The puzzle of protoplanetary disk masses

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1 Introduction

The cosmos is within us.
We are made of star-stuff.
We are a way for the universe to know itself.
Carl Sagan

Since the beginning of human history, men have raised their eyes to the night sky and wondered about the meaning of such a majestic show (Fig. 12.1). Ancient civilizations from different parts of the world, from Egypt to China, from Oceania to southern America, have given life to myths and legends about the constellations and nebulosities that they could spot in the sky. Even throughout our European history many poets, painters and artists have taken inspiration from celestial events. The astonishment in front of the sky has always been accompanied by the need to understand the link between mankind and the universe. Now that science and technology have advanced and we are able to explain the physical and chemical structure of astronomical objects, this question has not been abandoned. Science has revealed to us that the connection of the cosmos with our existence is much deeper than any pre-scientific vision had dared to imagine. For example our knowledge on our hosting galaxy tells us that all phenomena happening in the Milky Way, from the presence of a black hole to that of supernova explosions up to the actual location of our Solar System, have cooperated to allow life to evolve up to the current status. Also, the growing zoo of discovered exoplanets allows us to compare their characteristics with those of our planetary system. Despite the large statistics, it seems that the configuration of our own Solar System is very "special" as shown by Morbidelli & Raymond (2016). Based on exoplanet observational surveys, the Sun-Jupiter system is as common as one in a thousand. On the other hand theoretical modeling favors Jupiter as the fundamental player in the Solar System's evolution (Walsh et al. 2011; Izidoro et al. 2015).

Figure 1.1: The galactic center and dusty Milky Way as seen on March 26, 2017 on a new moon night from Cerro Paranal (photo taken by the author with Reflex camera, exposure 30s).

1.1 Star formation and protoplanetary disks

The question about our origins centers around star and planet formation. How do stars and planets orbiting around them form? What are the initial conditions needed to generate a planetary system similar to our own? Which roles do the physical architecture and chemical composition of these forming systems play?

On large scales, star formation begins with the formation of filamentary structures inside giant molecular clouds ($\sim 10 - 100$ pc). Observations have shown that filaments are elongated structures with widths of ~ 0.1 pc (André et al. 2010; Kennicutt & Evans 2012). Within these long filaments, typically several pc-long dozens of smaller fibers are created (Hacar et al. 2013) and eventually fragment into dense cores (Hacar & Tafalla 2011). These are defined as *prestellar cores* ($n \sim 10^4 - 10^5$ cm^{-3}), as they will likely collapse to form one or more stars. As the collapse proceeds, due to conservation of angular momentum a rotating disk-like structure is formed, through which matter accretes onto the forming protostar (Fig. 1.2). This is called either a *cir-*

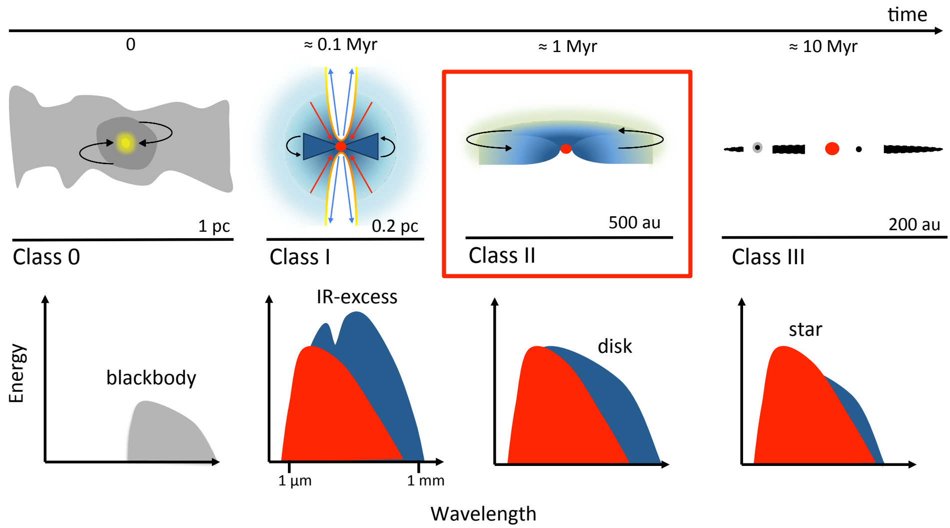


Figure 1.2: Sketch of the star and planet formation process in isolation. In the upper panel different evolutionary classes are sketched, while in the lower panel the respective observational features are shown through schematic SEDs. This thesis focuses on the stage of a pre-main sequence star with a disk, called the Class II stage.

cumstellar disk, or *accretion disk*, or *protoplanetary disk* depending on the community. The idea that the solar system was born from nebulous material was firstly introduced by Emanuel Swedenborg in 1734 and further developed by Immanuel Kant in 1755 as the *nebular hypothesis*. Afterwards, in 1796, Pierre-Simon Laplace proposed an independent but similar model, where the forming Sun was surrounded by a hot atmosphere. Such material would cool and flatten with time, creating rotating rings from which planets would form. This theory had some problems in explaining the angular momentum distribution between the Sun and planets.Therefore, Laplace's idea was abandoned at the beginning of the 20th century. The study of stellar accretion disks started then as a purely theoretical field in the 1970s from the work by Shakura & Sunyaev (1973). This was motivated by observations of accretion onto black holes in binary system, but the simple physical model proposed by Shakura & Sunyaev (1973) turned out to be applicable also for circumstellar disks. The first indirect observational evidence of circumstellar disks came then in the late 1980s at optical and mm wavelengths (Hartmann & Kenyon 1985, 1987; Sargent & Beckwith 1987). The advent of the *Infrared Astronomical Satellite* (IRAS) allowed a wider study of disk properties through their Spectral Energy Distributions (SEDs) published by Strom et al. (1989). This statistical work was followed-up with a survey at mm wavelengths by Beckwith et al. (1990) which provided the first disk mass estimates from continuum emission from cold dust. The first direct image of a protoplanetary disk was taken some years later by O'dell & Wen (1994) with the *Hubble Space Telescope* (HST), which allowed to study disk morphology in much detail thanks to its high angular resolution. Interestingly, the first direct image of a gas-poor disk, β Pic, around a young star was taken by Smith & Terrile (1984), earlier than for gas-rich classical disks.

Our physical understanding of the different stages of star and planet formation is linked to an observational classification done based on studies of the SED shapes of different Young Stellar Objects (YSOs) in the mid- to near-infrared (MIR to NIR). Historically, it was expected that the release of accretion luminosity would be very bright in the infrared (see Wynn-Williams 1982, as a review). Therefore, much work went into surveying protostars at such wavelengths, but the amount of extinction and radiation reprocessing provided by the infalling material was underestimated. As shown by the sketch in Fig. 1.2, three different SED slopes were detected and used to classify Class I, Class II and Class III objects (Lada 1987).

- **Class I** YSOs are typically visible in the near IR, but not in the optical, with a rising spectrum in the mid-Infrared (mid-IR), called IR-excess. This is interpreted as a contribution of the forming star and disk to the thermal emission due to the presence of warm dust. An extended structure, called envelope, is still present and emits at longer wavelengths but its mass is much smaller than the protostar mass.

- **Class II** YSOs are optically visible with a decreasing SED in the IR. At short wavelengths the emission is dominated by the star, while the disk component emits at larger wavelengths. At this stage the envelope is completely dissipated and the disk is gas rich.

- **Class III** YSOs are also optically visible but they do not show any IR-excess. The disk is gas poor and larger bodies, such as planets and asteroids, must be already formed at this stage.

- Subsequently a stage even less evolved than the Class I phase, i.e. **Class 0** YSOs, was defined observationally by André (1995) as embedded YSOs which have $L_{\rm submm}/L_{\rm bol} > 5 \times 10^{-3}$; $L_{\rm submm}$ is the sub-millimeter luminosity measured at wavelengths larger than 350 μm and $L_{\rm bol}$ is the total bolometric luminosity. Class 0 sources are not detected in the NIR, but most of their emission ($\gtrsim$99% of the luminosity) is in the far-infrared. Class 0 prostostars are bright in the 50-200 μm range, which however unfortunately cannot be observed from the ground. Moreover these embedded sources have strong emission in the sub-mm dominated by cool dust in the envelope ($T_{\rm dust} \sim$ 30-50 K). At this stage the envelope mass is much larger than the forming protostar mass.

The focus of this thesis is on protoplanetary disks in their gas rich Class II phase through the modeling of their bulk gas component. Disks are generally divided in two categories, depending on the type of protostar they are orbiting around: T Tauri or Herbig. Herbig Ae/Be protostars are the higher mass counterparts of T Tauri protostars, with spectral types A and B and masses $M_{\star} \gtrsim 2M_{\odot}$. T Tauri stars are more common (spectral types K and M) and often show a characteristic ultraviolet (UV) excess in addition to the stellar photosphere, which is more prominent than in Herbig stars. The Herbig stars are widely studied as they are very bright, and so are also their disks. The process of high-mass star formation is far less understood than the low-mass star formation and will not be considered in this PhD thesis. The same holds for Brown Dwarfs (BDs), whose formation process is not studied here.

Planet formation

How protoplanetary disks evolve from their gas rich phase to the formation of planetary systems is still an open question. Many planet formation theories have been developed so far, but none is able to correctly reproduce the needed timescales, or the properties observed in exoplanetary systems, as well as in our own solar system. The favorite scenario starts however with the coagulation of small (sub μm-sized) dust particles into larger pebbles, all the way out to planetary rocky cores (Hayashi 1981; Pollack et al. 1996). Dust growth can start already in the embedded phase (e.g. Miotello et al. 2014a) and as the ISM-like grains grow to larger sizes they start to decouple from the gas. They suffer a strong drag force and settle toward the midplane, where they can grow to even larger sizes due to the enhanced dust density. As they grow up to mm-cm sizes they start to drift inward and their velocity is maximized when they reach the meter size (at 1 au). As a consequence fragmentation due to collision becomes an important effect which stops the growth to larger bodies. Moreover the drift toward the central star becomes very fast, with timescales much shorter than those needed to grow larger bodies (Dullemond & Dominik 2005). This problem is known as the *meter size barrier* and was first formulated by Weidenschilling (1977).

A possible solution is found if a pressure maximum is present in the disk, which would trap the dust particles in a localized region of the disk (Whipple 1972). Such dust traps have been observed and modeled in protoplanetary disks and are thought to be created by gap-opening planets, vortices, or dead zones (Varnière & Tagger 2006; Armitage 2011; Zhu et al. 2011; Pinilla et al. 2012; Regály et al. 2012). Once the meter size barrier is overcome, as this must happen somehow, grain growth continues to reach planetesimal sizes, all the way to rocky planets. Once the planet core reaches 10 Earth masses, gas can be accreted to form giant gaseous planets, as predicted by the *core accretion model*. This must occur before the gaseous disk is dispersed. Alternatively gas giants could be formed via *gravitational instability*, a very fast process which could occur already in the embedded phases of protoplanetary disks when they are massive and cold enough (Helled et al. 2014). Both theories alone however fail to reproduce the statistics on exoplanets orbits. The core-accretion model is able to explain $\sim 90\%$ of the observed exoplanets, while the rest could be formed by gravitational instabilities (Matsuo et al. 2007).

Disk dispersal

Disks are traditionally thought to undergo viscous evolution, which redistributes angular momentum within the disk and leads to accretion of matter onto the central star. Mass accretion would then be responsible for the dissipation of the disk material. In particular the mass accretion rate $\dot{M}_{\rm acc}$ onto the central protostar is theoretically expected to scale with the disk mass, and there is observational support for this as shown by Manara et al. (2016b). The exact mechanism responsible for viscous evolution is not yet known, but the favorite candidate is magneto-rotational instability (see Turner et al. 2014, as a review). One key problem is that viscous evolution alone is not efficient enough to account for the fast disk dispersal timescales that are observed in young stellar clusters (~ 5 Myr, Fedele et al. 2010, and reference therein). A process has to take over disk dispersal at $2-6$ Myr as viscous evolution alone would imply disk dispersal timescales exceeding $10^7 - 10^8$ yrs.

Some other effects may modify or overtake viscous evolution in disks. For instance magnetically driven winds may be extremely efficient in removing material from the disk but quantitative constraints are not yet available (Armitage et al. 2013; Bai et al. 2016). On the other hand, photoevaporation from the central object, or from external sources, may play an important role in dispersing the disk and extensive studies have been carried out on this subject (Johnstone et al. 1998; Clarke et al. 2001; Adams et al. 2004; Owen et al. 2010; Anderson et al. 2013; Facchini et al. 2016). Finally, the environment can further affect disk evolution by physical encounters. A disk can be truncated by the gravitational encounter with another member of its star-forming region.

Main questions

One of the fundamental properties of disks is the total *mass*, as it determines their physics, evolution and the characteristics of the planetary outcomes. Nevertheless disk masses are not yet observationally determined with high confidence. Disks are composed of gas and dust grains, as are molecular clouds and cores. The dust does not have the ISM size distribution however, but the grains can easily reach mm-size and such grains, which dominate the dust mass in disks, are not necessarily well mixed with the gas. Accordingly the mass determination of the gaseous and dusty components should in principle be carried out independently. Most of the disk mass is expected to be in the form of molecular gas, essentially molecular hydrogen (H_2). However, H_2, under the disk thermo-physical conditions, is not easily excited and observable. Hence, traditionally, the presence of gas in disks has been constrained through carbon monoxide (CO) emission lines, easily excited in disks. However the emission is generally very optically thick, so using CO to measure accurately the gas mass is very difficult and model dependent. The main questions that are tackled in this PhD thesis are the following.

- Which is the best gas mass tracer in protoplanetary disks? Could the less abundant isotopologues of CO serve this purpose? Would hydrogen deuteride (HD) be a good alternative and what are its limitations?

- How can current and future ALMA observations be used to determine the masses of a statistically significant sample of disks?

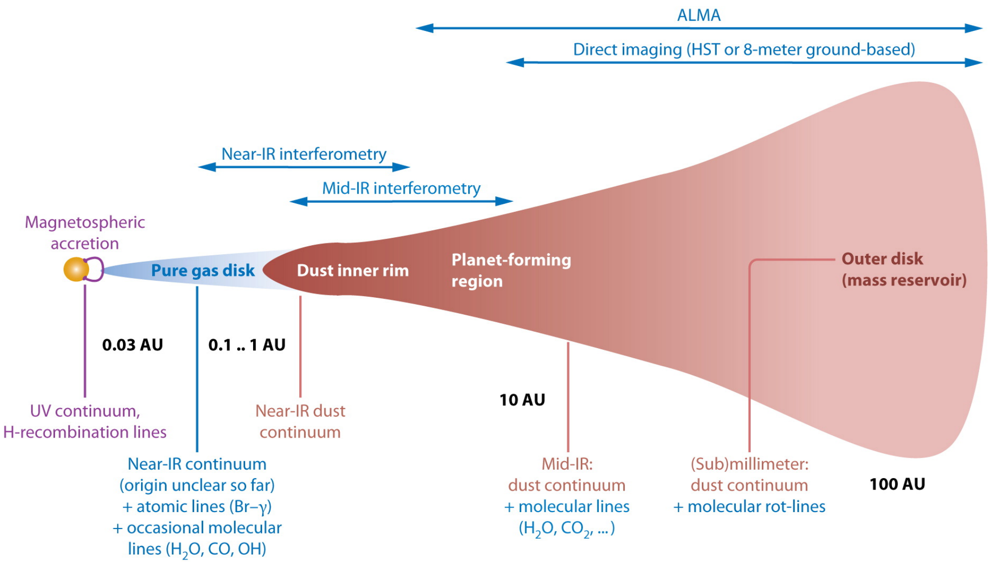
- What is the actual gas-to-dust mass ratio in disks and how is its determination affected by elemental carbon and oxygen depletion?

1.2 The Atacama Large Millimeter/submillimeter Array

Great improvements in the study of protoplanetary disks and their mass determination have been brought by the advent of ALMA, the Atacama Large Millimeter/submillimeter Array. This is a single facility composed of 66 high precision antennas located on the Chajnantor plateau, 5000 meters altitude in northern Chile.

ALMA[1] is sensitive to wavelengths where the bulk of the dust and molecular gas in disks emit (see Fig. 1.3). Moreover its extraordinary sensitivity and angular resolution allow to detect and resolve disk emission at high signal-to-noise (S/N) levels. It is very illustrative to compare ALMA current capabilities with some pre-ALMA interferometers, such as the Submillimerter Array (SMA), that has served the disk community for many years before. ALMA can achieve a continuum rms noise level below 0.1 μJy in less than one hour, while SMA would take approximatively 81 nights to reach the same sensitivity.

[1]ALMA is an international partnership of the European Southern Observatory (ESO), the U.S. National Science Foundation (NSF) and the National Institutes of Natural Sciences (NINS) of Japan, together with NRC (Canada), NSC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile.



Dullemond CP, Monnier JD. 2010.
Annu. Rev. Astron. Astrophys. 48:205–39

Figure 1.3: 2D sketch of a disk where its different regions are connected to the wavelength range in which it is observable. The top arrows show which techniques can spatially resolve which scales (from Dullemond & Monnier 2010). ALMA is very well suited to study the outer disk, where most of the mass is enclosed.

The ALMA disk community is following mainly two complementary observational strategies. On one hand complete surveys of disks are carried out to statistically study simultaneously the dust, through mm-continuum emission, and gas, through CO isotopologues (see Ansdell et al. 2016; Pascucci et al. 2016; Barenfeld et al. 2016; Ansdell et al. 2017, Fig. 1.4). Such surveys show that the bulk of the disk population is much fainter and possibly smaller than what we assumed as the average disk before the ALMA era. On the other hand the well studied large and bright disks, such as e.g. TW Hya (Fig. 1.5), HD163296, HL Tau, are now observed at extremely high angular resolution revealing exciting substructures that may be common in most if not all protoplanetary disks (ALMA Partnership et al. 2015; Andrews et al. 2016; Isella et al. 2016). Moreover, large cavities in gas and dust are observed in a subset of so-called *transitional disks* (see e.g. van der Marel et al. 2015, 2016). The results coming from both paths are transforming the field by complementing each other.

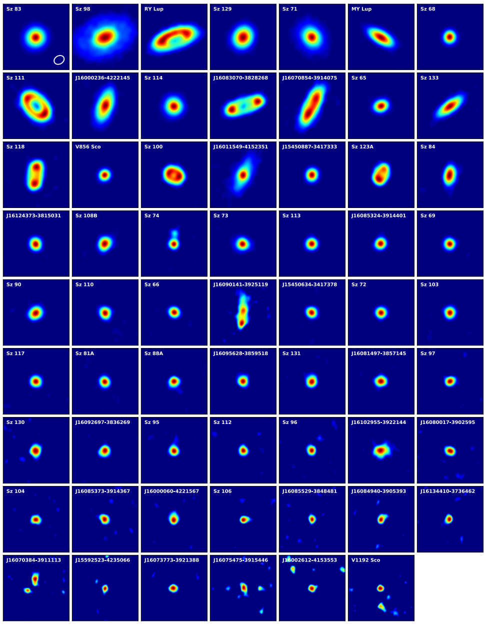


Figure 1.4: Dust continuum emission observed with ALMA in Band 7 for a large sample of disks in the Lupus star-forming region (d=150 pc) at a resolution of $\sim$ 0.3″ ($\sim$ 20 − 30 au radius Ansdell et al. 2016). Each panel is 2″×2″. This ″zoo″ presents very different disk morphologies and a surprisingly high fraction of sources which appear very compact at this resolution and S/N.

The *Lupus disk survey* with ALMA (PI: J. P. Williams, Ansdell et al. 2016, Fig. 1.4) has provided most of the new observational constraints that have been employed in this thesis. More details will be presented in Chapter 4.

1.3 Disk dust mass determination

Dust is traditionally assumed to account only for 1% of the total disk mass. This comes from the assumption that disks present the same gas-to-dust ratio as that found in molecular clouds. In clouds the combination of various types of analyses has suggested that a factor of 100 is correct. Nevertheless, the mm-sized grains thermally emit broadband continuum radiation at mm wavelengths. Therefore dust emission from protoplanetary disks can be very bright and readily detectable by

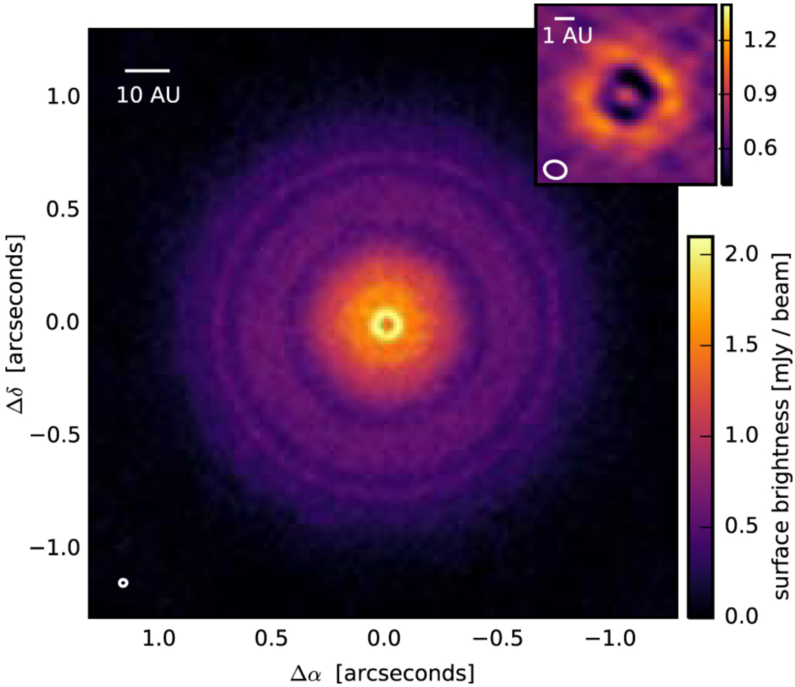


Figure 1.5: ALMA image of the 870 μm continuum emission from the closest disk, TW Hya. The circular beam FWHM is 30 milliarcseconds, corresponding to a resolution of 1.6 au. The top right panel shows a zoomed region which is 0.2″ wide (10.8 au), highlighting the 1 au gap seen in the inner disk. (Credit: S. Andrews - Harvard-Smithsonian CfA, Andrews et al. 2016)

(sub-)mm interferometers. A number of studies of dust in disks have been carried out, several already with pre-ALMA interferometers, and are summarized in recent reviews (Williams & Cieza 2011; Dutrey et al. 2014; Testi et al. 2014; Andrews 2015).

At mm-wavelengths the dust thermal emission is generally in the optically thin regime for surface densities of $\lesssim$ 3 g cm^{-2} and the Rayleigh-Jeans approximation holds (Beckwith et al. 1990). Therefore it is straightforward to derive the following relation:

$$M_{\rm dust} = \frac{F_\nu d^2}{\kappa_\nu B_\nu(T_{\rm dust})} \tag{1.1}$$

(Hildebrand 1983). The mass retained in mm-sized grains $M_{\rm dust}$ is directly proportional to the flux at mm wavelengths F_ν, where $\nu \sim 300$ GHz. The other three variables involved are the distance of the source d, the dust opacity κ_ν and the Planck function for a characteristic dust temperature $B_\nu(T_{\rm dust})$.

The large observational uncertainty on d is being overcome by the advent of the GAIA mission, which is providing a new distance catalog with micro-arcsecond precision on the parallaxes. The SED can provide constraints on the dust temperature $T_{\rm dust}(r, z)$, which is generally non constant throughout the disk. It is known that the disk temperature structure has vertical and radial gradients in the disk, making the surface layers much warmer than the midplane, which is however the region probed by mm-sized grains emission. There temperatures are generally low and constant and $T_{\rm dust}$ is often assumed to be ~ 20 K, as this is the average dust temperature found in the outer disk in the Taurus star forming region (Andrews & Williams 2005). The dust opacity κ quantifies the dust absorption cross-section per unit mass. The opacity can be approximated by a power law of the frequency,

$$\kappa_\nu = \kappa_0 \left(\frac{\nu}{\nu_0} \right)^\beta \tag{1.2}$$

(Draine 2006). The normalization κ_0 and the power law index β depend on the composition, shape and the size distribution of the dust grains (Pollack et al. 1994; Ossenkopf & Henning 1994). The latter can be constrained by multi-wavelength (sub-)millimeter continuum observations, as $\beta = \alpha - 2$ in the optically thin and Rayleigh-Jeans regime, where α is the measured spectral index (e.g. Ricci et al. 2010; Tazzari et al. 2016, and reference therein).

The total dust surface area is in the smallest sub-μm sized grains but the total dust mass is mostly within the larger mm-sized particles (Testi et al. 2014). Therefore, mm continuum emission is a good probe of the bulk of the dust component in disks. Anyway, such observations can only provide a lower limit of the total mass of solids, as larger bodies are completely invisible at these and other wavelengths.

Traditionally dust masses are then converted in total disk masses by multiplying for a constant gas-to-dust ratio of 100, as that found in the ISM (Goldsmith et al. 1997). Recent higher resolution disk observations carried out with ALMA have shown that this assumption is not necessarily correct, as dust and gas emission present two different distributions.

1.4 Disk gas mass determination

Dust mass measurements are important to determine the evolution of dust particles to larger solids, all the way to planet formation. However, as the gas is the disk's dominant constituent, this controls the disk dynamics and evolution, including that of the dust. It would be ideal thus to measure disk gas masses directly from a gaseous tracer and independently from dust mass measurements.

1.4.1 H_2, the main gaseous component

Molecular hydrogen (H_2) is the main gaseous species present in disks but it does not strongly emit due to its molecular physics (Field et al. 1966). H_2 is light and the energy spacings between its rotational levels in the ground vibrational state are large. Furthermore, being a symmetric molecule it has no dipole moment but only weaker quadrupole transitions.

The fundamental ground state transition of molecular hydrogen is the $J = 2 - 0$ or S(0) line, which has an energy spacing of 510 K at 28.2 μm. This large energy spacing combined with the weaker quadrupole Einstein A coefficient makes it hard for H_2 to emit appreciably in cold environments such as protoplanetary disks with typical gas temperatures $T_{\rm gas} = 20$ K. One would need much higher temperatures, $T_{\rm gas} > 100$ K, which can be found only in the inner disk regions. Within a few tens of astronomical units (au) from the central star the large dust column densities imply high dust optical depths at 28.2 μm, however. Thus, the emission of the warm gas where the ground state line of H_2 can be excited can be shielded by the optically-thick dust layer (Thi et al. 2001; Pascucci et al. 2006; Carmona et al. 2008; Bitner et al. 2008; Bary et al. 2008). Even if detected, H_2 is not a good tracer of the bulk of the disk mass which is retained in the outer disk regions (Pascucci et al. 2013).

Given that direct detection of molecular hydrogen is extremely difficult, one needs to find indirect tracers of the gas mass in protoplanetary disks.

1.4.2 Gas masses from HD observations

The closest molecule to H_2 is its less abundant isotopologue hydrogen deuteride (HD). HD chemistry is similar to that of H_2 as it does not freeze-out onto grains. Other molecules, e.g. CO and less volatile species, cannot survive in the gas phase at low temperatures but stick onto the icy grains through the so-called process of freeze-out (see Sect. 1.4.3). Also HD, like H_2, can self-shield itself from the photodissociating UV photons, but at reduced efficiency (Wolcott-Green & Haiman 2011). The abundance of HD with respect to H_2 is $\sim 3 \times 10^{-5}$, obtained assuming the local [D]/[H] value but accounting for the fact that 2 hydrogen atoms compose molecular hydrogen.

In contrast to H_2, HD has a small dipole moment which allows dipole transitions ($\Delta J = 1$). The energy difference between the first and second rotational levels of HD is of ~ 20 K and this means that at a temperature of $T_{\rm gas} \sim 20$ K the expected emission of HD is much larger than that of molecular hydrogen (see Fig. 1.6). The fundamental rotational transition of HD is at 112 μm (Müller et al. 2005) and it was first detected in the ISM by the *Infrared Space Observatory* (ISO, Wright et al. 1999). It was also covered with increased sensitivity by the PACS instrument on the *Herschel Space Observatory*. This transition has been targeted for a sample of close and bright

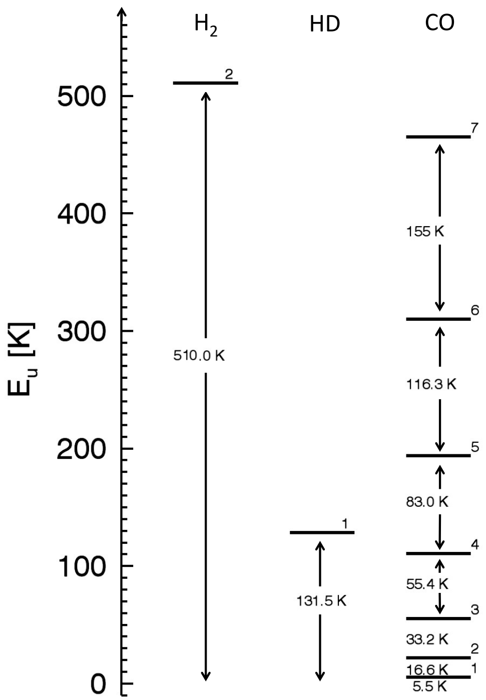


Figure 1.6: Rotational energy levels for H_2 (left), HD (middle) and CO (right). The energy needed to excite the different transitions are reported in Kelvin and are much higher for H_2, than for HD and CO. In particular, thanks to its low-J lines, CO is a good coolant even in cold environments such as disks.

protoplanetary disks, for a total of only 3 detections: TW Hya (Bergin et al. 2013), DM Tau, and GM Aur (McClure et al. 2016). The clear detection of HD in TW Hya was an important result as a very high disk mass, larger than $5 \times 10^{-2} M_{\odot}$, was determined for a relatively old disk (~ 10 Myr).

There are however some caveats in the conversion of HD into total disk mass. The main issue is that the emitting layer of the HD 112 μm line is elevated above the midplane, where the gas temperature is larger than 30 K. This implies that a good knowledge of the disk vertical structure is needed in order not to under- or over-estimate the disk mass. Proper physical-chemical modeling combined with tracers of the disk vertical extent are needed to reduce the uncertainty related to HD-based mass determinations (see Chapter 6).

1.4.3 CO as gas mass tracer

In disks, carbon monoxide (CO) is the second most abundant molecule after H_2 and it is the main gas-phase carrier of interstellar carbon. Furthermore, CO is chemically stable, it has a well studied chemistry and readily implemented in physical-chemical models, and is readily detectable. For these reasons carbon monoxide and its less abundant isotopologues are often used as tracers of gas properties, structure and kinematics in disks and in various other astronomical environments. In particular optically thin lines of less abundant isotopologues, which trace the gas column down to the midplane (van Zadelhoff et al. 2001), can be used as gas mass tracers. This however requires knowledge about the CO-H_2 abundance ratio. Surprisingly, the overall range of CO abundances in different environments such as molecular clouds, excluding the pre-stellar case where the effects of freeze-out are prevalent, is quite narrow between $CO/H_2 \sim 0.5 - 4 \times 10^{-4}$ (see review by Bergin & Williams 2017, and references therein). If isotopologue lines are used, the elemental isotopic ratio is then an additional unknown parameter.

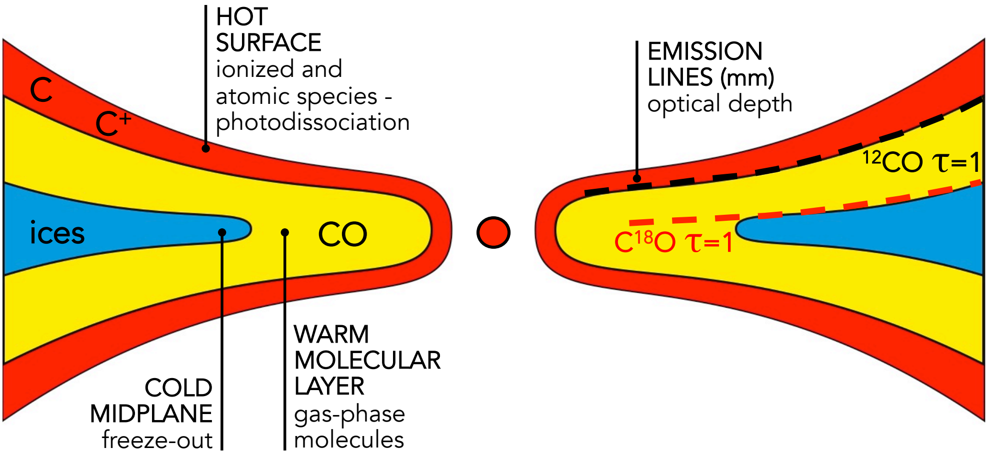


Figure 1.7: Simplified description of the disk thermo-chemical structure.

CO isotope-selective photodissociation and freeze-out

The main processes controlling the survival of carbon monoxide in the gas-phase in protoplanetary disks are CO *photodissociation* by UV photons and CO *freeze-out* onto dust grains (see Fig. 3.1).

CO photodissociation occurs through discrete (line-) absorption of UV photons into predissociative excited states, while absorption of continuum photons is negligible (Hudson 1971; Letzelter et al. 1987; Eidelsberg et al. 1992; Cacciani & Ubachs 2004). The energy needed to dissociate CO is 11.09 eV, thus CO photodissociation is initiated by photons at wavelengths between 911.75 Å and 1117.8 Å. The UV absorption lines are electronic transitions into vibrational levels of excited states and can become optically thick. This makes CO able to shield itself from photodissociating photons. More precisely the UV absorption lines of the main isotopologue ^{12}CO become optically thick at a CO column density $\sim 10^{15}\mathrm{cm}^{-2}$ (van Dishoeck & Black 1988). In disks, this column density is reached at the surface of the warm molecular layer (Fig. 3.1). At a given height in the disk the photodissociation rate drops and CO is able to survive, both because of self- shielding and absorption of FUV continuum attenuation by small dust grains or PAHs.

Photodissociation occurs in a similar manner also for rarer isotopologues (e.g., ^{13}CO, C^{18}O, and C^{17}O), which can self-shield from UV photons and also mutually shield each other (Visser et al. 2009). Being less abundant than ^{12}CO, self shielding happens at higher column densities for rarer isotopologues and accordingly closer to the disk mid-plane. There are regions in the disk where ^{12}CO is already self-shielded and can survive at high abundance, but the rare isotopologues are still photodissociated. There one would find isotopologue ratios (e.g. C^{18}O/ ^{12}CO) that are much lower than the corresponding elemental isotope ratio [^{18}O]/[^{16}O]. In chemical models of disks, the abundance of the rare isotopologues is usually obtained by simply scaling the ^{12}CO abundance with the local ISM elemental isotope ratio (Wilson & Rood 1994). However, in order to correctly interpret CO isotopologues observations, isotope-selective photodissociation needs to be included in the modeling.

Photodissociation rates are also affected by other effects in a depth-dependent manner. In particular, mutual-shielding adds to self-shielding when the UV absorption lines are blended with other species. More precisely, less abundant CO isotopologues can be mutually shielded by ^{12}CO, as well as by H and H_2, if their UV absorption lines overlap. Moreover, at greater depths, the UV continuum radiation is attenuated by small dust grains and PAHs. The photodissociation rate for a particular isotopologue ^{x}C^{y}O can be expressed by the following equation

$$k_{\mathrm{PD}} = \Theta\left[N(\mathrm{H}), N(\mathrm{H}_2), N(^{12}\mathrm{CO}), N(^{x}\mathrm{C}^{y}\mathrm{O})\right]\; k^{0}_{\mathrm{PD}}\;, \tag{1.3}$$

where Θ is a shielding function depending on the H, H_2, ^{12}CO, and ^{x}C^{y}O column densities, and k^0_{PD} is the unshielded photodissociation rate, calculated using the local continuum radiation field. Detailed shielding functions for the various CO isotopologues have been computed by Visser et al. (2009) and adopted in this work.

At the low dust temperatures reached in the disk midplane and far from the central star, CO can freeze-out onto grains. This would decrease the amount of CO in the gas-phase, reducing the line emission. CO freeze-out is a process of particular interest because CO ice is a starting point for prebiotic chemistry (Herbst & van Dishoeck 2009). Unlike photodissociation, freeze-out does not selectively affect different isotopologues, but it needs to be taken into account when modeling disk CO observations. The freeze-out temperature of carbon monoxide is $\sim$ 20 K for a pure CO ice with a binding energy of 855 K measured in the laboratory (Bisschop et al. 2006). It can vary between 17 K and 30 K varying the assumed density and binding energy in mixed ices (see Harsono et al. 2015, and reference therein).

[C]/[H] ratio and volatile carbon depletion

Both CO photodissociation and freeze-out are molecular processes that have been very well characterized in the laboratory and are readily implemented in physical-chemical codes. However, there are additional processes that play a role in reducing the CO abundance with respect to molecular hydrogen. In particular, chemistry can act to reduce the volatile carbon budget available to create CO.

TW Hya, the closest and probably best studied disk, has been observed in the fundamental rotational transition of hydrogen deuteride (HD) with the *Herschel Space Observatory* (Bergin et al. 2013). Comparing with SMA $C^{18}O$ data, Favre et al. (2013) found that the CO-based disk mass was two orders of magnitudes lower than the HD-based disk mass. This result has been confirmed by physical-chemical modeling of the source where freeze-out and isotope-selective photodissociation were treated explicitly (Kama et al. 2016b; Schwarz et al. 2016; Trapman et al. 2017, Chapter 6). This result has been interpreted as a large depletion of volatile carbon happening in the disk and leading to much fainter CO isotopologues lines. Similar results have then been more recently found in other two sources that were detected in HD (McClure et al. 2016).

Volatile carbon depletion may therefore be a more common process than what was initially thought. Which mechanism(s) is (are) responsible for carbon depletion in protoplanetary disks is still under debate. A possible explanation comes from gas-phase reactions initiated by X-ray and cosmic ray ionization of He. The resulting He^+ atoms can react with gaseous CO and gradually extract the carbon, which can then be processed into more complex and less volatile molecules that can freeze onto cold dust grains at higher temperatures than CO (Aikawa et al. 1997; Bruderer et al. 2012; Favre et al. 2013; Bergin et al. 2014; Kama et al. 2016b; Yu et al. 2016). In addition, oxygen will also be removed from the gas due to freeze out of H_2O, CO_2 and CO, even more than carbon (Öberg et al. 2011; Walsh et al. 2015). Accordingly, a way to test the level of carbon depletion in disks is to compare observations of CO isotopologues with species like C_2H and c-C_3H_2, whose gas-phase abundances are particularly sensitive to the gaseous carbon abundance and [C]/[O] ratio. Indeed, C_2H is observed to have very strong emission in the TW Hya disk (Kastner et al.

2015; Bergin et al. 2016) and is particularly strong when both elements are depleted but gaseous [C]/[O]>1 (Kama et al. 2016b). Alternatively, ice chemistry may be the fundamental process turning CO in more complex organics, such CH_3OH, or in CO_2 and CH_4 ice (see e.g. Fig. 3c in Eistrup et al. 2016). Finally, volatile elements, such oxygen and carbon, may be locked up in large icy bodies in the midplane (Bergin et al. 2010; Hogerheijde et al. 2011; Du et al. 2017; Schoonenberg & Ormel 2017). These large pebbles cannot diffuse upward and participate in the gas-phase chemistry (see Du et al. 2015; Kama et al. 2016b). Such a process is likely the cause of the under-abundance of gas-phase water in the surface layers of disks. Another way to trace the level of the volatile carbon available in the disk surface is through observations of the [CI] fine structure lines, as shown e.g. by Kama et al. (2016b).

1.5 Physical-chemical modeling

CO chemistry is fairly simple when compared with other molecules of astronomical interest. However, CO emission lines are sensitive to the gas and dust temperatures, which can vary significantly throughout the disk structure. A good thermo chemical-physical modeling of disks is therefore needed in order to interpret carbon monoxide observation in disks, and of its less abundant isotopologues. For this PhD thesis, the physical chemical code DALI (DustAndLInes Bruderer et al. 2012; Bruderer 2013; Bruderer et al. 2014, see 1.5.1) has been used. Similar modeling codes are ProDiMo (Protoplanetary Disk Modeling Woitke et al. 2009), developed for the interpretation of IR lines observed with *Herschel*, ANDES (Akimkin et al. 2013), and the models by Gorti & Hollenbach (2004); Jonkheid et al. (2004).

1.5.1 DALI

DALI is a powerful physical-chemical code developed by Dr. Simon Bruderer and designed to model CO and simple molecules in disks, with a focus on the gas-phase. As low-J CO lines arise from disk regions where the gas and dust temperatures are slightly decoupled, a proper modeling of the disk gas and dust thermal structure is needed and this is DALI's specialty. The modeling structure is presented in the flowchart in Fig. 1.8. Given a density structure and a stellar spectrum as inputs, the code solves the continuum radiative transfer using a 3D Monte Carlo method to calculate the dust temperature $T_{\rm dust}$ and local continuum radiation field from UV to mm wavelengths. A chemical network simulation then yields the chemical composition of the gas. The chemical abundances enter a non-LTE excitation calculation of the main atoms and molecules. The gas temperature $T_{\rm gas}$ is then obtained from the balance between heating and cooling processes. Since both the chemistry and the molecular excitation depend on $T_{\rm gas}$, the problem is solved iteratively. At each point

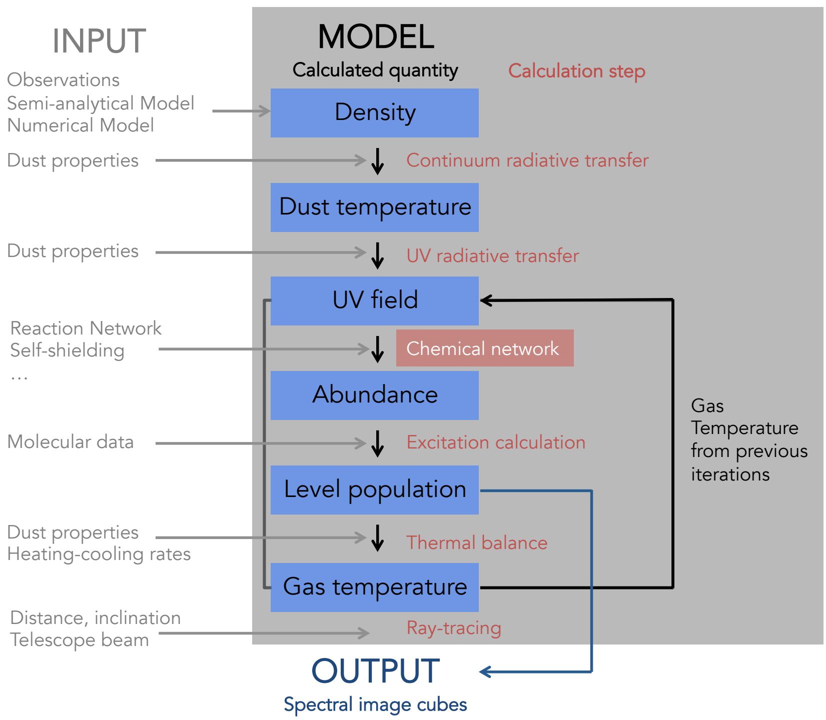


Figure 1.8: DALI modeling flowchart (Adopted from Bruderer et al. 2012). The chemical network calculation step is highlighted in red as this is the part of the code that has been augmented for this PhD thesis. More details are presented in Chapter 2 and 3.

in the disk $T_{\rm gas}$ is assumed to be equal to $T_{\rm dust}$, the heating-cooling balance is run to get a new $T_{\rm gas}$ and the loop runs until the input and output values converge. When a self-consistent solution is found, spectral image cubes are created with a raytracer.

For this PhD thesis, DALI has been extended with a complete treatment of isotope-selective processes. This includes a chemical network with different isotopologues taken as independent species (e.g., ^{12}CO, ^{13}CO, C^{18}O, and C^{17}O) and reactions that enhance or decrease the abundance of one isotopologue over the other. In particular photodissociation, the main process regulating the CO abundance in the gas phase, has been implemented self consistently for CO isotopologues. Also, a simple HD chemistry has been added. More details on the implementation of the new features are presented in Chapters 2, 3, and 6.

1.6 This thesis and future outlook

Determining disk gas masses has been the leading question of this PhD thesis since its origin. CO isotopologues have been promising gas mass tracer candidates for many years and with the advent of ALMA their detection in disks has become routine. The still open question is if chemical isotope-selective effects play a major role in setting the mutual abundance ratios of CO isotopologues and in the determination of disk masses. Therefore this thesis starts from the modeling perspective. Subsequently a larger sample of CO isotopologues observations in disks has been provided by the Lupus Disk Survey with ALMA (Ansdell et al. 2016). The grid of models presented in Chapter 3 has therefore been compared with observations and some more observation-motivated projects have been carried out.

- In Chapter 2 isotope-selective photodissociation, the main process controlling the relative abundances of CO isotopologues in the CO-emissive layer, was properly treated for the first time in a physical-chemical disk model. The chemistry, thermal balance, line, and continuum radiative transfer were all considered together with a chemical network that treats ^{13}CO, C^{18}O and C^{17}O isotopologues as independent species. The main result is that isotope selective processes lead to regions in the disk where the isotopologues abundance ratios are considerably different from the elemental ratios. Accordingly, considering CO isotopologue ratios as constants may lead to underestimating disk masses by up to an order of magnitude or more.

- In Chapter 3 the small grid of models used in Chapter 2 to investigate the effects of CO isotope-selective photodissociation has been expanded. More than 800 disk models have been run for a range of disk and stellar parameters. Total fluxes have been ray-traced for different CO isotopologues and for various low $J-$ transitions for different inclinations. This chapter shows that a combination of ^{13}CO and C^{18}O total intensities allows inference of the total disk mass, although with larger uncertainties, compared with the earlier work by Williams & Best (2014). These uncertainties can be reduced by employing spatially resolved observations, i.e. the disk's radial extent, inclination and flaring. Finally, total line intensities for different CO isotopologue and for various low-J transitions are provided as functions of disk mass and fitted to simple formulae. The effects of a lower gas-phase carbon abundance and different gas-to-dust ratios are investigated as well.

- In Chapter 4 the grid of physical-chemical models presented in Chapter 3 has been employed to analyze continuum and CO isotopologues (^{13}CO $J = 3 - 2$ and C^{18}O $J = 3 - 2$) observations of Lupus disks. Disk gas masses have been calculated for a total of 34 sources, expanding the sample of 10 disks studied by Ansdell et al. (2016). This chapter shows that overall CO-based gas masses are very low for disks orbiting a solar mass-like star, often smaller than $1M_{\rm J}$, if volatile carbon is not depleted. Accordingly, global gas-to-dust ratios are much lower than the expected ISM-value of 100, being predominantly between 1 and 10. Low CO-based gas masses and gas-to-dust ratios may indicate rapid loss of gas, or alternatively chemical evolution, e.g. via sequestering of carbon from CO to more complex molecules, or carbon locked up in larger bodies. The first hypothesis would imply that giant planet formation must be quick or rare, while for the latter the implication on planet formation timescales is less obvious.

- In Chapter 5 another important disk property has been investigated with DALI models, i.e. the gas surface density distribution $\Sigma_{\rm gas}$. Reliable observational measurements of $\Sigma_{\rm gas}$ are key to understand disk evolution and the relative importance of different processes, as well as how planet formation occurs. This chapter investigates whether ^{13}CO line radial profiles, such as those recently acquired by ALMA, can be employed as a probe of the gas surface density profile. By comparing with DALI simulations we find that ^{13}CO radial profiles follow the density profile in the middle-outer disk. The emission drops in the very inner disk due to optical depth, and in the very outer disk due to a combination of freeze-out and inefficient self-shielding. Ranges of radii and line emission fluxes are provided to observers, where fitting line emission radial profiles gives reliable value for the surface density power-law index γ.

- In Chapter 6 simple deuterium chemistry has been added to the chemical network in DALI to simulate HD lines in disks. The aim is to examine the robustness of HD as a tracer of the disk gas mass, specifically the effect of gas mass on the HD far infrared emission and its sensitivity to the disk vertical structure. The uncertainty on HD-mass determination due to disk structure is found to be moderate and HD observations should be considered as an important science goal for future far-infrared missions.

The main conclusions of this thesis are the following:

1. CO isotope-selective photodissociation needs to be properly considered when modeling rare CO isotopologues emission. Otherwise, C^{18}O lines emission could be overestimated and the derived gas masses could be underestimated by up to an order of magnitude or more.

2. Disk gas masses can be inferred by a combination of ^{13}CO and C^{18}O total intensities, although with non-negligible uncertainties, up to two orders of magnitude for very massive disks.

3. CO-based disk gas masses derived in Lupus are extremely low, often smaller than 1 M_J and the global gas-to-dust ratios are predominantly between 1 and 10. This may be interpreted as either rapid loss of gas, or fast chemical evolution.

4. The shape of the disk surface density distribution can be constrained by spatially resolved ^{13}CO observations, if optical depth, freeze-out and self shielding are properly considered in the modeling.

5. HD far-infrared emission can be used to determine disk gas masses with moderate uncertainty which depends mainly on the disk vertical structure. Such observations should be considered as an important science goal for future far-infrared missions.

The question on disk gas masses remains open. CO isotopologues are still promising mass tracers candidates, as their detection is routine for ALMA, but they need to be calibrated. This thesis shows that the process of isotope-selective photodissociation is important for a good interpretation of CO isotopologues as gas mass tracers. However photodissociation, at least for the case of TW Hya and possibly for other disks, is not the main process responsible for the observed faint CO isotopologues lines. In turn, volatile carbon depletion is a process that needs to be further investigated and understood. Where does the carbon go? The detection of slightly more complex molecules, such as the hydrocarbons C_2H and c-C_3H_2 could be a way to calibrate CO-based gas masses (see e.g., Bergin et al. 2016). Another option is to enlarge the sample of [CI] line detections, which allow inference of the volatile carbon abundance in the upper regions of the disk (see Kama et al. 2016b). Finally, if the HD fundamental lines can be covered at high enough spectral resolution with SPICA, their detection will provide an unique independent tracer of the disk mass.