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Observations of the Chemistry in Circumstellar Disks

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Abstract. Circumstellar disks around classical T Tauri stars have still large amounts of primary molecular gas and dust, which may evolve to form planetary systems. Although it is the remnant of the parental cloud, the gas component shows significant chemical evolution. Fundamental disk properties (kinematics, size, temperature profile) can be derived from observations of CO lines with mm arrays. Less abundant molecules have been discovered with the IRAM 30-m telescope, in the DM Tau and GG Tau disks. Despite the high depletion factors which are measured with respect to the nearby Taurus cloud, these molecules allow independent measurements of the disk density. These observations provide an overview of the properties of young (a few Myr) proto-planetary disks around low-mass stars as seen by current mm instruments.

1. Introduction

Understanding how planets and life appeared is one of the older dreams of mankind. Nowadays, circumstellar disks of gas and dust found around classical TTauri stars (CTTs) are intensively studied from the optical to the mm wavelengths. CTTs, also designated as Class II objects (Adams et al. 1987), are Pre-Main-Sequence (PMS) low-mass stars (around 0.5–2 $M_\odot$) of a few Myr which have already dissipated their envelopes and where the main outflow phase is over. They are analogous to our Sun when it was still surrounded by a flattened structure of rotating gas and dust: the so-called protosolar nebula which provided the material to build the Solar System. Therefore, understanding the physics, the chemistry and the evolution of these disks, is the important clue to find how planetary systems form around solar-type stars. The observation of circumstellar disks is not easy, due to their small sizes (radius of $\sim$2–5$''$ or 150–800 AU at 150 pc, the Taurus distance) and to confusion with foreground and background gas associated with parent molecular clouds. In such disks, except at a few AU from the star, the gas and the dust, heated by the central star, remain at relatively low temperatures and radiate at long wavelengths, from the far-infrared to millimeter waves. Therefore, in the last few years, many disks have been resolved in the thermal continuum of the dust and CO J=1–0 or J=2–1 lines by mm interferometers (Koerner et al. 1993; Dutrey et al. 1994). These observations reveal the disks to be large ($R_{out} \sim$ 300–800 AU) and in Keplerian rotation. The quality of the images allows in some cases the first quantitative analysis of the disk properties in terms of radial distributions for the temperature or the density. Moreover, observations also reveal that CO is underabundant (by factors around 5−20), making the optically thinner isotopomer $C^{18}O$ difficult to detect. In fact, current mm arrays (and large single-dish radiotelescopes) are not sensitive to the gas content at the scale of our Solar System. At the Taurus distance, current mm instruments allow to study the properties of the CO outer disk ($R > 30-50$ AU) or by reference to our own Solar System, the part of the gas disk which would be located beyond the Kuiper Belt. Information inferred from CO lines using present mm arrays are not directly relevant to the inner disk (within $R < 30-50$ AU).

Searching for other species than CO is even more difficult because one expects these species to be i) more depleted, and to have ii) optically thinner transitions and/or iii) sub-thermally excited lines. However, finding other tracers than CO or the thermal dust emission is of prime importance, not only to understand the chemistry of the disks and their evolution towards planet formation, but also to properly estimate the H_2 mass of the disks in a way which is free of assumptions about the dust properties and the gas-to-dust ratio.

2. Properties of CO Disks as Imaged by the IRAM Array

So far, gas disks around T Tauri stars are mostly observed in the rotational lines of CO because carbon monoxide remains the most abundant molecule in disks after H_2. The first rotational levels of CO are very easily populated by collision with H_2 and fully thermalized at the high H_2 densities ($\geq 10^6$ cm^{-3}) encountered in disks. CO observations also allow to study the kinematics which can only be addressed by spectroscopy.

2.1. Disk modelling

Quantitative physical information can be deduced from CO maps. This, however, requires (i) high signal-to-noise maps at high spectral resolution (~ 0.2–0.1 km s^{-1}); (ii) a realistic disk model; and (iii) a minimization procedure on the model parameters to determine not only the best parameters, but also the associated errors. Fortunately, Keplerian disks are relatively simple to model and constrain. Following Pringle (1981), a disk can be modeled by a geometrically thin disk in hydrostatic equilibrium where physical parameters such as the temperature, the density, and the velocity field are parameterized by power laws versus disk radius. Since CO lines are thermalized, LTE conditions can be assumed and the radiative transfer equation solved step by step along the line of sight (Dutrey et al. 1994). Performing a χ^2 minimization is the more difficult part of the work. Minimization must be performed directly inside the UV plane in order to avoid non-linearity effects associated to the deconvolution process. A complete description of a minimization process is given by Guilloteau & Dutrey (1998).

2.2. Results from CO maps

This process was first applied on DM Tau, a CTT star of age about $\sim 5 \times 10^6$ yr and spectral type M1, located in a region of the Taurus cloud devoid of CO emission. A Keplerian disk was first reported by Guilloteau & Dutrey (1994), and Guilloteau & Dutrey (1998) used the high sensitivity of the IRAM interferometer to map the gas disk in CO J=1–0. Fig. 1 displays the results of their

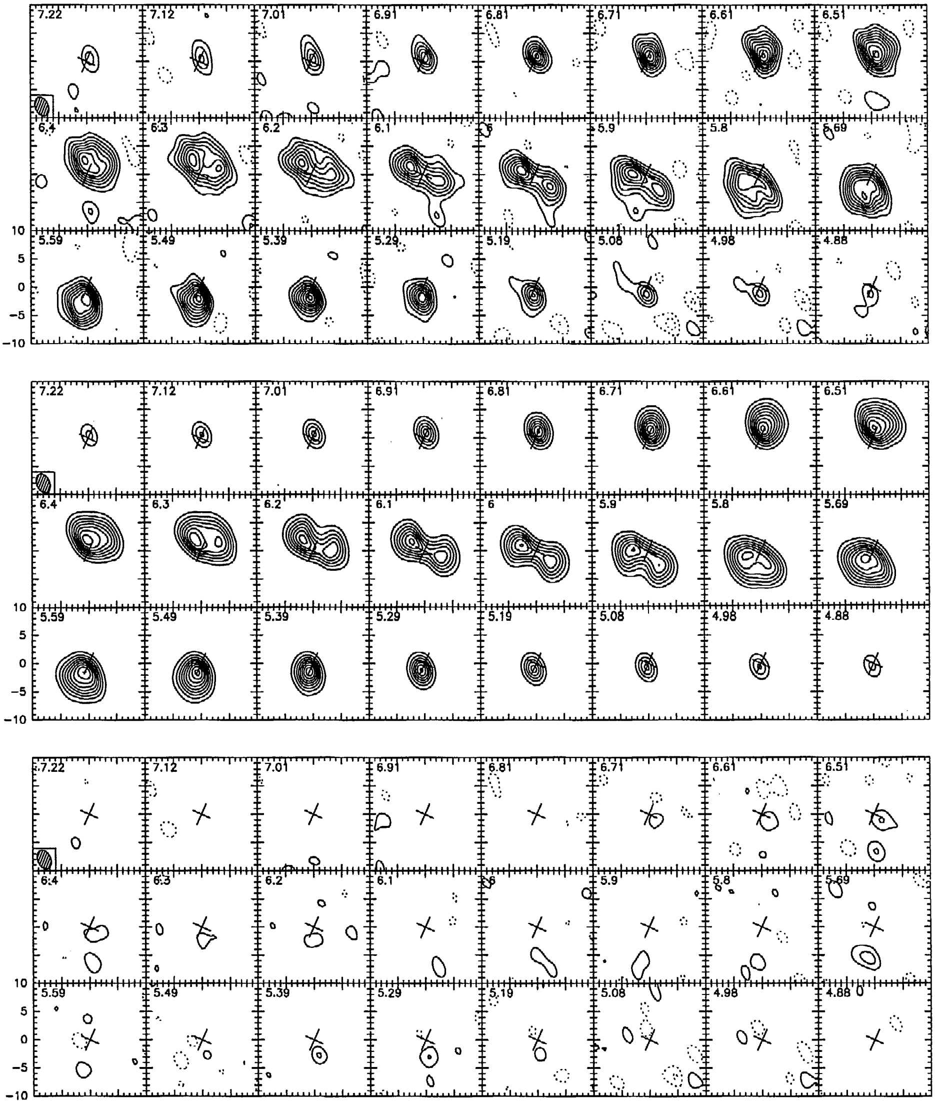

Figure 1. Channel map of the ^{12}CO J=1–0 toward DM Tau. The angular resolution is $3.5 \times 2.4''$ at PA 24°. Coordinates are offsets in $''$ from the continuum position, R.A. $04^h\,33^m\,48.735^s$, Dec. $18°\,10'\,10.2''$ (J2000.0). Contour spacing is 80 mJy/beam, or 0.9 K ($2\,\sigma$). The LSR velocity is indicated in each panel. The cross indicates the position of the continuum source, and the orientation of the disk axis. Middle: best model, with same contour levels. Bottom: difference between observations and best model (from: Guilloteau & Dutrey 1998).

analysis: the observed CO map (top), the best model obtained after χ^2 minimization (middle) and the difference between the data and the model (bottom).

Applying this method on a larger sample of stars (7 stars), Dutrey et al. (in prep.) find that:

1. The CO velocity laws are in good agreement with Keplerian rotation around the central objects with $V(r) \propto r^{-0.50\pm0.05}$.
2. The kinematic patterns indicate that the turbulence is small, of order ~ 0.1 km s^{-1} or less.
3. The temperatures typically scale as $T_k(r) \simeq 30 \times (r/100\ \mathrm{AU})^{-(0.60-0.65)}$, and are consistent with stellar heating in flared disks.

Since the rotation pattern is Keplerian, the velocity derived from CO provides a measurement of the stellar mass (neglecting the disk mass itself). Accuracies better than 10% (not including the distance uncertainties, the masses being proportional to the distance of the star) have been reached. However, since the ^{12}CO J=2–1 line is highly optically thick, the density profile in the disk, and *a fortiori* the H_2 mass cannot be measured.

3. Disk Mass Measurements: Towards Observable Chemistry

3.1. Classical methods to measure disk masses

Measuring the mass requires to have an optically thin tracer of known emission coefficient. This can be either (i) the thermal dust emission in the mm domain (the most usual method); or (ii) molecular species with optically thin emission lines. In the first case, a proper knowledge of the dust absorption coefficient is required, together with the gas-to-dust ratio. This proves to be difficult in protoplanetary disks, where grain properties are modified compared to the standard interstellar medium, and the gas-to-dust ratio could be anomalous. In the second case, both the molecular properties (line strength, excitation) and abundance relative to H_2 must be known. In disks around low-mass stars, the material is cold, and depletion by condensation of molecules on grains should occur for many molecules (Aikawa et al. 1997), making standard hypotheses on molecular abundances highly invalid.

The first attempt to estimate the CO depletion in a Class II object, using resolved interferometric images which reduce the beam dilution effects, was done in the GG Tau circumbinary ring. Dutrey et al. (1994) compared the H_2 mass of the disk deduced from the optically thin ^{13}CO J=1–0 image to those measured from the 2.7 mm dust map obtained simultaneously. They conclude that CO is depleted by a factor of ~ 20, assuming "standard" protoplanetary dust properties and gas-to-dust ratio (100).

3.2. Alternate mass measurement method: the excitation constraints

Molecular line excitation offers an alternate way to constrain the outer disk masses, independent of any assumption about the dust properties or molecular abundances. The basic idea (Dutrey et al. 1997) is to constrain the local H_2 density by measuring molecular lines of various critical densities. A lower limit

Table 1. Detections and upper limits (3σ) of molecules in the DM Tau disk

Molecules	TMC-1	Line	S_ν	M_D	R_{out}
^{12}CO	8(-5)	2-1	13.95(.43)	1.6(-5)	360
^{13}CO	4(-6)	2-1	5.40(.13)	1.4(-4)	230
$C^{18}O$	4(-7)	2-1	.68(.07)	1.5(-4)	80
HCN	2(-8)	1-0	.38(.05)	7.8(-5)	100
		3-2	<3.0	<3(-5)	<75
HNC	2(-8)	1-0	.16(.03)	3.7(-5)	90
CN	3(-8)	1-0	1.38(.24)	2.5(-4)	120
		2-1	8.7(0.4)	2.2(-4)	150
CS	1(-8)	3-2	.47(.07)	9.9(-5)	100
		5-4	.67(.11)	5.2(-5)	73
C^{34}	5(-10)	5-4	.38(.11)	6.1(-4)	56
H_2CO	2(-8)	2_{12}-1_{11}-o	.30(.04)	7.4(-5)	110
		2_{02}-1_{11}-p	.11(.04)	3.4(-5)	50
		3_{13}-2_{12}-o	.48(.04)	3.3(-5)	76
HCO^+	8(-9)	1-0	.82(.04)	2.1(-4)	220
		3-2	4.1(.5)	3.9(-5)	165
C_2H	8(-8)	1-0	.55(.08)	4.0(-4)	240
$H^{13}CO^+$	1.1(-10)	1-0	<.06	<1.3(-3)	<120
N_2H^+	5(-10)	1-0	<.45	<1.6(-3)	<220
SiO	$\leq$ 4(-12)	2-1	<.13	<1.6(-1)	<82
		5-4	<.36	<4.0(-2)	<59
SiS	1(-11)	5-4	< .09	<1.7(-1)	<65
		8-7	< .09	<6.4(-2)	<42
H_2S	$\leq$ 5(-10)	1_{10}-1_{01}	<.50	<3.5(-3)	<105
C_3H_2	$\leq$ 4(-10)	1_{10}-1_{01}	<.14	<5.5(-3)	<86
HC_3N	6(-9)	10-9	< .07	<8.0(-5)	<58
		16-15	<.15	<1.5(-4)	<55
CH_3OH	2(-9)	3_0-2_0	<.24	<2.8(-2)	<87
CO^+	$\leq$ 1(-11)	2-1	<.54	<1.2(-2)	<68
SO		6_5-5_4	<.28		
SO_2		25_{323}- 24_{420}	<.16		
SiC_2		4_{04}-3_{03}	<.15		
HNCS		12_{012}- 11_{011}	<.23		
HCO		1_{10}-0_{00}	<.12		
$HCOOCH_3$		20_{020}-19_{019}	<.40		
$HOHCS^+$		2-1	<.14		

S_ν is given in Jy km s^{-1}, M_D in $M_\odot$ and R_{out} in AU; see Dutrey et al. (1997) for details. Abundances measured in TMC-1 come from Ohishi et al. (1992) and Cernicharo & Guélin (1987). Standard isotopic ratios are assumed for $^{13}CO/C^{18}O$ =10, $CS/C^{34}S$=20, o-H_2CO/p-H_2CO=3. Areas have been obtained by fixing the position and linewidth to 6.05 and 1.4 km s^{-1} (derived from the best Gaussian fit to ^{13}CO J=2–1). T_k is taken equal to 20 K, as a reasonable average value (Guilloteau & Dutrey 1994). Upper limits are calculated as explained in Dutrey et al. (1997, Sec.3.)

on the H_2 density can be placed when excited lines such as HCO^+ J=3–2 are detected. On the other hand, an upper limit on the H_2 density is given by upper limits on higher excitation transitions (e.g. HCN J=3–2) provided: (i) the molecule is sufficiently abundant; and (ii) the limit is significant. In practice, these two conditions require to detect lower transitions from the same molecule (i.e. HCN J=1–0 in the example above). This direct measurement method thus naturally leads to the beginning of *observational chemistry*, since a larger number of observed molecular lines will provide more constraints on the H_2 density. A by-product of the observations is a direct measurement of the molecular abundances with respect to H_2.

3.3. Molecular species found in protoplanetary disks

The method was applied by Dutrey et al. (1997) to GG Tau and DM Tau. Using the IRAM 30-m, Dutrey et al. reported the detection of several transitions of HCO^+, CN, CS, HCN, HNC, H_2CO and C_2H, in addition to ^{13}CO and $C^{18}O$ (see Table 1 and Fig. 2). Not surprisingly, the detected molecules are the most abundant species found in the Taurus cloud. The higher excitation lines detected (CN J=2–1 or HCO^+ J=3–2) provided a minimum value for the H_2 density and the HCN J=3–2 gave an upper limit (since only HCN J=1–0 was detected). Comparing this *direct* measurement of the mean H_2 density with the observed H_2 column density, we were able to (i) derive *directly* the gas disk mass; and (ii) evaluate the molecular depletion by reference to molecular abundances measured in TMC1. Since the circumbinary disk of GG Tau has a density structure which is complicated by the binarity, we only estimated abundances and disk masses in the case of DM Tau. We assumed a simple power law model for the density distribution and a uniform temperature in agreement with CO J=1–0 data. The main results are:

1. CO is depleted by a factor of about $\sim 5-8$
2. Other molecules are depleted up to factors ~ 100 (HCN, H_2CO)
3. The mass of the DM Tau disk is about ~ 0.004 $M_\odot$, still 7 times smaller than the mass derived from the dust emission (~ 0.03 $M_\odot$)
4. Molecules specific for photon dominated regions (PDRs) such as CN or C_2H appear less depleted with depletion factors of about 10
5. On the contrary, HCN is strongly depleted by factors of about 100

The disagreement mentioned in (3) could imply that the gas-to-dust ratio differs from the canonical value of 100, and/or that the dust emissivity differs from the values quoted by Beckwith et al. (1990). Nonetheless, both continuum and molecular data suffer from different observational biases and a deeper analysis is required to solve the discrepancy.

Points (4) and (5) might be linked because CN is a photodissociation product of HCN. A photodissociation origin for CN could be realistic in a flared disk where the disk surface is intercepting the stellar UV field, in addition to the ambient UV field (see also Aikawa & Herbst, this volume). Only high angular resolution maps in CN and HCN giving the distribution of both molecules will permit to understand the origin of CN distribution.

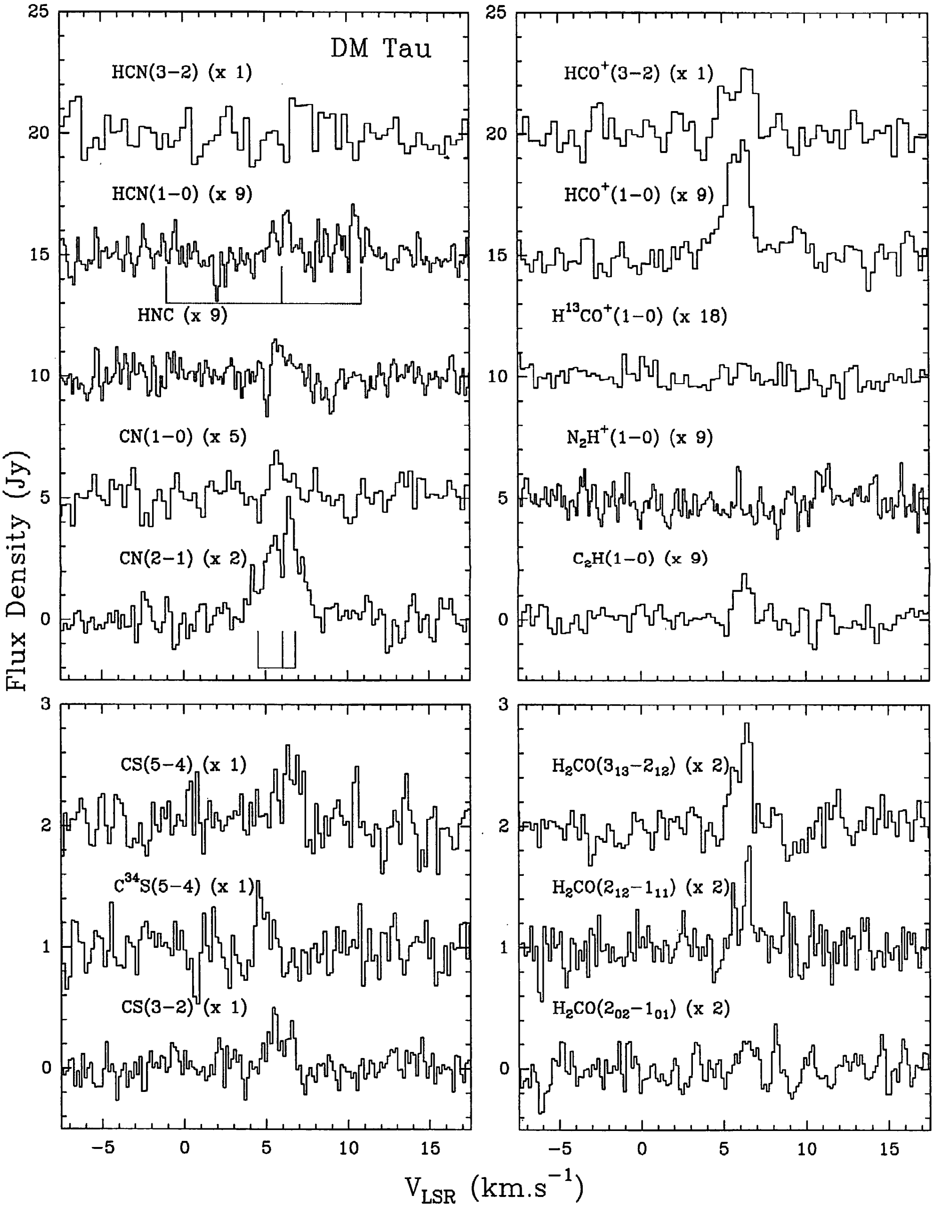

Figure 2. Molecular detections in the disk of DM Tau, done with the IRAM 30-m telescope (from: Dutrey et al. 1997).

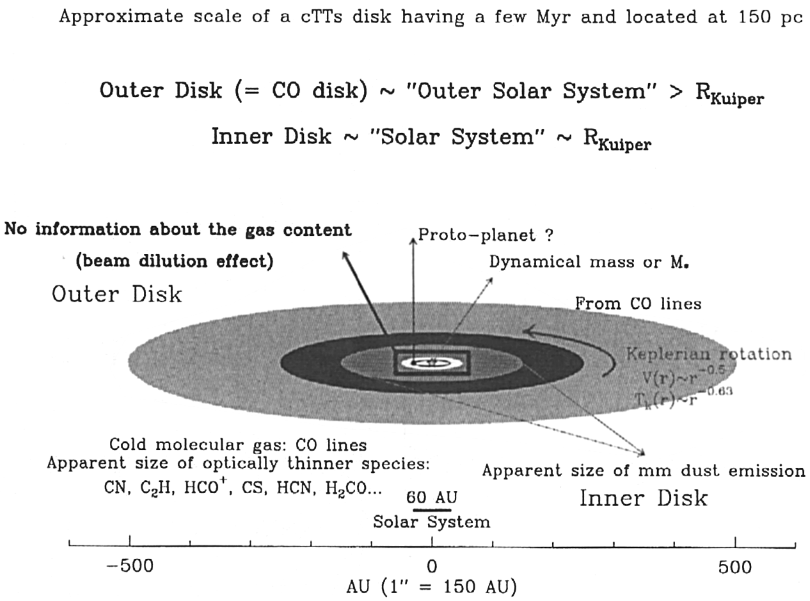

Figure 3. A montage showing which part of the disk is viewed with current mm arrays in continuum and in molecular lines. The disk is at 140 pc. For comparison the scale of our own solar system is mentioned.

4. Observational Overview and Prospects

Quantitative studies of the chemical processes in action in protoplanetary disks are limited by the sensitivity of current mm instruments. Understanding planetary formation requires (i) to map the gas in the inner part of the disk, at the scale of our solar system (30–50 AU); and (ii) to image molecular emissivity $E(r)$ in the *optically thin region* or $E(r) \propto T_k(r) \times \Sigma(r) \times X(r)$ (in the Rayleigh-Jeans approximation), $\Sigma(r)$ being the surface density law and $X(r)$ the molecular abundance.

The limited sensitivity does not allow to detect molecular species in the inner part of the disks, typically $R \leq 30$–80 AU (depending on the collecting area and integration time). Interferometers allow to map molecular emission, but the typical brightness sensitivity reached by current mm arrays (typically 1 K for sub-arcsecond resolutions) restrict these images to optically thick regions. The outer optically thin regions, at $R \geq 150$–250 AU or 1–2″ (Taurus distance), remain below the threshold of detection.

Fig. 3 gives an overview of the current possibilities and limitations. Observations of CO lines allow to determine the size of the disk, the nature of the rotation pattern and to measure the stellar mass. They also provide estimates of the kinetic temperature profile in the outer part of the disk. The inner part, strongly beam diluted and hidden to us, is still highly model dependent. Other molecular species mapped today are coming from the cold outer part, but the apparent sizes of their distribution are limited by the sensitivity of current arrays. The study of the chemistry of protoplanetary disks a few Myr old, in which the gas is a remnant of the parent cloud, remains strongly sensitivity limited. Older, more evolved objects which are in the process of dissipating their disks can only be searched in CO lines.

Further progress will require an increase in sensitivity, to enable observations of rarer molecular species, and in angular resolution, to enable studies of chemical stratification in the disk. Since spectral lines are Doppler broadened, these improvements can only result from a very significant increase in collecting area. With a collecting area of 7000 m^2, the Atacama Large Millimeter Array (ALMA) will open this domain to our understandings.

References

Adams, F.C., Lada, C.J., & Shu, F.H. 1987, A&A, 312, 788
Aikawa, Y. 1997, A&A, 476, 684
Beckwith, S.V.W., Sargent, A.I., Chini, R.S., & Guesten, R. 1990, AJ, 99, 924
Cernicharo, J. & Guélin, M. 1987, A&A, 176, 299
Dutrey, A., Guilloteau, S., & Simon, M. 1994, A&A, 286, 149
Dutrey, A., Guilloteau, S., & Guélin, M. 1997, A&A, 317, L55
Guilloteau, S. & Dutrey, A. 1994, A&A, 291, L23
——— 1998, A&A, 339, 467
Koerner, D., et al. 1993, Icarus, 106, 2
Ohishi, M., Irvine, W.M., & Kaifu, N. 1992, in The Cosmochemistry of Astronomical Phenomena, IAU Symposium 150, ed. P.D. Singh, 171
Pringle, J. 1981, MNRAS, 248, 754

Discussion

C. Qi: In your single dish surveys, have you detected any N_2H^+ lines?

A. Dutrey: We have searched for N_2H^+, both in DM Tau and GG Tau, but we did not detect it. The non detections are published in Dutrey et al. (1997).

Y. Aikawa: Are there any other molecules detected towards BP Tau except CO?

A. Dutrey: No, I am afraid that we need to wait for ALMA in order to do it.

E.F. van Dishoeck: Can you elaborate on the results from your HCO^+ 1–0 survey of disks?

A. Dutrey: We have detected and mapped HCO^+ 1–0 in the sources where we were able to do the χ^2 analysis of the ^{12}CO 2–1 data. HCO^+ seems to be a relatively good tracer of disks.

D. W. Koerner: Have you considered probing the inner disk by modeling emission in the line wings?

A. Dutrey: The sensitivity is still not available.