New Trends in Radio Astronomy in the ALMA Era:
The 30th Anniversary of Nobeyama Radio Observatory
ASP Conference Series, Vol. 476
Ryohei Kawabe, Nario Kuno, and Satoshi Yamamoto eds.

Molecular Line Observations of Protoplanetary Disks

E. Chapillon

Academia Sinica Institute of Astronomy and Astrophysics, P.O. Box 23-141, Taipei 10617, Taiwan

Abstract. Understanding the structure of the protoplanetary disks surroundings low to intermediate mass star is a prerequisite to constrain planets formation mechanism. The study of molecular lines emission is an efficient tool to investigate the disk structure, since different molecule exist in different physical conditions. Here I present and discuss the observations of molecular gas at very low temperature in T-Tauri disks, and the search for new molecular tracers, with the recent detection of HC_3N and upper limits on H_2D^+, CCS , H_2S and SO.

1. The Thermal Structure

The overall thermal structure of dust in disks can be roughly described by a simple model: near the mid-plane and below ~ 2 scale heights, the gas temperature is imposed by the dust temperature because of the very high densities. Somewhat above, when the density becomes low enough, the gas and dust temperature are decoupled. Even further above, a hot atmosphere surrounds the whole disk. This simplistic model does not take into account grain growth and sedimentation process, both process affecting disk thermal structure since grain temperatures depend on their size (e.g. Kruegel & Walmsley 1984).

Because of this thermal structure, chemical models predict a layered structure for the disk. In the mid-plane, the low temperatures and high densities, combined with the high extinction, which limits photo-desorption, lead to a region where most molecules stick on dust grains and are severely depleted in the gas phase. Above this cold layer, thermal (and photo) desorption creates a lukewarm, molecular rich, layer. Further above, the high incident UV flux from the central object photodissociates the molecules and leads to a (dense) PDR.

From a multi-isotope multi-transition study of CO in disks, Dartois et al. (2003) and Piétu et al. (2007) found that a substantial fraction of the gas-phase CO is at temperatures below 17 K, the freeze-out temperature of CO. Moreover, Henning et al. (2010) and Guilloteau et al. (2012) derived temperature as low as $6-15$ K at R=300 AU radius from CCH and CS observation in disks around T-Tauri stars.

Chapillon et al. (2012b) present IRAM-PdBI observation of the CN $J = 2 - 1$ and HCN $J = 1 - 0$ lines in two T-Tauri (DM Tau and LkCa 15) and one Herbig Ae stars (MWC 480). Molecular column densities and gas temperatures derived using a simple power-law parametric model (Diskfit, described in Piétu et al. 2007) are shown in Table 1. If the observed gas temperature is in the expected order of magnitude for the warm Herbig Ae ($\sim$ 30 K), it is surprisingly very low in the cooler T-Tauri ($<$ 10 K), whereas HCN and photodissociation product CN are expected to lay in the upper layers of the disks. This result may indicate that the lines are not thermalized (which is unlikely for CO and HCN $J = 1-0$ that are expected to originate from the the dense part of the disk), or that the molecular layer is indeed cooler than predicted. A chemical modelling of the disks using the Meudon PDR code (Le Petit et al. 2006) was performed to test the influence of several parameters : the UV field, the cosmic ray ionisation rate, the grain size distribution, and the gas-to-dust ratio. The majority of the CN column density is build at densities higher than 10^6 cm^{-3} (thus the emission should be thermal), and at temperature higher than 30 K, in contradiction with observations (Chapillon et al. 2012b). We do not succeeded to reproduce the observed temperature and column density.

In T-Tauri disks, these mm results were reinforced by the detection with HSO at a very low level of H_2O (e.g. Hogerheijde et al. 2011) which also suggests that the molecule rich medium is colder than expected.

Table 1. Column density and temperature distribution derived from observation.

Source	Molecule	$\Sigma_{R=300\,AU}$ [cm^{-2}]	p	Tk$_{R=300\,AU}$ [K]	q
MWC 480	HCN(1-0)	1.1 ± 0.4·10^{12}	2.4 ± 0.4	30^a	0^a
	CN(2-1)	10.4 ± 0.9 ·10^{12}	2.1 ± 0.1	30 ± 4	0^a
LkCa 15	HCN(1-0)	10.6± 1.5·10^{12}	1.1 ± 0.2	7.0 ± 0.6	0.55 ± 0.25
	CN(2-1)	58.0 ± 5.0 ·10^{12}	0.8 ± 0.1	8.8 ± 0.3	0.95 ± 0.05
DM Tau	HCN(1-0)	6.5 ± 0.9 ·10^{12}	1.0 ± 0.3	6.0 ± 0.4	0.00 ± 0.12
	CN(2-1)	35.0 ± 9.0 ·10^{12}	0.6 ± 0.06	7.5 ± 0.3	0.60 ± 0.05

Column density $\Sigma(r) = \Sigma_{R_0}(r/R_0)^{-p}$. Temperature $T(r) = T_{R_0}(r/R_0)^{-q}$.
^{a} : fixed parameter.

The protoplanetary disk mid-plane is expected to be a dense, cold medium depleted in molecules, especially CO (that should be frozen onto grain mantles).

The light molecule H_2D^+ is a tracer of cold and CO-depleted environments. It is therefore a good candidate to explore the disks mid-planes. Chapillon et al. (2011) performed a deep search for H_2D^+ in the disks surrounding the T-Tauri TW Hya and DM Tau using the APEX and JCMT telescopes. The o-H_2D^+ line at 372 GHz is not detected in both source, but the upper limit is improved by a factor of $\sim$ 3 compared to previous publication. The influence of the CO abundance in gas phase, the cosmic ray ionisation rate and the grain size on the column density of H_2D^+ has been tested thanks to a chemical model adapted to Deuterium chemistry (presented in Parise et al. 2011). No constrain on the remaining quantity of CO in gas-phase close to the disk mid-plane can be derived from these observations (see fig 1). H_2D^+ may not be a sufficiently sensitive tracer of the disk mid-plane.

2. Searching for New Molecular Tracers

The observation of new tracers will bring constraints on chemical models and physical models of disks, and is a necessary step towards the understanding of the molecular complexity in such environments.

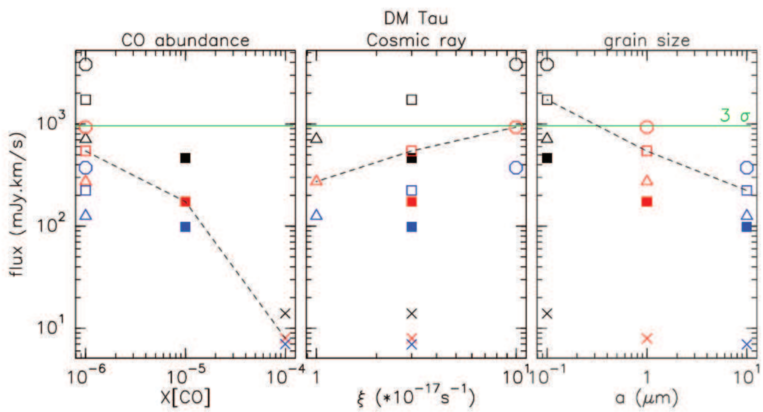

Figure 1. ortho-H_2D^+ line flux as function of CO abundance (left panel), cosmic ray ionization rate (central panel) and grain size (right panel) in the case of DM Tau. The green line shows the 3σ upper limit derived from observation.

Among potential new molecular tracers, H_2S and CS are interesting because they are observed in comets. H_2S is predicted to be abundant in gas phase by Pasek et al. (2005).

Dutrey et al. (2011) searched for CS, H_2S and SO using the IRAM-30m telescope. SO and H_2S were not detected, but the upper limits were improved by a factor 7. CS in detected in the T-Tauri disks (see Table 2). A chemical modelling was performed thanks to the gas-grain code Nautilus (Hersant et al. 2009). The order of magnitude of the predicted column densities of CS and SO is in agreement with the values derived from observations, but the predicted H_2S column density is overestimated in the chemical model by two order of magnitudes. Considering that grain surface chemistry is poorly constrained, an hypothesis to explain this result is that H_2S may be locked into grain mantles, and then react to form other molecules.

Table 2. Column densities (and 3 sigma limits) derived from observations

			$\Sigma_{R=300\,AU}$ [cm^{-2}]		
Souce	SO	H_2S	CS	HC_3N	CCS
LkCa 15	$\leq 1.9 \cdot 10^{12}$	$\leq 3.6 \cdot 10^{11}$	$8.7 \pm 1.6 \cdot 10^{12}$	$8 \pm 2 \cdot 10^{11}$	$\leq 1.4 \cdot 10^{12}$
GO Tau	$\leq 8.9 \cdot 10^{11}$	$\leq 1.8 \cdot 10^{11}$	$2.0 \pm 0.16 \cdot 10^{12}$	$13 \pm 2 \cdot 10^{11}$	$\leq 1.2 \cdot 10^{12}$
DM Tau	$\leq 7.5 \cdot 10^{11}$	$\leq 1.4 \cdot 10^{11}$	$3.5 \pm 0.1 \cdot 10^{12}$	$\leq 3.5 \cdot 10^{11}$	$\leq 1.1 \cdot 10^{12}$
MWC 480	$\leq 2.5 \cdot 10^{12}$	$\leq 4.1 \cdot 10^{11}$	$\leq 8.4 \cdot 10^{11}$	$6 \pm 1 \cdot 10^{11}$	$\leq 0.9 \cdot 10^{12}$

In addition, we searched for heavy molecules. These tracers are interesting not only to study chemistry but also to investigate in details the kinematic (as the line emission from an heavy molecule will be less sensitive to the thermal broadening).

Chapillon et al. (2012a) searched for CCS and HC_3N using the IRAM facilities (30m and PdBI). HC_3N was successfully detected in two T-Tauri and one Herbig Ae: GO Tau, LkCa 15 and MWC 480 (see table2) while CCS was not detected. Chemical models performed with the Nautilus code overestimate the HC_3N column density by more than an order of magnitude. The values derived for CCS are in agreement with the observations. This emphasizes the uncertainties on the nitrogen-bearing molecule chemistry.

3. Summary

A long-term study of chemistry in protoplanetary disk done mainly in the frame of the CID consortium has lead to several results. i) The observation of CO, CN, HCN, CCH, CS in gas phase at low temperature (∼10K) in T-Tauri disks, which challenges the current thermal structure predicted by thermo-chemical models. ii) The column densities of Sulphur and Nitrogen bearing molecules are not yet well reproduced by disk models. iii) The detection of new molecular species in disks is not easy, even with the new instruments. These results point out toward the importance of the grains For the chemistry in disks. Indeed dust grains play a role in the UV transfer (extinction curve), the thermal structure (grain temperature depend on theirs size, thermal coupling with gas...) and the chemistry (surface reaction, desorption process). In particular, the photo-desorption process may explain the observation of molecules at very low temperature (see the detection of cold water vapor in dense clouds by Caselli et al. 2012).

Acknowledgments. The author thanks all the members of the CID consortium.

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