Molecular line observations of protoplanetary disks

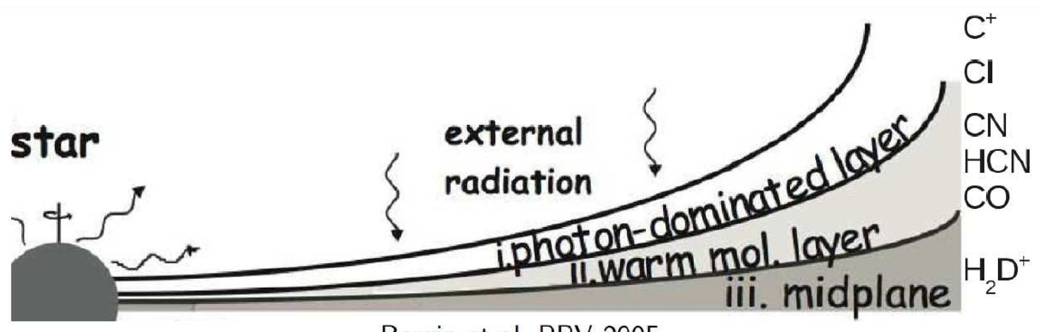
Edwige Chapillon (1) and the CID consortium : A. Dutrey (2), T. Henning (3), S. Guilloteau (2), V. Wakelam (2), F. Hersant (2), M. Guélin (4), F. Gueth (4), V. Piétu (4), N. Ohashi (1), Y .Boehler (5), M. Simon (6), D .Semenov (3), R. Lauhnardt (3), K. Schreyer (7), and P. Barise (8)

1: ASIAA, Taiwan, 2: LAB, France, 3 :MPIA, Germany, 4 : IRAM, France, 5 : UNAM, Mexico, 6 : SUNY Univ.,USA, 7 :Jena, Germany, 8 : MPIfR, Germany

We summarize in this poster a long-term study of the chemistry as a powerfull tool to constrain the protoplanetary disk physics. Most of the above results were obtained in the frame of the CID (Chemistry In Disks) consortium

Structure of the outer disk (R > 10 AU) from models

3 layer structures :
- **PDR surface**, chemistry is driven by UV radiation
- **Molecular layer** rich gas-phase chemistry
- Cold, dense, depleted **mid-plane**, with chemistry on grains ?



Bergin et al. PPV 2005

Already detected molecules in disks in mm domain : (cold clouds chemistry)
- CO, 13CO, C18O
- CN, HCN, HNC, CS, H2CO CCH and HC3N (e.g. Dutrey et al 1997,
- Henning et al 2010, Chapillon et al 2012)
- ions : HCO+, H13CO+, N2H+ (Qi et al 2008, Dutrey et al 2007)
- deuterated : DCO+, DCN (van Dishoeck et al 2004, Qi et al 2008)
- \+ H2O (Herschel, Bergin et al 2010, Hogerheijde et al 2011)

The gas temperature case

CN is the product of the photodissociation of HCN.
- CN is supposed to trace the PDR upper layers
- HCN is a tracer of the rich molecular layer

We observed the CN J=2-1 and HCN J=1-0 in two T-Tauri (DM Tau and LkCa 15) and one Herbig Ae stars (MWC 480) with PdBI. We analyzed the data using a simple power-law parametric model (Diskfit, describe in Piétu et al 2007). Results are presented in Tab 1.

Molecule	Σ_{300} 10^{12} cm^{-2}	p	T_k (K)	q
		MWC 480		
HCN 1-0	1.1 ± 0.4	2.4 ± 0.4	[30]	[0]
CN 2-1	10.4 ± 0.9	2.1 ± 0.1	30 ± 4	[0]
		LkCa 15		
HCN 1-0	10.6 ± 1.5	1.1 ± 0.2	7.0 ± 0.6	0.55 ± 0.25
CN 2-1	58 ± 5	0.8 ± 0.1	8.8 ± 0.3	0.95 ± 0.05
		DM Tau		
HCN 1-0	6.5 ± 0.9	1.0 ± 0.3	6.0 ± 0.4	0.00 ± 0.12
CN 2-1	35 ± 9	0.6 ± 0.06	7.5 ± 0.3	0.60 ± 0.05

Tab 1 Values of the molecular column density and temperature distribution derived from the PdBI observation. [fixed parameter]

- **Temperature very low in T-Tauri**
- OK in Herbig Ae

Cause ?
- CN (HCN) close to cold mid-plane ?
- "cold" molecular layer ?
- Is CN emission subthermal ?

▶ chemical modeling of disks

Chemical study with the Meudon PDR code
Test of the influence of several parameters :
- UV field (stellar + ISRF)
- Cosmic ray ionisation rate
- Grain size distribution
- Gas-to-dust ratio

gas-phase study only

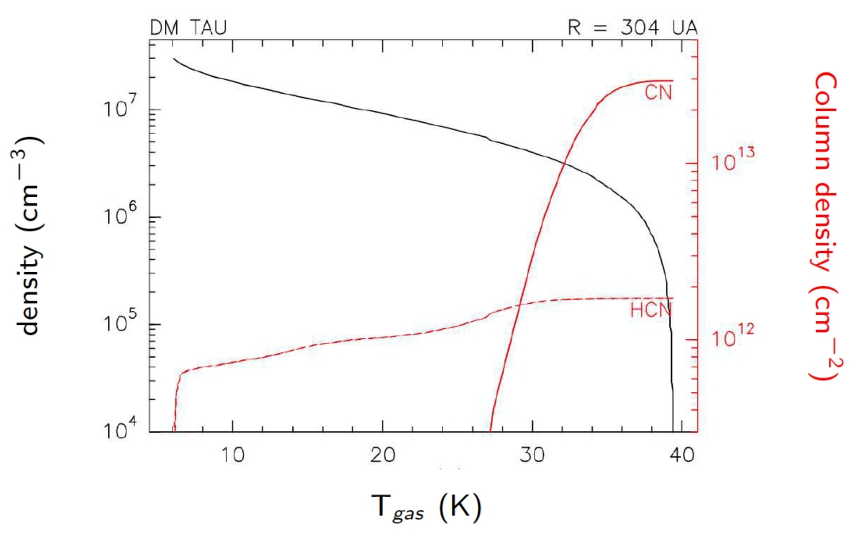


Fig 1 Distribution of density (black) andcummulated column desities (red) in functin of the temperture ar R=304 AU for DM Tau model. The vertical temperature gradient showned in the x axis goes from the mid-plane (left) to the atmosphere (right). The Column densities are integrated from the mid-plane (0) to the atmosphere (totale column density)

Fig 1 shows a typical result from the chemical modeling. The majority of the CN column density is build at densities higher than 10^6 cm^{-3} (so the emission should be **thermalised**) and temperature higher than 30 K, in contradiction with observations (Chapillon et al 2012).

Several gas-phase molecules are observed at low temperature in T-Tauri disks (~10K at 100 AU radius
- CO isotopologues (Dartois et al. 2003, Piétu et al 2007)
- CCH (Henning et al 2010)
- CN, HCN (Chapillon et al 2012)
- CS (Guilloteau et al 2012

▶ALMA proposals Cycle 0 & 1

Emphasis role of :
- Uncertainties on the gas-phase reaction rate of N-bearing molecules (Wakelam et al in prep.)
- Role of **grains**
  - Chemistry on grain
  - Extinction curve (UV penetration in disk)
- Photodesorption processes

H2D+, a mid-plane tracer ?

H2D+ trace medium cold and depleted in CO
- Trace the mid-plane
- Evaluate the amount of cold gas-phase CO in mid-plane

Observations of o-H2D+ 372 GHz in DM Tau (JCMT) and TW Hya (APEX)

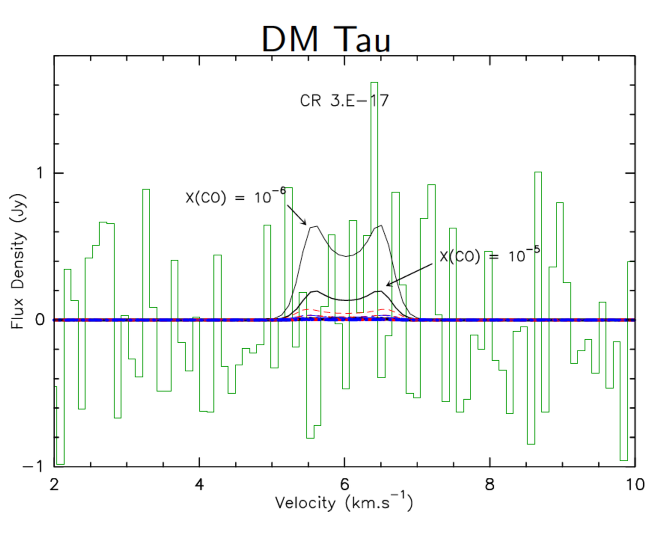


Fig 2 : Spectrum at 372 GHz toward DM Tau (green) and predicted spectrum from chemical models

Chapillon et al 2011

Chemical model : model adapted to Deuterium chemistry (Parise, Du)

Testing the influence of abuncance of CO (gas phase), cosmic ray ionisation rate and grain size (Fig 2)
- CR rate (1,3,10.10−17s−1)
- X(CO) (10−4, 10−5, 10−6)
- Grains sizes (0.1, 1, 10 μm)

▶ Observation not constraining

H2D+ may not be a sufficiently sensitive tracer of the disk mid-plane

Searching for other molecular tracers

1- S-bearing molecules

Deep search for Sulfur-bearing molecules with the IRAM 30-m : CS, SO, H2S
- H2S expected to be abundant in gas phase (Pasek et al 2005)
- H2S, CS, observed in comets.

- CS : detection in the T-Tauris
  No detection in Hae (Tab 2.)
- SO & H2S : upper limits (Tab 2.) (improvement factor 7)

Sources	Σ_{300} (cm^{-2}) SO	H_2S	CS
DM Tau	$\leq 7.5 \times 10^{11}$	$\leq 1.4 \times 10^{11}$	$3.5 \pm 0.1 \times 10^{12}$
LkCa15	$\leq 1.9 \times 10^{12}$	$\leq 3.6 \times 10^{11}$	$8.7 \pm 1.6 \times 10^{12}$
MWC480	$\leq 2.5 \times 10^{12}$	$\leq 4.1 \times 10^{11}$	$\leq 8.4 \times 10^{11}$
GO Tau	$\leq 8.9 \times 10^{11}$	$\leq 1.8 \times 10^{11}$	$2.0 \pm 0.16 \times 10^{12}$

Tab. 2 : Column densities (and 3 sigma limits) derived from observation, with Diskfit.

Chemical study with NAUTILUS, a gas-grain chemical code (Hersant et al 2009)

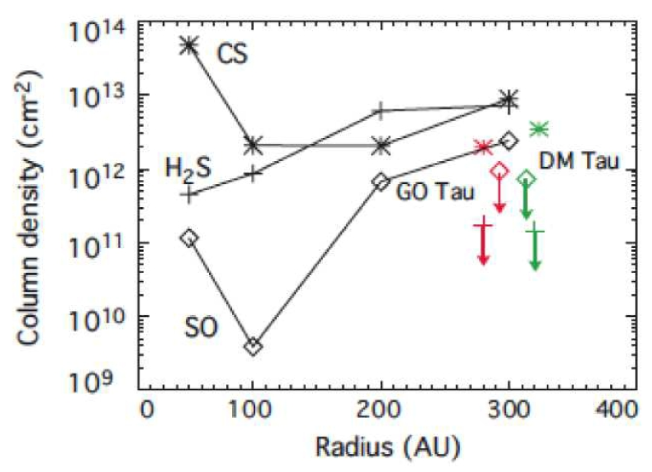


Fig 3 Predicted column densities (black) and observed calues (color) for GO Tau and DM Tau disks

- better agreement with initial abundances ratio C/O = 1.2 (Hincelin et al 2011)
- CS and SO OK
- H2S failed (Fig. 3)

▶ emphasis importance of **grain surface chemistry.**
H2S may be locked into grain mantle and react to form other molecules

Dutrey et al 2011 (CID V)

2- Heavier molecules

Deep search with the IRAM 30-m and PdBI for heavier molecules.
- CCS : no detection
- **HC3N : 5 sigma detection in GO Tau LkCa 15 (Fig. 4) and MWC 480**
- Not detected on DM Tau.

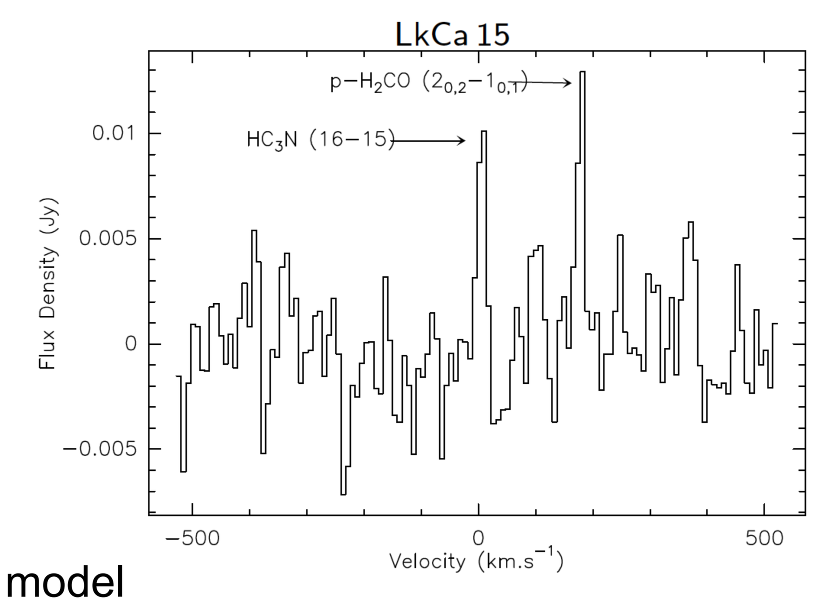


Fig 4 : PdBI spectrum of HCCCN toward LkCa15

Chemical study with NAUTILUS
CCS upper limit compatible with chemical model
N(HC_3N) are 2 orders of magnitude lower than predicted (Tab. 3)

- HC3N sensitive to UV ?
  - strong UV field
  - grain growth
  - dust settling
- Accuracy of reaction rates ?

Chapillon et al 2012 (CID VII)

Souce	Σ_{300} (cm^{-2}) HC_3N Derived	HC_3N Predicted	CCS Derived	CCS Predicted
LkCa 15	$8 \pm 2 \cdot 10^{11}$	$5.2 \cdot 10^{13}$	$\leq 1.4 \cdot 10^{12}$	$2.9 \cdot 10^{11}$
GO Tau	$13 \pm 2 \cdot 10^{11}$	$4.4 \cdot 10^{13}$	$\leq 1.2 \cdot 10^{12}$	$3.7 \cdot 10^{11}$
DM Tau	$\leq 3.5 \cdot 10^{11}$	$4.4 \cdot 10^{13}$	$\leq 1.1 \cdot 10^{12}$	$3.7 \cdot 10^{11}$
MWC 480	$6 \pm 1 \cdot 10^{11}$	$6.4 \cdot 10^{11}$	$\leq 0.9 \cdot 10^{12}$	$3.1 \cdot 10^{11}$

Tab.3 Molecular column densities(and upper limits) derived from observations and predicted by chemical model.

Observation of molecular lines is a powerful tool to study disk structure

- CO, CN, HCN, CCH, CS in gas phase at low temperature (~10K) in T-Tauri disks
  ▶ challenge thermal structure predicted by thermo-chemical models
- Column densities of S- N-bearing molecules not well reproduced by disk models

Points out toward :
- Up-to-date gas-phase reaction rate
- Importance of the grains to explain chemistry in disk
- UV transfer (grain growth, settling)
- Chemistry on grains
- Photodesorption (UV, CR) see also detection of cold water vapor in dense cloud by Caselli et al 2012

And with ALMA ?
- Detailled structure of disks (physical and thermal), turbulence
- Search for new molecules ? How far can we go in molecular complexity ?
- Increase sample of sources