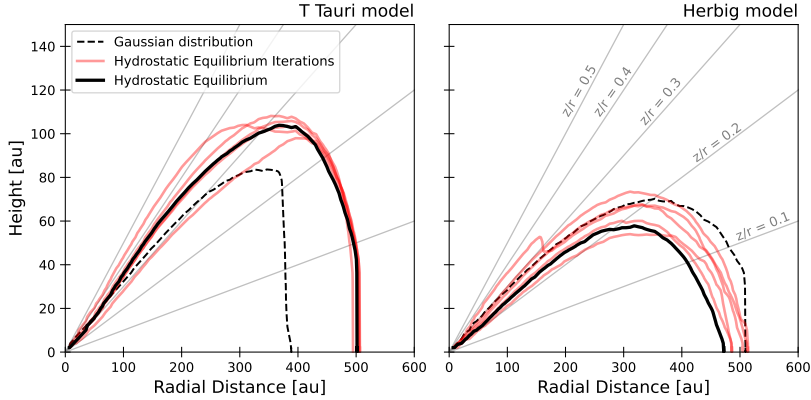


Figure 5.2: Variation of the ^{12}CO $\tau = 1$ surface when considering the hydrostatic equilibrium model solutions. Left panel shows the output for a T Tauri system and Right panel the results for a Herbig system. Both models correspond to a disk mass of $10^{-2}M_\odot$. The dashed lines trace the surface from the parametric gaussian distribution and the solid black line the final hydrostatic equilibrium solution considered. Each red line represents a model iteration of hydrostatic equilibrium in DALI.

When accounting for hydrostatic equilibrium, the $\tau = 1$ surface varies both in its vertical and radial extent from the surface extracted from the parametric model. Figure 5.2 indicated the variations for the $\tau = 1$ layer in a $10^{-2}M_\odot$ disk around a $1M_\odot$ and $1L_\odot$ star (T Tauri model) compared to the same disk mass around a $2M_\odot$ and $17L_\odot$ star (Herbig model). As the hydrostatic equilibrium solution depends on the stellar mass, temperature and density distribution, it is expected that the surfaces will be different in each case. Convergence is reached rapidly after a couple of iterations, therefore all presented models in this work will consider the output from the 6th iteration of the self-consistent hydrostatic equilibrium solver.

5.3 Results

As has been shown in multiple studies, CO molecular surfaces can be parametrized through an exponentially tapered power-law (Law et al. 2021b, 2023b; Paneque-Carreño et al. 2023). To model each ^{12}CO $\tau = 1$ surface from the self-consistent DALI outputs after solving the hydrostatic equilibrium equations, we select the following prescription,

$$z(r) = z_0 \times \left(\frac{r}{100 \text{ au}} \right)^\phi \times \exp \left[\left(\frac{-r}{r_{\text{taper}}} \right)^\psi \right] \quad (5.8)$$

The best fit values for z_0 , ϕ , r_{taper} and ψ are obtained using a Monte Carlo Markov Chain (MCMC) sampler as implemented by emcee (Foreman-Mackey et al. 2019). Each surface is then identified based on its characteristic z/r value, which corresponds to the best-fit line of constant z/r that traces the height profile within 80% of r_{taper} (Law et al. 2023b). This assures us that we are characterizing the rising portion of the ^{12}CO surface, as exemplified in Figure 5.3 where a schematic of the method is shown.

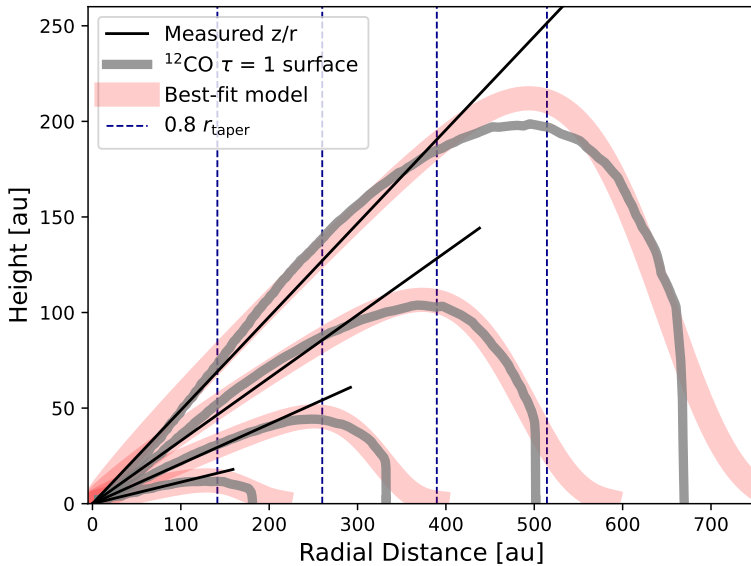


Figure 5.3: Schematic of the method use to measure the ^{12}CO surface z/r values. Each surface traced by the grey line is the output of a T Tauri model, in order of increasing height and radial extent they have disk masses of 10^{-4} , 10^{-3} , 10^{-2} and $10^{-1} M_{\odot}$. The shaded red curve shows the best-fit parametric model fitted to the molecular surface, from where r_{taper} is the taper radius. The measured z/r is obtained by fitting the surface region within 80% of r_{taper} , this distance is indicated by the vertical dashed line. The characteristic z/r is traced by the straight black line for each surface.

5.3.1 Parameters that affect vertical CO surface

Our fiducial models for each stellar type are indicated in Table 5.1. To determine which parameter variation most strongly affects the measured z/r we compute additional models with a varied stellar luminosities and temperatures as reported in Table 5.2 covering the range of reported values from the comparison observations. Disk structure values for the flaring angle (φ), small-to-large dust grain fraction (f), PAH abundance, surface density characteristic radius (R_c), total disk mass (M_d) and volatile carbon abundance (C_{abu}) are also sampled. For each model the characteristic z/r is computed as described at the beginning of Section 3. Figure 5.4 presents the percentual variation from the fiducial model for disk masses of $10^{-3} M_\odot$ and $10^{-2} M_\odot$. The full vertical profiles for each parameter can be found in Figures 5.A.1 and 5.A.2.

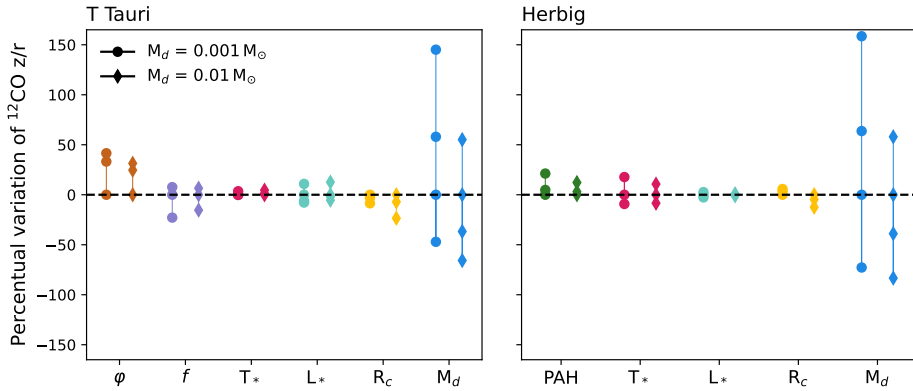


Figure 5.4: Percentual variation of the ^{12}CO surface z/r caused by various stellar and disk parameters. Left panel indicates the results for the T Tauri system and right panel for the Herbig system. Each parameter corresponds to a specific color. The circle markers indicate the effects on a disk with mass $10^{-3} M_\odot$ and the diamond markers the effects on a disk with mass $10^{-2} M_\odot$. Specific details on the parameter range and properties are shown in Table 5.2.

The largest variation in z/r is caused by varying the total disk mass, which is sampled at $10^{-4} M_\odot$, $10^{-3} M_\odot$, $10^{-2} M_\odot$ and $10^{-1} M_\odot$. An order of magnitude change in the disk mass can vary the emission height by more than 50%. Volatile carbon abundance also presents a strong effect in the emission surfaces. Indeed, an order of magnitude decrease in the assumed volatile carbon abundance with respect to the ISM can lower the characteristic z/r by $\sim 30\%$ and two orders of magnitude in carbon depletion produce z/r variations beyond 50%. These two parameters have a degenerate contribution to the vertical surface, as can be seen from Figure 5.5. Increasing disk mass will push the CO emission layer higher, while for the same disk mass a lower volatile carbon abundance (higher depletion) will push the emitting layer towards the midplane. This effect of carbon abundance in the vertical structure had been previously observed in Calahan et al. (2021) when constraining the disk model of TW Hya.

Across all masses, for the same degree of carbon depletion, the T Tauri systems display a larger z/r than the Herbig disks (see Fig. 5.5). This is expected due to the larger stellar mass of the Herbig model, which will translate into a higher gravitational potential (equation 5). The parameter space between our models is covered using a cubic spline which we use to extrapolate our results beyond our mass grid, to nearby values. We refer to this result as the z/r - M_d relationship, noting that volatile carbon depletion will shift it and must be accounted for.

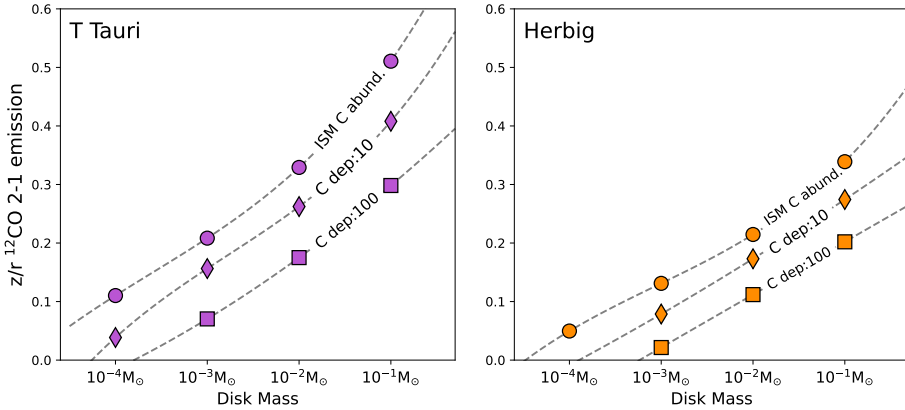


Figure 5.5: Relation between the ^{12}CO surface z/r and the total disk mass (z/r - M_d relationship) with a dependence on the volatile carbon abundance. Left panel shows results for T Tauri systems and right panel for Herbig systems. Circles indicate ISM-like carbon abundance (no depletion), diamonds trace a carbon depletion of 10 and squares a depletion of 100, with respect to the ISM.

All other parameters, including order of magnitude variations in stellar accretion rate and PAH abundance (see Table 5.2), cause a variation of less than $\sim 30\%$. We stress that these results only hold for the ^{12}CO 2 – 1 surface z/r , other molecules, particularly those more sensitive to UV fields are likely more significantly affected by some of the sampled parameters.

5.3.2 Model comparison to observations

In order to benchmark our model results and the z/r - M_d relationship, we estimate the gas masses and expected z/r in an observational sample of 19 disks, as indicated in Table 5.3. The studied disks all have estimates of their total disk mass from dust continuum observations, additionally some of them have disk mass estimates from modelling of CO, HD and N_2H^+ fluxes and dynamical analysis of rotation curves.

Most disk mass values from dust continuum emission are extracted by converting the total continuum flux into a dust mass, assuming a dust temperature and grain opacity and then using the canonical assumption of a gas-to-dust ratio of 100 (Hildebrand 1983; Ansdell et al. 2016; Andrews et al. 2013; Barenfeld et al. 2016; Pascucci et al. 2016; Stapper et al. 2022). Excluding the sources from the MAPS

Table 5.3: Observational sample, stellar parameters and estimated total disk masses

Star	M _*	L _*	T _*	Previous disk mass estimates [M _⊙]				References
	[M _⊙]	[L _⊙]	[T _⊙]	Dust continuum	CO flux	HD emission	Dynamical	
T Tauri Disks								
MY Lup	1.27	0.87	5129	1.5×10 ⁻²	8.3×10 ⁻⁵	-	-	4 , 3, 12, 5
AS 209	1.2	1.41	4266	7.5×10 ⁻²	4.5×10 ⁻³	-	2×10 ⁻⁴	1, 13, 16, 18
WaOph 6	1.12	2.9	4169	1.4×10 ⁻²	-	-	-	4, 3, 14
IM Lup	1.1	2.57	4266	3.67×10 ⁻¹	2×10 ⁻¹	-	1.1×10 ⁻¹	1, 13, 16, 18
GM Aur	1.1	1.2	4350	7.3×10 ⁻²	2×10 ⁻¹	-	1.2×10 ⁻¹	1, 13, 16, 18
DoAr 25	1.06	0.95	4266	4.2×10 ⁻²	-	-	-	4, 3, 5
LkCa 15	0.7	1.098	4162	2.7×10 ⁻²	-	-	-	5
GW Lup	0.62	0.33	3631	1.5×10 ⁻²	9.6×10 ⁻⁵	-	-	4, 3, 12, 5
Sz 91	0.55	0.26	3720	2.2×10 ⁻³	-	-	-	4, 10, 5
DM Tau	0.50	0.24	3705	1.6×10 ⁻²	-	-	-	4, 9, 5
Elias 2-27	0.46	0.91	3890	3.4×10 ⁻²	-	-	8×10 ⁻²	2, 3, 5, 17
Herbig Disks								
HD 100546	2.10	23.4	9750	1.2×10 ⁻²	3.2×10 ⁻²	<8×10 ⁻²	-	4, 8, 11, 15, 19
HD 97048	2.70	44.2	10500	4.7×10 ⁻²	1×10 ⁻¹	<9.4×10 ⁻²	-	4, 8, 11, 15, 19
HD 100453	1.66	6.31	7400	5.3×10 ⁻³	3.2×10 ⁻²	<1×10 ⁻²	-	6, 11, 15, 19
HD 34282	1.59	13.64	8625	2.6×10 ⁻²	1.2×10 ⁻¹	-	-	7, 11, 15
MWC 480	2.1	21.9	8250	1.2×10 ⁻¹	1×10 ⁻¹	-	1.5×10 ⁻¹	1, 13, 15, 16
HD 163296	2.0	17.0	9332	8.4×10 ⁻²	1×10 ⁻¹	<6.7×10 ⁻²	1.3×10 ⁻¹	1, 13, 15, 16, 19
HD 142666	1.73	9.1	7500	7.6×10 ⁻³	3.2×10 ⁻²	-	-	4, 8, 11, 15
Ak Sco	1.2	2.4	6250	1.8×10 ⁻³	2.3×10 ⁻³	-	-	8, 11, 15

References. (1) Öberg et al. 2021b (2) Veronesi et al. 2021 (3) Andrews et al. 2018 (4) Law et al. 2022 (5) Manara et al. 2023 (6) Rosotti et al. 2020 (7) Merín et al. 2004 (8) Fairlamb et al. 2015 (9) Pegues et al. 2020 (10) Tsukagoshi et al. 2019 (11) Stapper et al. 2022 (12) Miotello et al. 2017 (13) Sierra et al. 2021 (14) Brown-Sevilla et al. 2021 (15) Stapper et al. 2024 (16) Martire et al. 2024 (17) Veronesi et al. 2021 (18) Zhang et al. 2021 (19) Kama et al. 2020

program (Öberg et al. 2021b), the total disk masses estimated from CO millimeter emission for the Herbig sample are calculated in Stapper et al. (2024) based on an extensive grid of models, as is the case of MY Lup and GW Lup from the T Tauri sample (Miotello et al. 2017). For the disks in the MAPS program (AS 209, IM Lup, GM Aur, MWC 480, HD 163296 Öberg et al. 2021b) the total disk mass calculated from dust continuum accounts for dust scattering processes and has a more accurate fitting of the thermal conditions (Sierra et al. 2021), on the other hand, the CO disk masses come from detailed thermochemical modelling of Zhang et al. (2021). Upper limits of disk mass from HD emission were also calculated using thermochemical disk models to match the non-detection threshold (Kama et al. 2020). Through the combination of N_2H^+ and $C^{18}O$ emission, thermochemi-

cal models assuming a degree of disk ionization have computed the total disk mass and expected carbon depletion (Trapman et al. 2022). Dynamical masses have been obtained for some disks, through the detection of super-keplerian motion in the outer radius of the disk rotation profile using isothermal (Veronesi et al. 2021) and thermally stratified (Martire et al. 2024) vertical disk prescriptions.

This sample has been constructed from mid-inclination disks with available $^{12}\text{CO } 2-1$ data cubes from which the surfaces have been extracted and published in previous works (Law et al. 2022, 2023b; Stapper et al. 2023; Paneque-Carreño et al. 2023). In all cases, the vertical structure from the observations is obtained following the methodology presented in Pinte et al. (2018a), where the surfaces are constrained based on the emission maxima across the molecular channel maps. All ^{12}CO surfaces for the Herbig disk sample are taken from Stapper et al. (2023), where the ALFAHOR code (Paneque-Carreño et al. 2023) is used to extract the vertical profile. For the T Tauri disks, part of the sample (AS 209, WaOph 6, IM Lup, GM Aur, Elias 2-27) is presented in Paneque-Carreño et al. (2023), also using ALFAHOR. The remainder of the T Tauri disks are published in Law et al. (2023b) using an initial version of the DISKSURF code (Teague et al. 2021b) that in some cases underestimated the vertical profiles due to contamination from the back side of the disk (Paneque-Carreño et al. 2023). In order to do a uniform analysis, the disks previously studied using DISKSURF (MY Lup, DoAr 25, LkCa 15, GW Lup, Sz 91, DM Tau) are re-analysed using the ALFAHOR, yielding comparable results but with a lower scatter. All vertical profiles from the observational sample are presented in Figures 5.A.3 and 5.A.4, compared to the vertical profiles from the fiducial DALI models of varying disk mass with ISM-like carbon abundance.

As done for the DALI models, the vertical profiles of the observational sample are processed to obtain their characteristic z/r . To accurately account for the spread in the vertical profile, z/r is calculated for the mean value and also for the lower and upper limits of the profiles, which indicate the dispersion within radial bins and will give the uncertainty on the characteristic z/r .

Based on the $z/r - M_d$ relationship shown in Figure 5.5 we estimate the expected z/r for the reported total disk mass derived from dust continuum and available HD upper limits, assuming an ISM-like carbon abundance. These values are compared against the observationally derived z/r values in Figure 5.6. For the majority of the sample, if we assume an ISM-like carbon abundance, our measured z/r is below the expected value based on the dust masses considering a gas-to-dust ratio of 100. The only exceptions are DM Tau, Elias 2-27, HD 97048 and HD 34282. Throughout the sample, the differences are more noticeable in the T Tauri systems, as Herbig systems have better agreement within the uncertainty of our method. We note that taking into consideration carbon depletion would lower the expected z/r of the literature mass measurements (see Fig. 5.5), obtaining a better agreement with the observational emission heights.

Overall, these results may indicate that the assumed gas-to-dust ratio in the systems is much lower than 100 (effectively lowering the literature estimates from the dust flux) or that our model assumptions are failing to account for a significant factor affecting the z/r value, such as the presence of carbon depletion. We favor

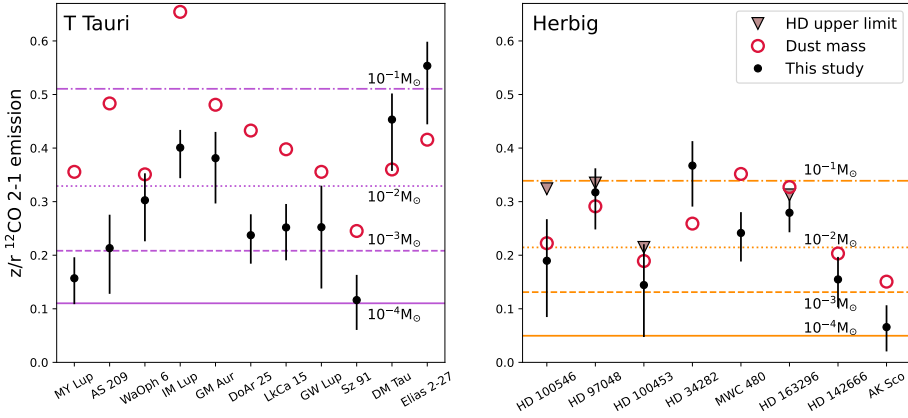


Figure 5.6: Comparison between the measured ^{12}CO surface z/r for a sample of disks and their expected values, based on literature total disk mass estimates from dust continuum observations. Black dots indicate the z/r values obtained in this study for our disk sample, open red circles trace the expected z/r values estimated from the dust continuum total disk masses and downwards triangles the expected upper limits of z/r from HD measurements. Left panel shows the results for a T Tauri system and right panel for a Herbig system. Each horizontal line indicates the z/r of our DALI models with disk masses of $10^{-4} M_{\odot}$, $10^{-3} M_{\odot}$, $10^{-2} M_{\odot}$ and $10^{-1} M_{\odot}$, in increasing z/r order respectively.

the second scenario as dust-derived masses are expected to be lower limits of the total disk mass due to the assumptions on uncertain dust properties required for their calculation and usually unaccounted for effects such as optical depth and scattering (see discussion and references in Miotello et al. 2023). Additionally, dynamical estimates of total disk mass have shown typical gas-to-dust ratios $\gtrsim 100$ (Lodato et al. 2023; Martire et al. 2024), further indicating that the total disk mass derived from dust measurements should be a lower limit to the actual value.

5.3.3 Accounting for volatile carbon depletion

The initial abundance of volatile carbon in our models will determine the amount of CO formed in each case. We have shown in the previous sections that this also has a significant effect in the extracted vertical CO surfaces, with low-carbon models producing shallower emission layers. There is independent observational motivation to assume carbon depletion for our disk sample, as measurements of CO abundance in some of the sources have shown depletion factors of 10-100 from the typically assumed ISM value of $\sim 10^{-4}$ (Zhang et al. 2019, 2021).

Figure 5.7 compares the published masses from various methods (Table 5.3) to the derived disk mass from our z/r values, calculated accounting for varying degrees of carbon depletion in the $z/r - M_d$ relationship. For disks that show a large scatter in their literature values we focus on the total disk mass extracted from the dust mass assuming a gas-to-dust ratio of 100 as main indicator of the

expected value.

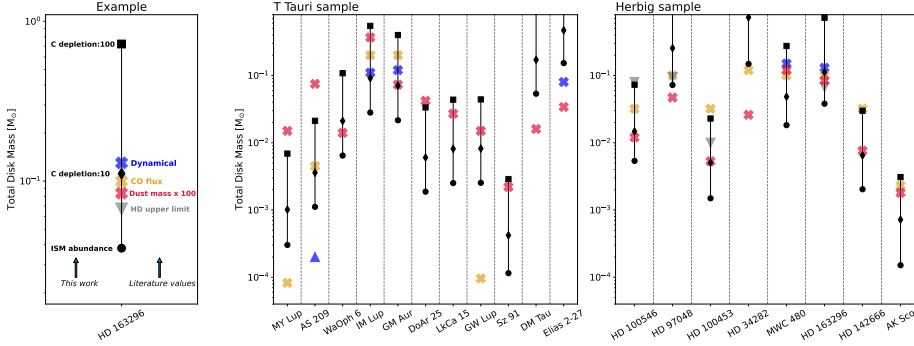


Figure 5.7: Estimated total disk masses from z/r analysis compared to literature values. Left panel shows the results for the T Tauri systems and right panel for the Herbig sources. For each disk the available literature values of the disk mass are shown in colored crosses and grey triangles for the HD upper limits. Black symbols correspond to the estimates from the characteristic z/r , where circles, diamonds and squares have been calculated using the $z/r - M_d$ relationship curves for 0, 10 and 100 values of volatile carbon depletion, respectively.

In some disks it is sufficient to consider a volatile carbon depletion of 10 to match the dust masses, however many require carbon depletion of 100 to be in agreement, particularly in the T Tauri systems. We briefly discuss here the case of HD 163296 and MWC 480, which have well constrained CO depletion profiles from optically thin C¹⁸O and C¹⁷O emission (Zhang et al. 2021). The HD 163296 literature analysis indicates an almost constant CO abundance profile, depleted by a factor 10 with respect to the ISM value beyond ~ 50 au and MWC 480 follows a similar pattern going towards even lower values of CO depletion beyond ~ 100 au (Zhang et al. 2021). Our analysis indicates that for HD 163296 a global volatile carbon depletion of ~ 10 is required to match the literature disk mass estimates to those derived from the CO z/r . For MWC 480 the preferred carbon depletion from our results ranges between 10-100, also in agreement with the spatially resolved values of Zhang et al. (2021).

For all disks, the inferred total mass we obtain from the characteristic z/r , for each carbon depletion value, are presented in Table 5.4 together with the preferred carbon depletion. The volatile carbon depletion value should be taken with caution, as it has been visually estimated based on comparison to the dust-derived total disk mass. In the optimal scenario it may be a lower limit of the disk integrated volatile carbon depletion with respect to the ISM.

Table 5.4: Studied systems, their calculated characteristic ^{12}CO z/r and associated total disk mass for various volatile carbon depletion scenarios.

Star	Characteristic $^{12}\text{CO } z/r$	Total disk mass [$\log(M_{\odot})$]			Preferred carbon depletion
		ISM C abundance	C depletion: 10	C depletion: 100	
T Tauri Disks					
MY Lup	$0.16^{+0.03}_{-0.05}$	$-3.52^{+0.38}_{-0.48}$	$-2.99^{+0.37}_{-0.44}$	$-2.16^{+0.33}_{-0.44}$	100
AS 209	$0.21^{+0.05}_{-0.08}$	$-2.95^{+0.53}_{-0.85}$	$-2.45^{+0.55}_{-0.81}$	$-1.67^{+0.49}_{-0.74}$	-
WaOph 6	$0.30^{+0.05}_{-0.07}$	$-2.19^{+0.34}_{-0.63}$	$-1.67^{+0.35}_{-0.64}$	$-0.97^{+0.36}_{-0.59}$	10
IM Lup	$0.40^{+0.03}_{-0.05}$	$-1.55^{+0.17}_{-0.34}$	$-1.02^{+0.18}_{-0.35}$	$-0.26^{+0.21}_{-0.39}$	10-100
GM Aur	$0.38^{+0.05}_{-0.08}$	$-1.67^{+0.27}_{-0.56}$	$-1.13^{+0.27}_{-0.57}$	$-0.40^{+0.32}_{-0.6}$	10
DoAr 25	$0.24^{+0.03}_{-0.05}$	$-2.73^{+0.32}_{-0.50}$	$-2.22^{+0.33}_{-0.49}$	$-1.48^{+0.30}_{-0.43}$	100
LkCa 15	$0.25^{+0.04}_{-0.06}$	$-2.60^{+0.34}_{-0.56}$	$-2.09^{+0.35}_{-0.56}$	$-1.36^{+0.33}_{-0.49}$	100
GW Lup	$0.25^{+0.08}_{-0.11}$	$-2.60^{+0.59}_{-1.1}$	$-2.09^{+0.6}_{-1.08}$	$-1.36^{+0.58}_{-0.96}$	10-100
Sz 91	$0.12^{+0.04}_{-0.06}$	$-3.94^{+0.47}_{-0.52}$	$-3.38^{+0.43}_{-0.46}$	$-2.54^{+0.42}_{-0.55}$	100
DM Tau	$0.45^{+0.05}_{-0.09}$	$-1.27^{+0.22}_{-0.53}$	$-0.73^{+0.23}_{-0.54}$	-	0
Elias 2-27	$0.55^{+0.05}_{-0.09}$	$-0.82^{+0.17}_{-0.49}$	$-0.27^{+0.17}_{-0.50}$	-	0
Herbig Disks					
HD 100546	$0.19^{+0.08}_{-0.1}$	$-2.27^{+0.74}_{-1.31}$	$-1.83^{+0.76}_{-1.09}$	$-1.14^{+0.84}_{-1.15}$	10
HD 97048	$0.32^{+0.04}_{-0.07}$	$-1.14^{+0.27}_{-0.52}$	$-0.57^{+0.41}_{-0.66}$	-	0
HD 100453	$0.14^{+0.08}_{-0.09}$	$-2.83^{+0.87}_{-1.18}$	$-2.30^{+0.76}_{-1.03}$	$-1.64^{+0.83}_{-1.06}$	10
HD 34282	$0.37^{+0.04}_{-0.08}$	$-0.83^{+0.24}_{-0.49}$	-	-	0
MWC 480	$0.24^{+0.04}_{-0.05}$	$-1.74^{+0.32}_{-0.53}$	$-1.31^{+0.37}_{-0.52}$	$-0.56^{+0.41}_{-0.57}$	10-100
HD 163296	$0.28^{+0.02}_{-0.04}$	$-1.42^{+0.18}_{-0.29}$	$-0.94^{+0.23}_{-0.34}$	$-0.14^{+0.14}_{-0.39}$	10
HD 142666	$0.15^{+0.05}_{-0.05}$	$-2.69^{+0.48}_{-0.65}$	$-2.19^{+0.42}_{-0.53}$	$-1.52^{+0.45}_{-0.56}$	10-100
Ak Sco	$0.07^{+0.03}_{-0.05}$	$-3.82^{+0.48}_{-0.46}$	$-3.14^{+0.43}_{-0.49}$	$-2.51^{+0.43}_{-0.48}$	100

5.4 Discussion

5.5 Discussion

5.5.1 Low gas-to-dust or high carbon depletion?

It has been previously discussed in the literature that current CO gas models compared to observations do not allow us to distinguish between a low gas-to-dust system (lower gas mass than dust-derived total disk mass) or a high volatile carbon depletion scenario (Miotello et al. 2017; Calahan et al. 2021). Our results are in agreement with this entanglement, however we favor the high carbon depletion over low gas-to-dust due to evidence for CO abundance evolution over time in young stars (Bergner et al. 2020; Zhang et al. 2020), measurements of CO depletion in sources from our sample (Zhang et al. 2019, 2021) and results from dynamical

mass estimates that indicate gas-to-dust ratios $\gtrsim 100$ (Martire et al. 2024) rather than much less than 100.

As discussed in Miotello et al. (2023), various methods can yield orders of magnitude differences in the calculated disk mass. This is particularly apparent for the literature total disk mass values of T Tauri systems MY Lup and GW Lup. For these disks our analysis indicates that a high carbon depletion of ~ 100 is needed to reach the reported dust-derived mass value, but the reported gas mass, which is several (~ 2) orders of magnitude lower in both cases, was extracted without accounting for carbon depletion (Miotello et al. 2017). It is therefore likely that a higher carbon depletion rate would put all values in agreement, an alternative that was suggested by Miotello et al. (2017) to account for the low gas-to-dust ratios that the measurement would otherwise entail.

We note that for the Herbig sample, the gas mass estimates used in this work were mostly obtained from DALI models of isotopologue CO emission (Stapper et al. 2024), measuring the fluxes and disk radii in these tracers. These models assumed an ISM volatile carbon abundance, with a parameter space similar to our models, however they obtain mass values higher than the dust-based masses, consistent with a gas-to-dust ratio $\gtrsim 100$ (see right panel of Figure 5.7). We are confident that carbon depletion must happen at least for MWC 480 and HD 163296, as it has been measured independently through dedicated models and observations (Zhang et al. 2021). HD 100546 also has estimates of volatile carbon depletion between 2-10, consistent with our results (Bruderer et al. 2012; Kama et al. 2016). The overall discrepancy between our work and analysis using models of CO isotopologue fluxes is the consideration of hydrostatic equilibrium in our models. We show in Figure 5.B.1 that for high disk masses, when the gas emission becomes optically thick, not accounting for hydrostatic equilibrium can underestimate the CO flux, therefore overestimating the calculated disk masses. Due to the optical depth, the use of model fluxes in the high disk mass regime also leads to large uncertainties of up to an order in magnitude in the calculated mass, which also affects the comparison (Miotello et al. 2017; Stapper et al. 2024). Overall, this highlights the sensitivity of vertical surfaces as a probe for total disk mass and volatile carbon depletion.

5.5.2 Synergy with other methods

Using our $z/r - M_d$ relationships can be useful to have an initial idea on the system properties, contrary to other methods, we are able to utilize a bright and readily detected molecule to have a first-order joint constraint of disk mass and carbon abundance. Indeed, if the calculated z/r is ≥ 0.3 then the total disk mass is $\geq 10^{-2} M_\odot$. For lower z/r , the uncertainty on the carbon abundance creates a span of several orders of magnitude in the total disk mass value. However, if gas-to-dust ratio of at least 100 is assumed, which is reasonable from accretion rate values that point towards gas-rich disks (Manara et al. 2016, 2023) and dynamical mass estimates (Lodato et al. 2019; Martire et al. 2024), this work has shown that the total mass calculated from the dust continuum flux may be used as an anchor to estimate the lower limit of carbon depletion (see section 3.3).

Combining the information from CO surfaces with dynamical mass estimates, as has been done for a small sample in this work would put strong constraints on the overall carbon depletion. Furthermore, the use of rarer CO isotopologues and C-abundance-sensitive tracers such as N_2H^+ has demonstrated to be a good tool to discern between the effects of varying disk mass and volatile carbon depletion (Anderson et al. 2019, 2022; Trapman et al. 2022). N_2H^+ models have the uncertainty of the disk ionization rate and complication of relying on a fainter molecular line, however in combination with measurements of the CO vertical profile it could be possible to determine all three parameters, key for understanding protoplanetary disk conditions. We highlight that our results for DM Tau and GM Aur using the CO surface and dust-derived disk masses are in great agreement with the total disk mass and carbon depletion values determined in Trapman et al. (2022) through N_2H^+ and C^{18}O flux analysis.

5.5.3 Caveats and future perspectives

While exciting and very useful for an initial overview of the disk conditions, there are a few caveats to our results. In particular, the studied models have been developed using a full-disk prescription, a standard radial density profile and a single disk-integrated volatile carbon depletion value. However observations show disks with a plethora of substructure (e.g. Andrews et al. 2018; Andrews 2020; Long et al. 2019) and that CO abundance profiles varies radially (Zhang et al. 2019, 2021). Highly structured or transition disks such as AS 209 and LkCa 15 are likely not accurately represented by our models. Future work, beyond the scope of this paper, will test the effect of large cavities and other substructure on the vertical profile and z/r - M_d relationship.

We note that emission surfaces obtained at high enough spatial resolution may give direct information on the surface density profile, allowing for a more accurate description of the material distribution without the need to use a characteristic z/r (see for example, Paneque-Carreño et al. 2023). Through this approach, the total disk mass may be more accurately determined and scaled depending on the carbon abundance in a source-by-source analysis, without the uncertainties of general models.

Most importantly, future work must focus on different molecular tracers, such as rarer CO isotopologues and bright optically thin molecules, for example CN and C_2H , that have been proposed to be sensitive tracers of the upper disk regions (Cazzoletti et al. 2018; Bergin et al. 2016; Paneque-Carreño et al. 2021, 2024). Our results in this work are only applicable to the CO emitting layer, however it is likely that tracing the vertical structure with other molecular species will give direct insight into varied ongoing disk processes.

5.6 Conclusions

In this work we have presented a z/r - M_d relationship, linking the vertical extent of CO 2 – 1 to the disk mass and volatile carbon abundance. This was done through

the study of thermochemical DALI models, computed accounting for hydrostatic equilibrium. Our models tested the effect of various stellar and disk parameters on the vertical structure and our theoretical predictions were benchmarked on a set of observations. The main findings and conclusions are the following:

1. We determine that for T Tauri and Herbig systems, the total disk mass and volatile carbon abundance are the main parameters that set the location of the CO 2 – 1 emission surface. This surface can be characterized by a constant characteristic z/r tracing the rising portion of the vertical profile.
2. The z/r - M_d relationship for T Tauri systems is different than that of disks around Herbig stars. For the same disk mass and assumed volatile carbon abundance, material around T Tauri stars extends further vertically, as expected due to the difference in the stellar masses and gravitational potential.
3. Using the total disk masses inferred from continuum dust observations (assuming a gas-to-dust ratio of 100) we are able to calibrate the z/r - M_d relationship for each individual system and estimate the order of magnitude of carbon depletion.
4. Fifteen out of the nineteen studied systems (79%) show indicators of volatile carbon depletion (compared to the ISM abundance). For disks with previous constraints on their carbon abundance, our results yield comparable values. T Tauri disks seem to be more carbon depleted than Herbig systems.

Overall, this study has demonstrated the utility of a bright and readily-detected molecular tracer, CO 2–1, that may be used to probe two of the most fundamental disk parameters through its vertical extent: total disk mass and carbon abundance. As the sample of disks with high resolution data grows, studies of vertical layering in mid-inclination disks will be used to deepen our understanding not only on the thermal and density conditions, but also on the amount and composition of the materials available for planet formation.

Appendix

5.A Full emission surfaces from models and observational sample

In the main text our results are expressed in z/r . For visual comparison, here we show the full vertical profiles extracted for the CO emission surfaces in models and observations. Figures 5.A.1 and 5.A.2 show the emission surfaces tracing the $\tau = 1$ layer, as extracted from the DALI model output of the fiducial models and models varying specific parameters (see Table 5.2 for details).

Figures 5.A.3 and 5.A.4 display the emission surfaces extracted from the CO channel map emission of each disk using ALFAHOR (Paneque-Carreño et al. 2023; Stapper et al. 2023). For comparison, the location of the $\tau = 1$ layer from the

fiducial models using $R_c = 100$ au of each sampled disk mass are plotted in each panel.

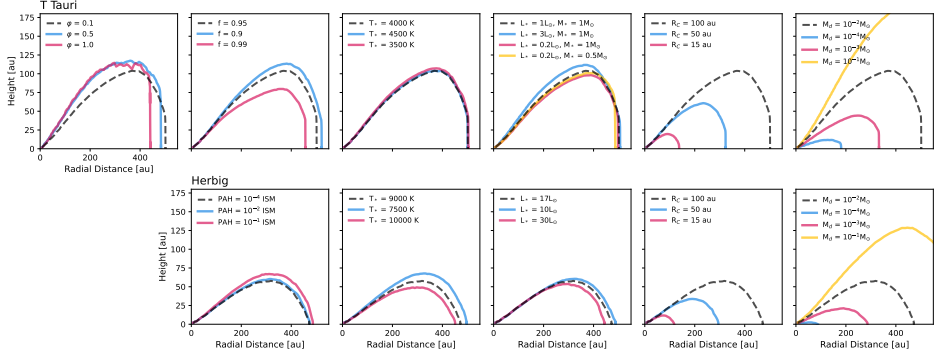


Figure 5.A.1: Vertical profiles tracing $\tau = 1$ layer of the DALI model grid for $M_{\text{disk}} = 10^{-2} M_{\odot}$. Top row shows the sampled parameters for the T Tauri systems and bottom row for Herbig. In each panel the black dashed line corresponds to the fiducial model and only one parameter is varied, as indicated by the legend and colors.

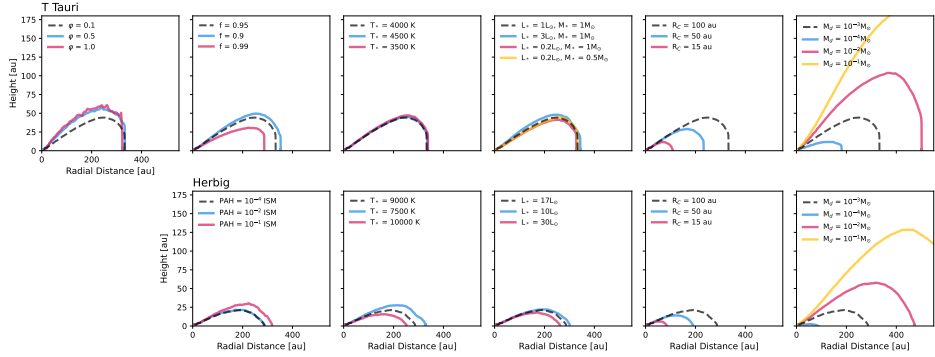


Figure 5.A.2: Same as Figure 5.A.1 but for fiducial model with $M_{\text{disk}} = 10^{-3} M_{\odot}$.

5.B CO isotopologue model fluxes using hydrostatic equilibrium solver

When using the hydrostatic equilibrium solver in DALI, the disk density converges to a physical structure given by the equilibrium between the stellar gravitational potential and the thermal structure. The disk integrated fluxes may vary when comparing the hydrostatic equilibrium output to the models with static gaussian distributions. For optically thin emission in low-mass disks, the fluxes will be larger in the static models, which means the disk masses will be underestimated in

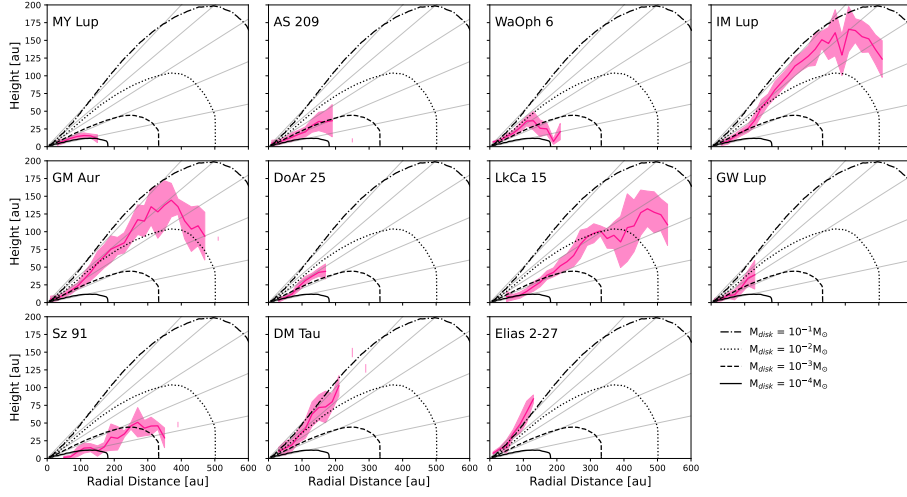


Figure 5.A.3: Observational CO emission surfaces for the T Tauri disk sample. Magenta lines indicate the observational results and data vertical dispersion, black lines show the $\tau = 1$ layer from the fiducial DALI models using $R_c = 100$ au for different disk masses indicated by different line styles. Grey lines mark constant z/r surfaces of 0.1, 0.2, 0.3, 0.4 and 0.5.

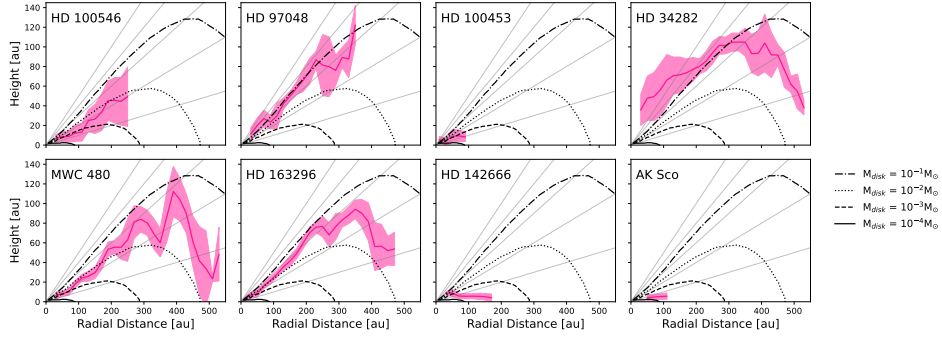


Figure 5.A.4: Same as Figure 5.A.3, but for the Herbig sample and models.

comparison to those obtained from model fluxes when hydrostatic equilibrium is considered. In the case of high-mass disks the reverse happens, the static gaussian models underestimate the fluxes, therefore overestimate the disk masses.

Figure 5.B.1 shows this effect displaying the total flux difference and percentual variation. This flux variation explains the generally higher masses of Stapper et al. (2024) and the lower masses obtained by Miotello et al. (2017) for MY Lup and GW Lup compared to our mass values assuming an ISM carbon abundance (see Fig. 5.7).

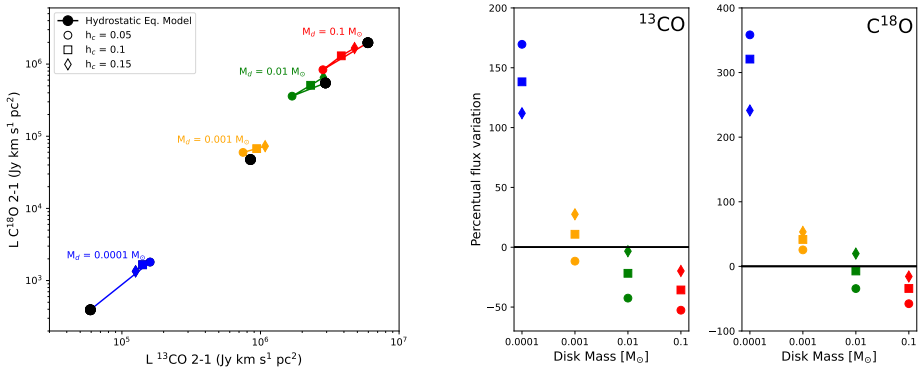


Figure 5.B.1: Comparison of retrieved fluxes from DALI models when using hydrostatic equilibrium and not. Left panel shows the ^{13}CO and C^{18}O emission fluxes, black dots corresponds to models obtained after iterating and solving the hydrostatic equilibrium equations. Colored dots show the fluxes from models with a single iteration using a static gaussian material distribution. Right two panels display the percentual variation of the model flux from the static models compared to the one which uses hydrostatic equilibrium to determine its thermal and density structure.

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Nederlandse samenvatting

In het noorden van Chili biedt de Atacama-woestijn, door de natuurlijke omstandigheden op die plek en de isolatie van de buitenwereld, een unieke mogelijkheid om het universum te observeren. Gedurende vele eeuwen keken de lokale inheemse volken, die in hun taal *Lickan Antay* worden genoemd en in het huidige Spaans *Atacameños*, naar de sterrenhemel en concentreerden zich niet alleen op de heldere sterren maar ook op de donkere gebieden die contrasteerden met de heldere achtergrond. We weten nu dat deze regio's donker zijn omdat kleine stofdeeltjes het zichtbare sterlicht absorberen en dat deze donkere wolken worden geassocieerd met stervormingsgebieden. Terwijl onze ogen niet in staat zijn om door het stof te kijken, kunnen instrumenten zoals de Atacama Large Millimeter/submillimeter Array (ALMA) hun geheimen onthullen. ALMA is gebouwd op het Chajnantor-plateau, een heilige plaats voor de *Lickan Antay* in de Atacama-woestijn, wat “plaats van vertrek” betekent in hun taal. Het is een van de belangrijkste wetenschappelijke doelen van ALMA, gelegen op een hoogte van 5000 meter, om deze donkere en koude gebieden te onderzoeken om de processen te begrijpen die leiden tot ster- en planeetvorming.

De analyse en resultaten die gepresenteerd worden in dit proefschrift zijn mogelijk gemaakt door de capaciteiten van ALMA, die sinds het begin van de waarnemingen in 2013 hebben gezorgd voor een revolutie in het veld van planeetvorming. Door waarnemingen en theoretische voorspellingen van het universum op (sub-)millimetergolflengtes hebben we de unieke kans om terug te kijken naar onze oorsprong. Hoe is de aarde gevormd? Zien andere planetenstelsels er vergelijkbaar uit? Wat zijn de belangrijkste processen in deze eerste periodes?

Ster- en planeetvorming

Het proces van planeetvorming is intrinsiek verbonden met stervorming. Eerst vormen sterren uit het inkrimpende materiaal van een moleculaire wolk die samen trekt tot een prestellaire kern. Van kern naar planetenstelsel worden jonge sterren (YSO's) ingedeeld in Klassen (0, I, II of III). In de vroegste Klasse 0/I-fase zal een protoster actief materiaal accumuleren uit zijn omringend protostellair omhulsel, waarna, door behoud van hoekmoment, het binnenvallende materiaal zich zal verspreiden in de vorm van een draaiende, schijfvachtige structuur rond de protos-

ter. Deze schijven worden protoplanetaire of planeetvormende schijven genoemd, omdat ze de geboorteplaatsen en het materiaalreservoir zijn van planetenstelsels.

De Klasse II protoplanetaire schijffase duurt 1-10 miljoen jaar en eindigt wanneer het meeste van het schijfmateriaal ofwel op de ster is gevallen, ofwel planeten heeft gevormd ofwel is verspreid, waarna een Klasse III planetenstelsel wordt onthuld. Dit proefschrift richt zich op de protoplanetaire schijffase, waar het planeetvormende materiaal met hoge resolutie kan worden waargenomen op (sub-)millimetergolflengten.

Protoplanetaire schijven

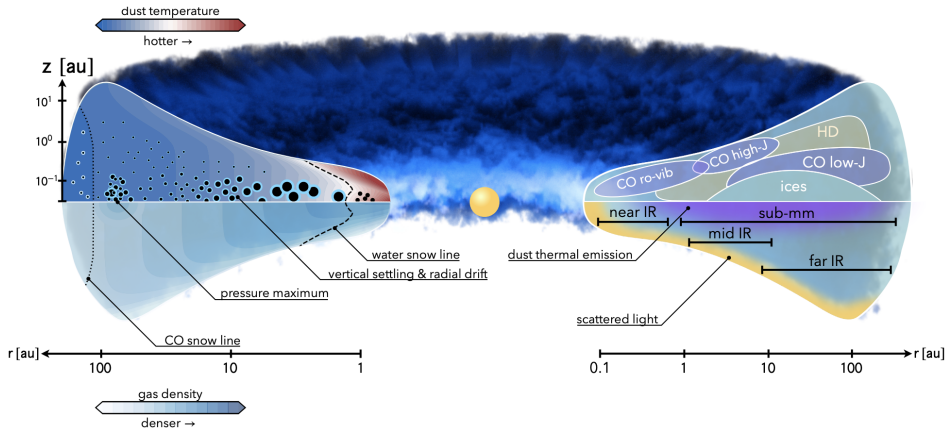
Net als de wolk waaruit ze geboren zijn, zijn protoplanetaire schijven gasrijke structuren met vaste deeltjes (stof) die slechts enkele procenten van hun massa uitmaken. Het grootste deel van het gasvormige schijfmateriaal is moleculair waterstof (H_2), maar de emissie hiervan is extreem zwak en ontoegankelijk met de huidige telescopen. Koolmonoxide (CO) is na H_2 het meest voorkomende molecuul en wordt vaak gedetecteerd, waardoor het veelvuldig gebruikt wordt om het gasreservoir te bestuderen. Andere moleculen in de gasfase die vaak zijn waargenomen in protoplanetaire schijven zijn: CN , HCN , H_2CO , CS , HCO^+ , N_2H^+ , H_2O en C_2H .

Figuur 6 toont de radiële en verticale materiaalverdeling binnen een schijf, samen met de belangrijkste kenmerken en processen. Radieel gezien wordt de schijf verdeeld tussen een heet binnendeel ($<20\text{au}$) en koude buitengebieden. ALMA waarnemingen kunnen de buitenste delen van de schijf zien met een ruimtelijke resolutie van enkele astronomische eenheden. Het begrijpen van de morfologie, eigenschappen en dynamiek van eventuele radiële, azimutale of verticale structuren is een belangrijk doel van planeetvormingsstudies om de heersende processen direct te onderzoeken.

De hoogte van de schijf wordt bepaald door hydrostatisch evenwicht. Dit betekent dat de balans tussen de zwaartekracht van de ster en de thermische ondersteuning van het materiaal hun verticale verdeling zal vormgeven. Daarom bevat de verticale verdeling van protoplanetaire schijven informatie over belangrijke fysische eigenschappen zoals de thermische- en dichtheidsstructuur. De verticale structuur kan ook gebruikt worden om de ionisatiestructuur en de aanwezigheid van hydrodynamische instabiliteiten en winden vast te stellen. Het waarnemen van de verticale dimensie in een groot aantal schijven is echter pas de afgelopen jaren mogelijk geworden en, in het bijzonder, door de resultaten van dit proefschrift.

Het bestuderen van de verticale schijfstructuur

Of de verticale dimensie van protoplanetaire schijven met ALMA te zien is, hangt af van de inclinatiehoek waaronder de schijf vanaf de aarde wordt bekeken. Er zijn twee extreme gevallen; 1) schijven met grote inclinaties ($\gtrsim 75^\circ$) en 2) schijven met kleine inclinaties ($\lesssim 35^\circ$). In deze beide gevallen kunnen slechts twee dimensies worden bekeken: voor schijven met grote inclinatie de verticale en radiële, voor schijven met kleine inclinatie de radiële en azimutale. De rest van

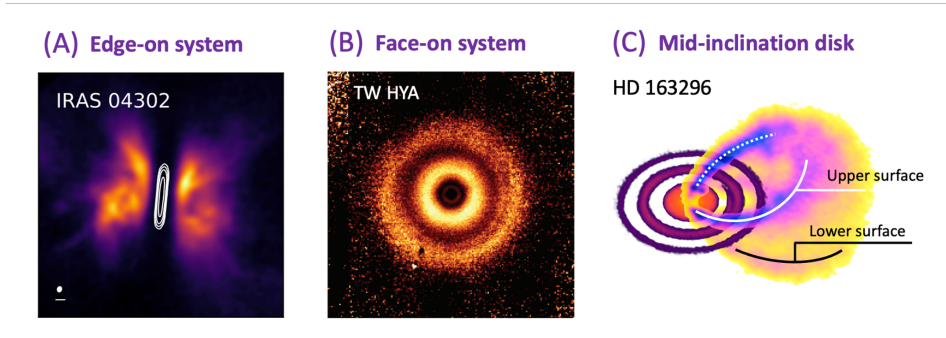


Figuur 1: Deze illustratie van Miotello et al. (2023) geeft de emissiegebieden, relevante schalen, stoftemperatuur en gasdichtheid in protoplanetaire schijven aan. De linkerkant toont de verdeling van stofdeeltjes als zwarte cirkels met verschillende groottes waarbij de grote cirkels grotere stofdeeltjes voorstellen. De rechterkant toont een vereenvoudigd beeld van de moleculaire gelaagdheid voor de belangrijkste moleculen in de gasfase. Onderin worden de gebieden waar warmtestraling en verstrooid licht vandaan komen aangegeven in paars en geel.

de protoplanetaire schijven met waargenomen inclinaties tussen $\sim 35\text{--}70^\circ$ worden geclassificeerd als schijven met een gemiddelde inclinatie. Ons werk richt zich op deze bronnen, omdat ze een nauwkeurige weergave van de lopende processen in hun volledige driedimensionale structuur mogelijk maken, inclusief de verticale as. Figuur 4 toont elk van de inclinatiescenario's.

In schijven met gemiddelde inclinatie die door ALMA worden waargenomen, kan de verticale dimensie direct worden onderzocht via de emissiekaarten door de emissiemaxima te volgen, zoals weergegeven in het rechter paneel van Figuur 4. Deze methode is gevoelig voor eventuele substructuren of asymmetrieën die aanwezig kunnen zijn en is geïmplementeerd in algoritmes zoals ALFAHOR dat publiek beschikbaar is (zie Hoofdstuk 3 van dit proefschrift).

De directe toepassingen van het meten van de verticale moleculaire lagen in protoplanetaire schijven zijn talrijk, afhankelijk van de geselecteerde moleculen, de resolutie en de beschikbare informatie uit eventuele radiële of azimutale structuren. De temperatuurstructuur kan worden getraceerd door de piek van de helderheidstemperatuur van de CO-isotopologen, wat sterke beperkingen oplegt aan het ijken van thermochemische modellen en nauwkeurige temperatuurmetingen, die cruciaal zijn voor het bepalen van de turbulentie (zie Hoofdstuk 4 van dit proefschrift voor een toepassing). Als ruimtelijk opgeloste snelheidsinformatie beschikbaar is, kunnen recent ontwikkelde methoden de radiële, azimutale en verticale richtingen van de snelheid van het materiaal onderscheiden. In combinatie met metingen van de locatie van de verticale emissieoppervlakken kan de aanwezigheid van meridionale stromen of schijfwinden direct bepaald en getest worden, iets wat cruciaal is voor



Figuur 2: Drie protoplanetaire schijven met verschillende kijkhoeken. Voor IRAS 04302 (grote inclinatie) laten de kleuren de verdeling van de kleine stofkorrels, die goed gekoppeld zijn aan het gas, zien terwijl de witte contouren de mm-continuüm straling van het stof tonen (van't Hoff et al. 2020). De TW Hya schijf (kleine inclinatie) wordt waargenomen in ALMA mm-continuüm (Andrews 2020). De HD 163296 schijf (gemiddelde inclinatie) toont stof ringen in ALMA mm-continuüm waarnemingen die het middenvlak van de schijf traceren terwijl een kaart van het CO gas op één specifieke snelheid de bovenste en onderste emissieoppervlakken laat zien die zich verticaal uitstrekken.

het begrijpen van schijfdynamica. Recent zijn de eerste onderzoeken uitgevoerd om de hoogte en eigenschappen van het hete bestraalde schijfoppervlak te bepalen met behulp van atomaire koolstof.

Dit proefschrift

Aangezien het karakteriseren van de verticale structuur van protoplanetaire schijven belangrijk is om de omstandigheden en belangrijkste processen van planeetvorming beter te begrijpen, presenteert dit proefschrift een diepgaande analyse van zowel waarnemingen als de theoretische aspecten van de verticale dimensie. Hieronder volgt een overzicht van de hoofdstukken en conclusies van dit werk,

Hoofdstuk 2: Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk. We analyseren CN $N = 3 - 2$ ALMA data in twee verschillende overgangen en vergelijken dit met de emissie van CO-isotopologen. Onze resultaten tonen aan dat de verticale locatie van CN en CO in Elias 2-27 gelaagd is en consistent is met de voorspellingen van thermochemische modellen. De gemeten CN-kolomdichtheid, lage optische diepte ($\tau \leq 1$) en de locatie nabij het schijfoppervlak komen overeen met thermochemische modellen voor schijven waar de vorming van CN wordt geïnitieerd door de reactie van N met UV-gepompt H_2 . Deze studie benadrukt het belang van het traceren van de verticale locatie van verschillende moleculen om de fysische schijfomstandigheden te bepalen.

Hoofdstuk 3: Directly tracing the vertical stratification of molecules in protoplanetary disks. De ALFAHOR-code wordt gepresenteerd. Dit is een implementatie van de Pinte et al. (2018a) methode en leidt tot nauwkeurige verticale

profielen, zelfs voor moleculen met een lage signaal-ruisverhouding, met behulp van interactief maskeren van emissiekaarten. Met behulp van ALFAHOR bestuderen we de moleculaire emissieoppervlakken in Elias 2-27, WaOph 6 en de vijf bronnen van het MAPS ALMA Large Program. De temperatuurstructuur, karakteristieke hoogte door de gasdruk, substructuren en modulaties in de verticale profielen en relaties met de chemische oorsprong van elk waargenomen molecuul worden besproken. Over het geheel genomen tonen we aan dat het mogelijk is de verticale locaties van meerdere moleculaire soorten te traceren en deze informatie te relateren aan een breed scala van fysische en chemische eigenschappen van de schijf.

Hoofdstuk 4: High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C₂H emission. Het bepalen van turbulentie in schijven is cruciaal voor het begrijpen van de evolutie van schijven, maar metingen van turbulentie vereisen kennis van de thermische omstandigheden die invloed hebben op de moleculaire emissie. Door de informatie over de ruimtelijk opgeloste temperatuurstructuur te combineren met de informatie die kan worden verkregen uit de analyse van de verticale structuur, presenteren we een nieuwe manier om direct turbulentie te meten. Deze methode is geijkt met behulp van CN en C₂H moleculaire emissie van de protoplanetaire schijf rond IM Lup. Onze analyse toont hoge turbulentie van Mach 0.4-0.6 aan bij $z/r \sim 0.25$. Deze studie presenteert het eerste empirische bewijs voor een verticale gradiënt in de schijfturbulentie, wat een belangrijke voorspelling is van magneto-rotatie instabiliteiten.

Hoofdstuk 5: Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion. Met behulp van thermochemische modellen bestuderen we de eigenschappen van protoplanetaire schijven en hun jonge sterren die het meeste invloed hebben op de verticale locatie van CO $J = 2 - 1$ emissieoppervlakken. De voorspellingen van de modellen worden geijkt met behulp van de gegevens van CO-emissie van negentien schijven. We vinden dat het CO-emissieoppervlak het meest wordt beïnvloed door de totale schijfmassa (M_d) en de hoeveelheid vluchtig koolstof, wat leidt tot een z/r - M_d relatie. Om de schattingen van de totale schijfmassa op basis van de karakteristieke z/r in overeenstemming te brengen met de waarden die zijn verkregen op basis van analyse van het stofcontinuüm, is een koolstofdepletie van 10-100 (ten opzichte van het ISM) nodig voor het grootste gedeelte van de bronnen.

Toekomstperspectief

Studies van verticale schijfstructuur in grote getalen bevinden zich in een vroeg stadium. Tot op heden zijn van slechts ~ 20 schijven verticale CO-oppervlakken gekarakteriseerd en slechts ~ 8 schijven (Paneque-Carreño et al. 2023; Law et al. 2024) hebben gemeten verticale profielen van meer dan drie verschillende moleculen. Het algehele werk in dit proefschrift heeft aangetoond dat het mogelijk is om ALMA-waarnemingen te gebruiken om de verticale moleculaire gelaagdheid te

bestuderen en deze te relateren aan een aantal fysische processen.

Toekomstig werk moet zich richten op het uitbreiden van het aantal schijven waarin de moleculaire oppervlakken gekarakteriseerd zijn en het combineren van de chemische informatie met kennis over de verdeling van stofkorrels om schijfprocessen nauwkeurig te karakteriseren. Dit vereist waarnemingen op hoge ruimtelijke en spectrale resolutie van moleculen anders dan CO, wat doorgaans tijdrovend is vanwege de lage signaal-ruisverhouding van zeldzamere moleculen. De aankomende ALMA Wideband Sensitivity Upgrade in het volgende decennium zal ons in staat stellen deze studies in minder tijd en voor grotere groepen schijven uit te voeren.

Over het geheel genomen biedt de mogelijkheid om de materiaalverdeling van protoplanetaire schijven in alle drie de dimensies te bestuderen unieke inzichten in het proces van planeetvorming. Observationele studies halen nu de theoretische modellen in, die moeten worden herzien om de totaliteit van waargenomen kenmerken te verklaren. Op dezelfde manier als studies zich de afgelopen jaren hebben gericht op het verklaren van het bestaan van radiële en azimutale substructuren, moeten we nu naar de derde dimensie kijken en de informatie begrijpen die daaruit voortkomt. De technieken en resultaten van dit proefschrift hebben de basis gelegd voor veel toekomstige studies die zeker de vragen zullen beantwoorden die we nu open laten.

English summary

In the north of Chile, due to its natural conditions and isolation, the Atacama desert is a unique window to observe the universe. For many centuries the local native indigenous groups, called in their language *Lickan Antay* and in current spanish *Atacameños*, looked up at the universe and focused not only on the bright stars, but on the dark areas that contrasted against the glow. We now know that these regions are dark because small dust grains absorb the starlight at optical frequencies and that these dark clouds are associated with star-forming regions. While our eyes are not able to see past the dust, instruments such as the Atacama Large Millimeter/submillimeter Array can reveal their secrets. ALMA is built on the Chajnantor plateau, a sacred place for the *Lickan Antay* in the Atacama desert, that means “place of departure” in their language. Located at an altitude of 5000 meters, one of the main science goals of ALMA is to look into these dark and cold regions to understand the processes that lead to star and planet formation.

The analysis and results presented in this thesis have been possible due to the capabilities of ALMA, that since the start of its operations in 2013 has revolutionized the view of planet formation. Through observations and theoretical understanding of the universe as traced at (sub-)millimeter wavelengths we have the unique opportunity to look back towards our origins. How did the earth form? May other planetary systems have similar conditions? What are the key processes that govern the initial epochs?

Star and planet formation

The process of planet formation is intrinsically linked to stellar formation. First, stars form from the collapsing material of molecular clouds that contracts into a pre-stellar core. From core to planetary system, young stellar objects (YSOs) are classified into Classes (0, I, II or III). In the earliest Class 0/I stage, a protostar will be actively accreting material from its surrounding protostellar envelope, then, due to conservation of angular momentum, the infalling material will spread out to form a rotating disk-like structure around the protostellar system. These disks are named protoplanetary or planet-forming disks, as they are the birthplaces and host the material reservoir of planetary systems.

The Class II protoplanetary disk stage lasts ~ 1 -10 million years and ends when

most of the disk material has either accreted onto the star, formed planets or dispersed, after which a Class III planetary system is revealed. This thesis focuses on the protoplanetary disk phase, where the primordial planet-forming material can be observed at high resolution (sub-)millimeter wavelengths.

Protoplanetary disks

Like their parent clouds, protoplanetary disks are gas-rich structures with solid particles (dust) that account for only a few percent of their mass. The bulk of the gaseous disk material is molecular hydrogen (H_2), however its emission is extremely faint and inaccessible with current telescopes. Carbon monoxide (CO) is the second most abundant molecule after H_2 and frequently detected, making it the preferred probe of the material reservoir. Other gas tracers commonly observed in protoplanetary disks are; CN , HCN , H_2CO , CS , HCO^+ , N_2H^+ , H_2O and C_2H .

Figure 6 presents the radial and vertical material distribution within a disk, together with the main features and ongoing processes. Radially, the disk is divided between a hot inner disk (<20 au) and a cold outer disk. ALMA observations can access the outer disk at a spatial resolution of a few astronomical units. Understanding the morphology, properties and dynamics of any radial, azimuthal or vertical substructures is a key goal of planet-formation studies in order to directly probe ongoing processes.

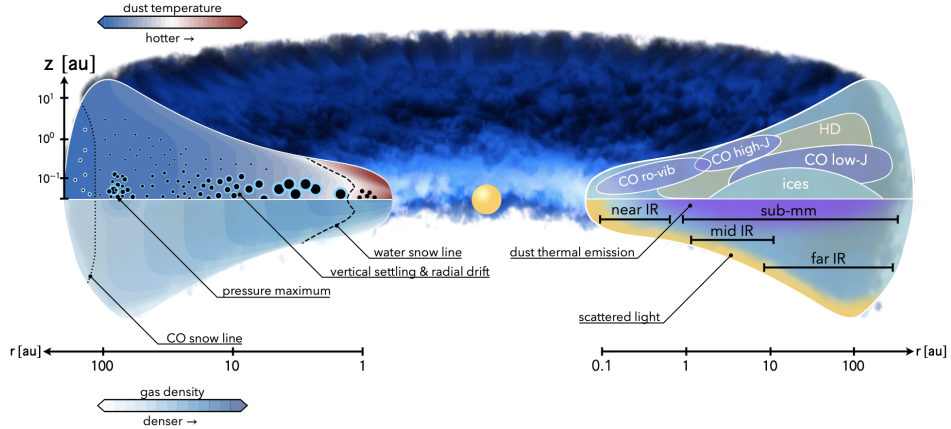


Figure 3: Illustration from Miotello et al. (2023) indicating the emission regions, relevant scales, dust temperature and gas density structure in protoplanetary disks. Left side shows the distribution of dust particles in black circles with different sizes represented as symbol size. Right side presents a simplified view of the molecular layering for the main gas-phase molecules. In the bottom the dust thermal and scattered light emission regions are highlighted in purple and yellow.

In their vertical dimensions, disks have an extent that is set by hydrostatic equilibrium. This means that the balance between the gravitational potential of the star and thermal support of the material will shape their vertical distribution.

Therefore, the vertical distribution of protoplanetary disks contains information on key physical properties such as the thermal and density structure. Vertical structure may also be used as a probe for the ionisation field and the presence of hydrodynamical instabilities and winds. However, observationally probing the vertical dimension in large disk samples has only been possible over the past few years and, in particular, through the results of this thesis.

Studying the disk vertical structure

Accessing the vertical dimension of protoplanetary disks with ALMA will depend on the inclination angle at which the disk is viewed from earth. There are two extreme cases; 1) edge-on disks with high inclinations ($\gtrsim 75^\circ$) and 2) face-on disks at low inclinations ($\lesssim 35^\circ$). In both cases only two dimensions can be accessed, for edge-on disks the vertical and radial, for face-on disks the radial and azimuthal. The remainder of the protoplanetary disk sample, with observed inclinations between ~ 35 - 70° are classified as mid-inclination disks. Our work focuses on these sources, as they allow for an accurate representation of the ongoing processes throughout their whole three-dimensional structure, including the vertical axis. Figure 4 shows each of the inclination scenarios.

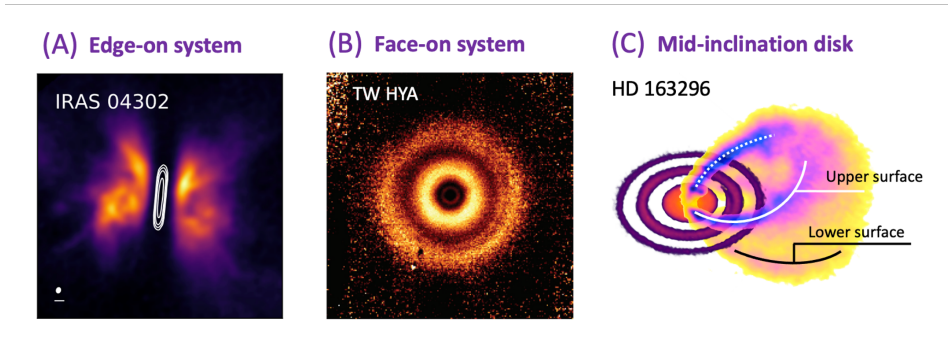


Figure 4: Three protoplanetary disks systems with different viewing inclinations. For IRAS 04302 colors trace the small dust grain distribution, which is well coupled to the gas, and white contours show the mm-continuum disk (van’t Hoff et al. 2020). TW Hya is observed in ALMA mm-continuum (Andrews 2020). HD 163296 shows the rings from ALMA mm-continuum tracing the disk midplane and a single CO gas channel where the upper and lower emission surfaces extend vertically.

In mid-inclination disks observed by ALMA, the vertical dimension can be directly probed through the emission channel maps by tracing the emission maxima, as shown in the right panel of Figure 4. This methodology is sensitive to any sub-structure or asymmetry that may be present and has been implemented in public algorithms such as ALFAHOR (see Chapter 3 of this Thesis).

The immediate applications of measuring the vertical molecular layers in protoplanetary disks are many, depending on the selected tracers, the resolution and the available information from any radial or azimuthal structures. The temper-

ature structure can be traced through the peak brightness temperature of CO isotopologues, providing strong constraints to benchmark thermochemical models and precise temperature measurements, which are critical in turbulence studies (see Chapter 4 of this thesis for an application). If spatially resolved kinematic information is available, recent methods allow to separate the radial, azimuthal and vertical components of the material motion, combining this with the location of the vertical emission surfaces it is possible to directly trace and test the presence of meridional flows or disk winds which are crucial for understanding disk dynamics. Most recently, by tracing the vertical location of atomic carbon, early studies are being conducted to understand the location of the hot irradiated disk surface and the properties of this region.

This thesis

Recognizing the importance of characterizing the vertical protoplanetary disk structure to further understand the conditions and governing processes of planet formation, this thesis presents an in-depth observational and theoretical analysis of the vertical dimension. Here is an outline of the upcoming chapters and conclusions of this work,

Chapter 2: Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk. We analyse CN $N = 3 - 2$ in two different transitions and compare it to CO isotopologue emission. Our results show that the vertical location of CN and CO in Elias 2-27 is layered and consistent with predictions from thermochemical models. The inferred CN column densities, low optical depth ($\tau \leq 1$), and location near the disk surface agree with thermochemical disk models where CN formation is initiated by the reaction of N with UV-pumped H_2 . This study highlights the importance of tracing the vertical location of various molecules to constrain the physical disk conditions.

Chapter 3: Directly tracing the vertical stratification of molecules in protoplanetary disks. The ALFAHOR code is presented, this is an implementation of the Pinte et al. (2018a) method and obtains accurate vertical profiles even for low signal-to-noise molecules using interactive masking of emission channel maps. Using ALFAHOR we study the molecular emission surfaces of Elias 2-27, WaOph 6, and the five sources from the MAPS ALMA Large Program. Thermal structure, gas pressure scale heights, substructure and modulations in the vertical profiles and relations to the chemical origin of each observed molecule are discussed. Overall, we show that it is possible to trace the vertical locations of multiple molecular species and relate this information to a wide variety of physical and chemical disk properties.

Chapter 4: High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C_2H emission. Constraining turbulence in disks is key to understanding their evolution, however its measurement relies on knowledge of the thermal conditions for the molecular emission. Com-

binning the information on the physically resolved temperature structure that can be obtained from the vertical structure analysis, we present a new way of directly measuring turbulence. This method is benchmarked using CN and C₂H molecular emission from the protoplanetary disk of IM Lup. Our analysis retrieves high turbulence of Mach 0.4-0.6 at $z/r \sim 0.25$. This study presents the first empirical evidence for a vertical gradient in the disk turbulence, which is a key prediction of magneto rotational instabilities.

Chapter 5: Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion. Using thermochemical models we study the protoplanetary disk and stellar host properties that most affect the vertical location of CO $J = 2 - 1$ emission surfaces. The modelling predictions are benchmarked against data of CO emission from nineteen disks. We find that the CO emission surface is most affected by the total disk mass (M_d) and volatile carbon abundance, which leads to a z/r - M_d relationship. In order to reconcile total disk mass estimates from the characteristic z/r and the values obtained based on dust continuum analysis, a volatile carbon depletion of 10-100 (with respect to the ISM) is needed for the majority of sources.

Future outlook

Studies of vertical disk structure in large samples are in early stages, to date only ~ 20 disks have vertical CO surfaces characterized and ~ 8 (Paneque-Carreño et al. 2023; Law et al. 2024) have measured vertical profiles of more than three different molecules. The overall work from this thesis has shown that it is possible to use ALMA observations to study the vertical molecular layering and relate it to a number of physical processes.

Future work must focus on expanding the sample of disks with characterized molecular surfaces and combine the chemical information with knowledge on the dust grain distribution to accurately characterize disk processes. This requires high spatial and spectral resolution observations of molecules beyond CO, which is typically time consuming due to the low signal-to-noise of less abundant tracers. The upcoming ALMA Wideband Sensitivity Upgrade in the next decade will allow us to do these studies in less time and for larger samples.

Overall, the possibility of studying the protoplanetary disk material distribution across all three dimensions offers unique insight into the process of forming planets. Observational constraints are now catching up to theoretical models, which must be revised in order to explain the totality of observed features. In the same way that for the past years studies have focused on explaining the existence of radial and azimuthal substructure, we must now look at the third dimension and understand the information that comes from it. The techniques and results from this thesis have laid the foundations for many future studies that will for sure answer the questions we now leave open.

Resumen en Castellano

En el norte de Chile, debido a sus condiciones naturales y aislamiento, el desierto de Atacama es una ventana única para observar el universo. Durante muchos siglos, las comunidades indígenas locales, llamados en su idioma *Lickan Antay* y en castellano actual *Atacameños*, miraban al universo y se enfocaban no solo en las estrellas brillantes, sino en las áreas oscuras que contrastaban con el resplandor. Ahora sabemos que estas regiones son oscuras porque pequeños granos de polvo absorben la luz estelar en frecuencias ópticas y que estas nubes oscuras están asociadas con regiones de formación estelar. Mientras que nuestros ojos no pueden ver más allá del polvo, instrumentos como el Atacama Large Millimeter/submillimeter Array pueden revelar sus secretos. ALMA está construido en el llano de Chajnantor, un lugar sagrado para los *Lickan Antay* en el desierto de Atacama, que en su idioma significa “lugar de partida”. Ubicado a una altitud de 5000 metros, uno de los principales objetivos científicos de ALMA es investigar estas regiones oscuras y frías para entender los procesos que conducen a la formación de estrellas y planetas.

El análisis y los resultados presentados en esta tesis han sido posibles gracias a las capacidades de ALMA, que desde el inicio de sus operaciones en 2013 ha revolucionado la visión sobre la formación de planetas. A través de observaciones y el estudio teórico del universo a longitudes de onda (sub-)milimétricas, tenemos una oportunidad única de mirar hacia nuestros orígenes. ¿Cómo se formó la Tierra? ¿Podrían otros sistemas planetarios tener condiciones similares? ¿Cuáles son los procesos clave que rigen estas épocas iniciales?

Formación de estrellas y planetas

El proceso de formación de planetas está intrínsecamente ligado a la formación estelar. Primero las estrellas se forman a partir de nubes moleculares que colapsan contrayéndose y creando un núcleo pre-estelar. Pasando de núcleo hasta sistema planetario, los objetos estelares jóvenes (YSO) se clasifican en Clases (0, I, II o III). En la fase más temprana de Clase 0/I, la protoestrella estará activamente acumulando material de una envoltura protoestelar alrededor de ella, luego, debido a la conservación del momento angular, el material circundante se extenderá para crear una estructura en forma de disco rotatorio alrededor del sistema proto-

estelar. Estos discos se denominan discos protoplanetarios, ya que son los lugares de nacimiento y albergan el reservorio de material de futuros sistemas planetarios.

La fase de disco protoplanetario se conoce como Clase II, dura entre 1-10 millones de años y termina cuando la mayor parte del material del disco ha caído hacia la estrella, formado planetas o se dispersado, tras lo cual se revela un sistema planetario de Clase III. Esta tesis se centra en la fase de disco protoplanetario, donde el material primordial puede ser observado en alta resolución a longitudes de onda (sub-)milimétricas.

Discos protoplanetarios

Al igual que sus nubes moleculares progenitoras, los discos protoplanetarios son estructuras ricas en gas con apenas un pequeño porcentaje de su masa correspondiente a partículas sólidas (polvo). La mayor parte del material gaseoso del disco es hidrógeno molecular (H_2), sin embargo, su emisión es extremadamente débil e inaccesible con los telescopios actuales. El monóxido de carbono (CO) es la segunda molécula más abundante después de H_2 y es frecuentemente detectado, lo cual lo convierte en un trazador preferido del reservorio total de material. Otros trazadores comúnmente observados en discos protoplanetarios son: CN, HCN, H_2CO , CS, HCO^+ , N_2H^+ , H_2O y C_2H .

La Figura 6 presenta la distribución radial y vertical del material dentro de un disco protoplanetario, junto con las principales características y procesos en curso. Radialmente, el disco se divide en un caliente disco interior ($<20,ua$) y un disco exterior frío. Las observaciones de ALMA pueden acceder al disco exterior con una resolución espacial de unas pocas unidades astronómicas. Comprender la morfología, propiedades y dinámica de cualquier subestructura radial, azimutal o vertical es un objetivo clave de los estudios de formación de planetas para investigar directamente los procesos en curso a través de dichas estructuras.

En sus dimensiones verticales, los discos tienen una extensión que está determinada por el equilibrio hidrostático. Esto significa que la distribución del material en el eje vertical será moldeada por el equilibrio entre el potencial gravitacional de la estrella y el soporte térmico del material. Por lo tanto, la distribución vertical de los discos protoplanetarios contiene información sobre propiedades físicas clave, como la estructura térmica y de densidad. La estructura vertical también puede utilizarse como una sonda para el campo de ionización y la presencia de inestabilidades hidrodinámicas y vientos. Sin embargo, estudiar observacionalmente la dimensión vertical en muestras amplias de discos solo ha sido posible en los últimos años y, en particular, a través de los resultados de esta tesis.

Estudio de la estructura vertical del disco

El acceso a la dimensión vertical de los discos protoplanetarios con ALMA dependerá del ángulo de inclinación con el que sean vistos desde la Tierra. Hay dos casos extremos; 1) discos vistos de canto con altas inclinaciones ($\gtrsim 75^\circ$) y 2) discos vistos de frente con bajas inclinaciones ($\lesssim 35^\circ$). En ambos casos solo se puede acceder a dos dimensiones, para los discos vistos de canto, las dimensiones vertical

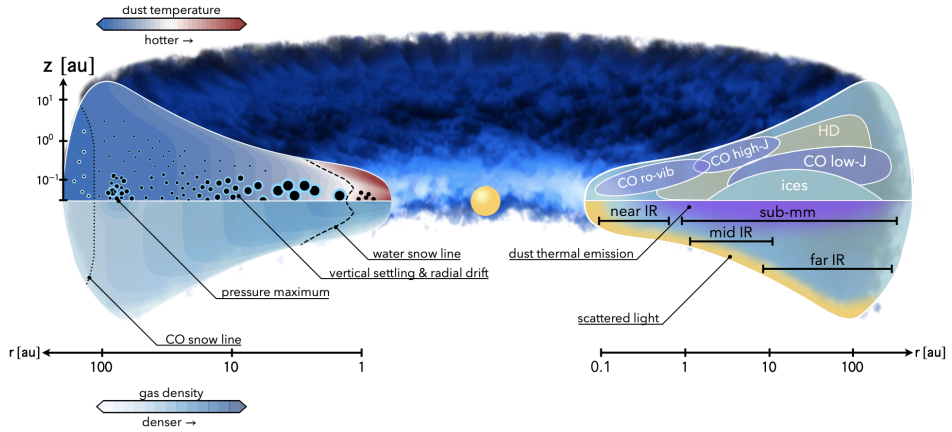


Figura 5: Ilustración de Miotello et al. (2023) que indica las regiones de emisión, escalas relevantes, temperatura del polvo y estructura de densidad del gas en discos protoplanetarios. El lado izquierdo muestra la distribución de partículas de polvo con círculos negros de diferentes tamaños. El lado derecho presenta una vista simplificada de la estratificación molecular para las principales moléculas en fase gaseosa. En la parte inferior se destacan las regiones de emisión térmica y de luz dispersa del polvo en púrpura y amarillo.

y radial, y para los discos vistos de frente, las dimensiones radial y azimutal. El resto de la muestra de discos protoplanetarios, con inclinaciones observadas entre $\sim 35\text{-}70^\circ$, se clasifican como discos de inclinación media. Nuestro trabajo se centra en estas fuentes, ya que permiten una vista de los procesos en curso en toda su estructura tridimensional, incluyendo el eje vertical. La Figura 4 muestra cada uno de las clasificaciones según inclinación.

En los discos de inclinación media observados por ALMA, la dimensión vertical puede ser sondeada directamente a través de los mapas de canales de emisión trazando los máximos de emisión, como se muestra en el panel derecho de la Figura 4. Esta metodología es sensible a cualquier subestructura o asimetría que pueda estar presente y ha sido implementada en algoritmos públicos como ALFAHOR (ver Capítulo 3 de esta Tesis).

Las aplicaciones inmediatas de medir las capas moleculares verticales en discos protoplanetarios son varias, dependiendo de los trazadores seleccionados, la resolución y la información disponible de cualquier estructura radial o azimutal. La estructura termal del disco puede ser trazada a través de la temperatura de brillo de los isotopólogos de CO, ofreciendo información fundamental para la calibración de modelos termodinámicos y mediciones de temperatura precisas, que son críticas en estudios de turbulencia (ver el Capítulo 4 de esta tesis para una aplicación). Si existe información cinemática, los métodos actuales permiten separar las componentes radiales, azimutales y verticales del movimiento del material, combinando esto con la ubicación de las superficies verticales es posible trazar y estudiar directamente la presencia de movimientos meridionales o vientos, que son cruciales

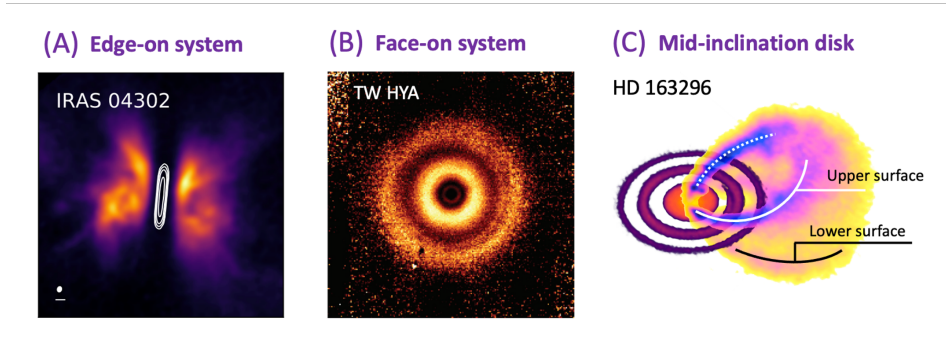


Figura 6: Tres sistemas de discos protoplanetarios con diferentes inclinaciones. Para IRAS 04302 los colores rastrean la distribución de pequeños granos de polvo, que están bien acoplada al gas, y los contornos blancos muestran el disco en emisión milimétrica (van't Hoff et al. 2020). TW Hya ha sido observado en el milimétrico con ALMA (Andrews 2020). HD 163296 muestra los anillos en emisión milimétrica de ALMA, que rastrea el plano medio del disco. Además la figura muestra un solo canal de gas CO donde las superficies de emisión superior e inferior se extienden verticalmente.

para entender la dinámica del disco. Recientemente, la ubicación vertical del carbono atómico está siendo utilizada para comprender la ubicación de la superficie irradiada del disco y las propiedades de esta región.

Esta tesis

Reconociendo la importancia de caracterizar la estructura vertical del disco protoplanetario para comprender las condiciones y procesos que rigen la formación de planetas, la siguiente tesis plantea un análisis observacional y teórico en profundidad de la dimensión vertical. A continuación se presenta un resumen de los próximos capítulos y conclusiones de este trabajo,

Capítulo 2: Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk. Analizamos CN $N = 3 - 2$ en dos transiciones diferentes y lo comparamos con la emisión de isotopólogos de CO. Nuestros resultados muestran que la ubicación vertical de CN y CO en Elias 2-27 está estratificada y es consistente con las predicciones de los modelos termodinámicos. Las densidades de columna de CN inferidas, la baja profundidad óptica ($\tau \leq 1$) y la ubicación cerca de la superficie del disco coinciden con los modelos termodinámicos de disco donde la formación de CN se inicia por la reacción de N con H_2 bombeado por UV. Este estudio destaca la importancia de trazar la ubicación vertical de varias moléculas para restringir las condiciones físicas del disco.

Capítulo 3: Directly tracing the vertical stratification of molecules in protoplanetary disks. Se presenta el código ALFAHOR, que es una implementación del método de Pinte et al. (2018a) y obtiene perfiles verticales precisos

incluso para moléculas con baja señal-a-ruido utilizando el enmascaramiento interactivo de canales de emisión. Usando ALFAHOR estudiamos las superficies de emisión molecular de Elias 2-27, WaOph 6 y las cinco estrellas del Programa MAPS de ALMA. Se discuten la estructura termal, las escalas de presión de gas, las subestructuras y modulaciones en los perfiles verticales y las relaciones con el origen químico de cada molécula observada. En general, mostramos que es posible trazar las ubicaciones verticales de múltiples especies moleculares y relacionar esta información con una amplia variedad de propiedades físicas y químicas del disco.

Capítulo 4: High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C₂H emission. Determinar el grado de turbulencia en los discos es clave para entender sus procesos de evolución, sin embargo, su medición depende de conocer las condiciones térmicas de la emisión molecular. Combinando la información sobre la estructura termal que se puede obtener del análisis de la estructura vertical, presentamos una nueva forma de medir directamente la turbulencia. Este método se calibra utilizando la emisión molecular de CN y C₂H del disco protoplanetario de IM Lup. Nuestro análisis recupera una turbulencia alta de Mach 0.4-0.6 en $z/r \sim 0.25$. Este estudio presenta la primera evidencia empírica de un gradiente vertical en la turbulencia del disco, que es una predicción clave de la inestabilidad magneto-rotacional.

Capítulo 5: Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion. Utilizando modelos termodinámicos estudiamos las propiedades del disco protoplanetario y de la estrella anfitriona que más afectan la ubicación vertical de las superficies de emisión de CO $J = 2 - 1$. Las predicciones de los modelos se calibran con los datos de emisión de CO de diecinueve discos. Determinamos que la superficie de emisión de CO es principalmente afectada por la masa total del disco (M_d) y la abundancia de carbono volátil, lo que conduce a una relación z/r - M_d . Para reconciliar las estimaciones de masa total del disco a partir del z/r característico y los valores obtenidos en base al análisis del polvo en longitudes milimétricas, se necesita una disminución de carbono volátil de 10-100 (con respecto al ISM) para la mayoría de las fuentes.

Perspectivas Futuras

Los estudios de la estructura vertical del disco en grandes muestras están en etapas tempranas, hasta la fecha solo ~ 20 discos tienen superficies verticales de CO caracterizadas y ~ 8 (Paneque-Carreño et al. 2023; Law et al. 2024) tienen perfiles verticales medidos en más de tres moléculas diferentes. El trabajo de esta tesis ha demostrado que es posible utilizar observaciones de ALMA para estudiar la estratificación molecular en el eje vertical y relacionarla con una serie de procesos físicos.

El trabajo futuro debe centrarse en expandir la muestra de discos con análisis de sus superficies moleculares y combinar la información química con el conocimiento de la distribución de granos de polvo para caracterizar con precisión los procesos del disco. Esto requiere observaciones de alta resolución espacial y es-

pectral de moléculas más allá del CO, que generalmente requieren mayor tiempo de integración debido a la baja señal-a-ruido de trazadores menos abundantes. La pronosticada actualización de la sensibilidad de banda ancha de ALMA en la próxima década nos permitirá realizar estos estudios en menos tiempo y para muestras más grandes.

En general, la posibilidad de estudiar la distribución de material del disco protoplanetario en las tres dimensiones ofrece una visión única del proceso de formación de planetas. La calidad e información entregada por las observaciones están alcanzando la precisión de los modelos teóricos, que deben revisarse para explicar la totalidad de las características observadas. De la misma manera que en los últimos años los estudios se han centrado en explicar la existencia de subestructuras radiales y azimutales, ahora debemos mirar la tercera dimensión y comprender la información que proviene de ella. Las técnicas y resultados de esta tesis han sentado las bases para muchos estudios futuros que seguramente responderán las preguntas que ahora dejamos abiertas.

Publications

Refereed publications as first author

1. *High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C₂H emission*
Paneque-Carreño, T., Izquierdo, A. F., Teague, R., Miotello, A., Bergin, E. A., Loomis, R., van Dishoeck, E. F., 2024, *Astronomy & Astrophysics*, 684, A174.
2. *Directly tracing the vertical stratification of molecules in protoplanetary disks*
Paneque-Carreño, T., Miotello, A., van Dishoeck, E. F., Tabone, B., Izquierdo, A. F., Facchini, S., 2023, *Astronomy & Astrophysics*, 669, A126.
3. *Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk*
Paneque-Carreño, T., Miotello, A., van Dishoeck, E. F., Pérez, L. M., Facchini, S., Izquierdo, A. F., Tychoniec, L., Testi, L., 2022, *Astronomy & Astrophysics*, 666, A168.
4. *Spiral arms and a massive dust disk with non-Keplerian kinematics: Possible evidence for gravitational instability in the disk of Elias 2-27*
Paneque-Carreño, T., Pérez, L. M., Benisty, M., Hall, C., Veronesi, B., Lodato, G., Sierra, A., Carpenter, J. M., Andrews, S. M., Bae, Jaehan, Henning, Th., Kwon, W., Linz, H., Loinard, L., Pinte, C., Ricci, L., Tazzari, M., Testi, L., Wilner, D., 2021, *The Astrophysical Journal*, 914, 2, 88.

Submitted publications as first author

1. *Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion*
Paneque-Carreño, T., Miotello, A., van Dishoeck, E. F., Rosotti, G., Tabone, B., submitted to *Astronomy & Astrophysics*.

Refereed publications as co-author

1. *Gravitational instability in a planet-forming disk*
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3. *CI traces the disk atmosphere in the IM Lup protoplanetary disk*
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4. *The Disc Miner. II. Revealing gas substructures and kinematic signatures from planet-disc interaction through line profile analysis*
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5. *Mapping protoplanetary disk vertical structure with CO isotopologue line emission*
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6. *Deuterium-enriched water ties planet-forming disks to comets and protostars*
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7. *Dynamical mass measurements of two protoplanetary discs*
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 12. *Predicting the kinematic evidence of gravitational instability*
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Published books (science outreach)

1. *Universo Según Carlota: Galaxias lejanas y materia oscura*
Paneque-Carreño, T., 2024, in press, Editorial Planeta Chile.
2. *Universo Según Carlota: Vida extraterrestre y exoplanetas*
Paneque-Carreño, T., 2023, Editorial Planeta Chile.
3. *Universo Según Carlota: Agujeros negros y explosiones estelares*
Paneque-Carreño, T., 2024, Editorial Planeta Colombia.
Paneque-Carreño, T., 2022, Editorial Planeta Chile.
4. *Universo Según Carlota: Asteroides y estrellas fugaces*
Paneque-Carreño, T., 2022, Editorial Planeta Colombia.
Paneque-Carreño, T., 2021, Editorial Planeta Chile.

Curriculum Vitae

I was born on the 15th of November, 1997, in Madrid, Spain. My parents, originally from Cuba and Chile, where in Spain doing their PhD studies in molecular genetics (dad) and immunology (mum). We stayed in Spain for five years, during which I bonded with my godparents and their sons, whom to this day are a second family to me. In January of 2003 we moved to Glasgow, Scotland where my parents worked as postdoctoral investigators. I started school without knowing a word of english, but thanks to the excellent public system managed to learn how to read, write and speak within the first six months. During our first years in Glasgow my two brothers where born. My life at this point was filled with books, I greatly enjoyed reading fantastic literature and the library was my favorite place. At school I was interested in all topics, from maths to english and also, at the insistence of my dad, learnt how to play the violin.

In April of 2007 my family moved to Chile. On one hand it was great to reconnect with my family from my mother's side, but it was very hard for me to leave my friends and life in Glasgow. After some struggles I managed to feel comfortable in my new high school and joined a program called PENTA UC. PENTA is an initiative of Universidad Católica in Chile that focuses on students with academic talent, offering classes on topics beyond the high school curriculum. Through PENTA I discovered robotics, computer science, astronomy and complex math. While for a long time my intention was to study to become a school teacher, I had a never ending curiosity and wished to also be a life-long student, therefore I decided to become a scientist like my parents, but in the topic of astronomy.

In March of 2014 I enrolled in the faculty of physical and mathematical sciences of Universidad de Chile. Here I was one of over 800 first year students interested in various engineering and scientific majors. I didn't know much about astronomy beyond the fact that it was a branch of physics that studied the processes of objects in the universe. My first approach was on the topic of planet formation and it filled me with curiosity and eagerness to learn more on the subject. During the four years of my undergraduate I worked as teaching assistant to various physics classes, my favorite being Mechanics, which was taught in the third semester and introduced cylindrical and spherical coordinates. During the weekends I worked as assistant professor in PENTA courses and volunteered as referee to a nation-wide robotics competition. I graduated from Astronomy in December of 2017 and, filled

with impostor syndrome, doubted about following an academic career beyond the bachelor. Thankfully my friends pushed me to apply for a Master degree and I was accepted to start in March of 2018 at Universidad de Chile.

The Master degree changed my view of academia and my place in it. I worked with Prof. Dr. Laura Pérez on the analysis of new ALMA data from the protoplanetary disk surrounding the young star Elias 2-27. At that point Prof. Dr. Myriam Benisty was also working at Universidad de Chile and both her and Laura became excellent role models of what it means to be a woman in academia. I became involved in the Dustbusters collaboration, which allowed me to travel in early 2019 to Università degli Studi di Milano and the University of Leicester to work alongside Prof. Dr. Giuseppe Lodato and Dr. Cassandra Hall in the modelling of gravitational instabilities. During these visits I also met the person who would become one of my PhD supervisors, Dr. Anna Miotello.

After successfully defending my Master thesis virtually during the 2020 pandemic, I moved to Germany in November of 2020 to start my PhD at the European Southern Observatory with Anna. In parallel, I worked with the group led by Prof. Dr. Ewine van Dishoeck at Leiden Observatory, as my position was shared between both institutions. I was introduced to the amazing world of astrochemistry, the various temperatures (brightness, kinetic, effective, rotational) that confused me for a long time and the power of understanding the conditions of emission for the gas observations that I was working with. We uncovered and dived deep into the vertical structure of protoplanetary disks, discovering new avenues and methods to understand the conditions of planet formation through the surfaces traced by molecular gas observations.

In parallel to the scientific production, since early 2020 I started to dedicate a large portion of my “spare” time to do astronomy outreach on social media. I began uploading videos in spanish to different social media platforms explaining astronomy concepts and when I was in Germany my following numbers grew unexpectedly. Currently I have over one million followers accross platforms, have written four astronomy outreach books for a juvenile audience that are used as reading materials in schools in Chile and was named UNICEF good will ambassador in Chile. To me, scientific outreach is a key part of my scientific research, as it helps me to use the astronomical knowledge to give back to society and promote critical thinking. I also think it is a way of connecting with my initial wish to be a teacher, only that instead of a blackboard I appear on a telephone screen.

In September of 2023 I left Germany and moved to the Netherlands to complete my last PhD year at the University of Leiden and work in person with people that for years had been virtual collaborators. Now, after my thesis defence I will continue doing astronomical research through a joint fellowship of 51 Pegasi b and Michigan Society of Fellows at the University of Michigan in the group of Prof. Dr. Ted Bergin.

Acknowledgements

My experience during this PhD has been largely filled by support, encouragement and collaboration. The list of people that have been part of this would be too long to put here, however I will do my best to name some of the key players.

First, some words for my nuclear family. Mamá y Papá you have always been my biggest supporters and shown me unconditional love that no amount of geographical distance can stop. To my not-so-little siblings, Carlos and Miguel, I am beyond proud of watching you both grow and conquer every challenge that you face. Huge recognition for my large extended family, but particularly to both my abuelitas, Nivia and Norma son mi inspiración máxima.

I was fortunate to divide my PhD between the European Southern Observatory in Garching working directly with Anna Miotello and Leiden Observatory with Ewine van Dishoeck. Anna, I appreciated our weekly meetings and your concern from the very first day. Even in a pandemic lockdown you were always present and available to have a conversation on science and life. It has been a delight to be a founding member of the Miotello group that will for sure grow largely in the coming years. Ewine, your sharp thoughts and experience always sparked new ideas in our research meetings. It has been very inspiring to learn astrochemistry with you. I am thankful to both my advisors for trusting me not only in my research, but also in my outreach endeavours and for being present in some of the key moments of my life both personal and professional.

To some of the many amazing people I worked with during these four years. My first office mate and favourite brazilian, Cami, it was lovely sharing this PhD adventure with you, the good and the bad. Luca, it has been all laughs with you since the first day, I thank you for your sincerity and constant support and I am so happy I will now get to see you every time I go to Chile! Victor, I will always look forward to having one of our talking sessions and I hope in the future we get to share more time together again. Andrés, from the start we got on great talking about kinematics and trying to figure out how to do crazy science, there is still a lot of work to be done! Gemma, Sam, Stephen, Simon, Juliet, Amanda, you were some of my closest friends at ESO and I hope the future brings us more opportunities to make new memories. Nelma, I appreciate your unwavering support and dedication, ESO would not have been the same without you. To all the ESO SPF team, Aashish, Domi, Alice, Rik, Adrien, Haochang, Pietro, Chi

Yan, Hala, Mari-Liis, Enrique, Carlo, Justyn, Claudia, Marta, Claudio, Karina, Leonardo, it has been amazing to be part of the Monday meetings all these years! To my fellow collaborators around the world, Rich, Giovanni, Benoit, Ilse, Myriam, Stefano, Ted solving science challenges together has been a delight.

Even though we only shared physical office space for the last year, the Leiden team was fundamental throughout this period. Margot, you have been my guide in the world of physical-chemical models and my dutch best friend, I am very grateful for all your kindness. Sierra and Alice, as postdocs in the team you were great support and role models, I am excited to keep collaborating and crossing paths with you both in the US. Lucas, Ardjan, Milou, Marissa, Andrew, Nashanty, Martijn, Lisa, Melissa, Michiel, Nienke, Will, Logan, Katie and Lukasz, thank you for welcoming me first virtually and then in person to the land of marvellous cheese, stroopwafels and bitterballen.

To the people that have been with me since the start. Elena, Julio, Juan, Abi, Amira, for being my second family, offering a house full of happiness and always having polvorones in store. Cele, Cata, Pame, Scarlett, it has been ten years since we left the school classrooms and we are still going strong, it is an honour to have such powerful girlfriends. Simón, Coni, Mathi, Sca, Bica, since university and through different stages of my life you have been there, and I deeply appreciate you all. I must also mention the investigation group at Universidad de Chile, led by Laura Pérez, who was first my mentor and is now also an esteemed collaborator and friend, I look forwards to many more projects together.

To the huge online community that follows @terepaneque, the boys and girls that read my books and the teachers that take me to their classrooms I deeply value your trust. Together we are building a brighter and better future through scientific education and critical thinking.

Finally, to the person that has held my hand every step of the way. Sacha, home is wherever you are. Your constant trust and love has pushed me through the bad times and celebrated in the good ones, I can't wait for the next chapter in our story to begin.