MM/subMM Molecular Observations of Circumstellar Disks

Anne Dutrey (LAB, France)

IAU 280, Toledo, June 1 2011

With inputs from CiD « Chemistry In Disks » consortium

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Circumstellar Disks around low-mass PMS Stars

c),d) Proto-planetary Disks

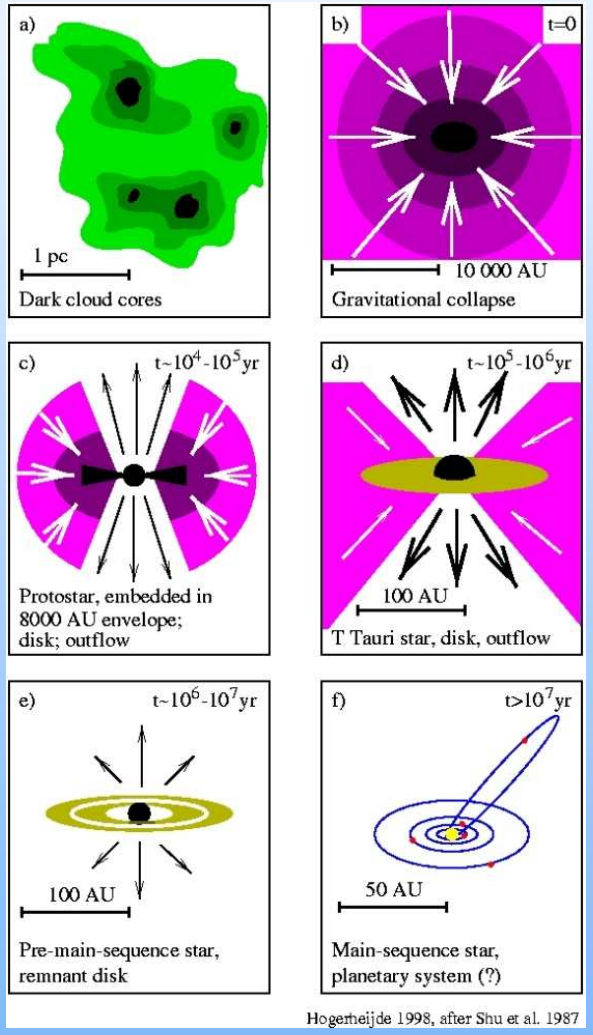
→ Dust emission opt. thick at λ= 1 μm

→Should contain enough gas to form a “proto-Jupiter”
Total disk mass ~ a few 0.01 Msun

→ Most of the disk mass in gas phase - G/D ~ 100 (?)
H_2 not easy to detect (rot. lines in the IR, where the dust is optically thick)

→Age ~ a few Myrs

TTauri stars 0.5 to 2 Msun



Hogerheijde 1998, after Shu et al. 1987

Towards Planet Formation

- Molecular Gas Properties
→CO as « cold »gas tracer
-Morphology/Kinematics
(disks in Keplerian rotation)

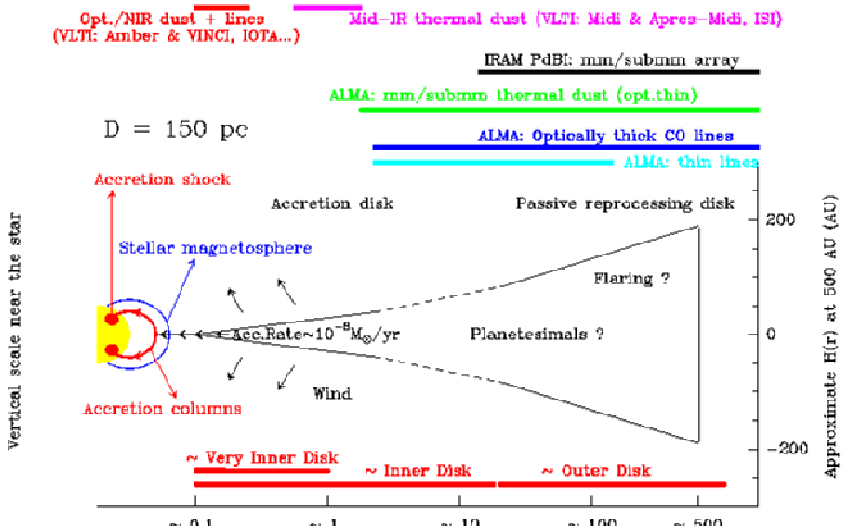
- Gas Density / Temperature
(excitation should be known)
- Turbulence ?

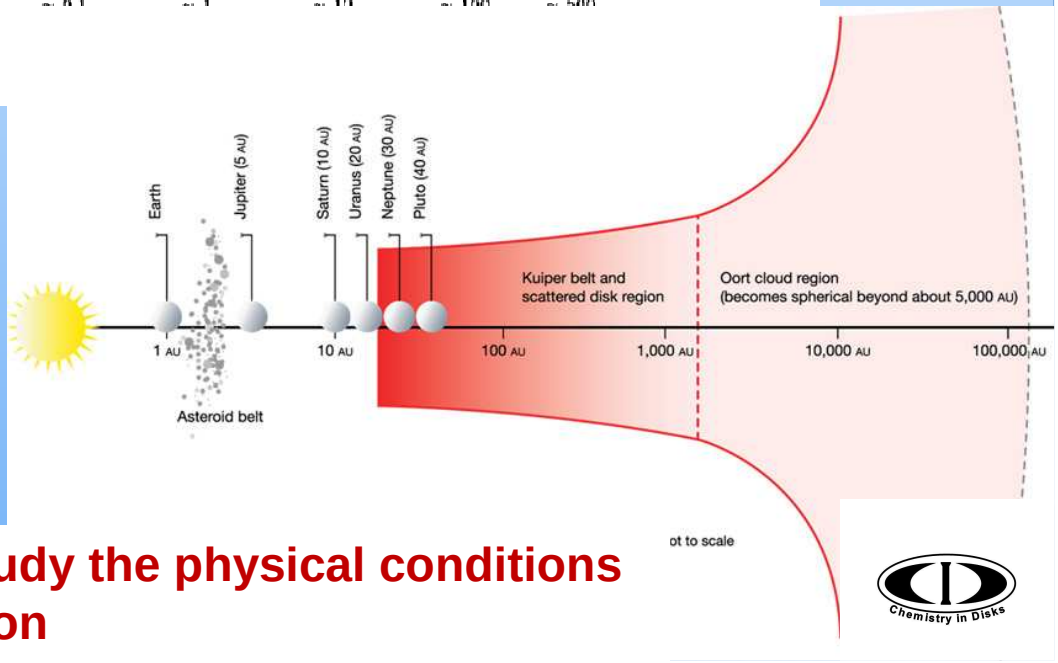
- Ionisation ?

-Deuteration ?
-Molecular Complexity ?

- Gas/Dust ratio ?
- Impact of Grain properties ?

-Modelling: See Dima Semenov's talk





Chemistry as a tool to study the physical conditions leading to planet formation

Detected cold Molecules, so far ...

- **Detection**

CO, ^{13}CO, $C^{18}O$ (several papers)
HCO^+, CN, HCN, HNC, CS, H_2CO and C_2H (Dutrey et al 1997: DM Tau & GG Tau, Henning et al 2010, **CID**, Chapillon et al 2011, **CID**: MWC480, DM Tau, LkCa15)

DCO^+ (van Dishoeck et al 2004: TW Hya, Guilloteau et al 2006, DM Tau), DISCS

N_2H^+ (Dutrey et al 2007, DM Tau, LkCa 15, **CID**), DISCS

DCN (Qi et al 2008: TW Hya), DISCS

$H^{13}CO+$ (Qi et al 2008: TW Hya), DISCS

H_2O (Herschel, Bergin et al 2010)

- **Deep Search**

H_2D^+ (Chapillon et al 2011, submitted: DM Tau & TW Hya)

Sulfur-bearing molecules (Dutrey et al 2011, **CID**, submitted)

• **Mm/Submm Interferometry:**
PdBI (CID)

-**Best angular resolution**
→ 0,35'' ≡ 50 AU @ D=140 pc

-**Super-resolution when high Spec. Resol.**
→dv = 0.1 km/s ≡ 10 AU @ r=100 AU
for 0.5 Msun star

→**See also presentations** - **DISCS survey by E.Bergin**
- **H_2O in Disks with Herschel**

Detected

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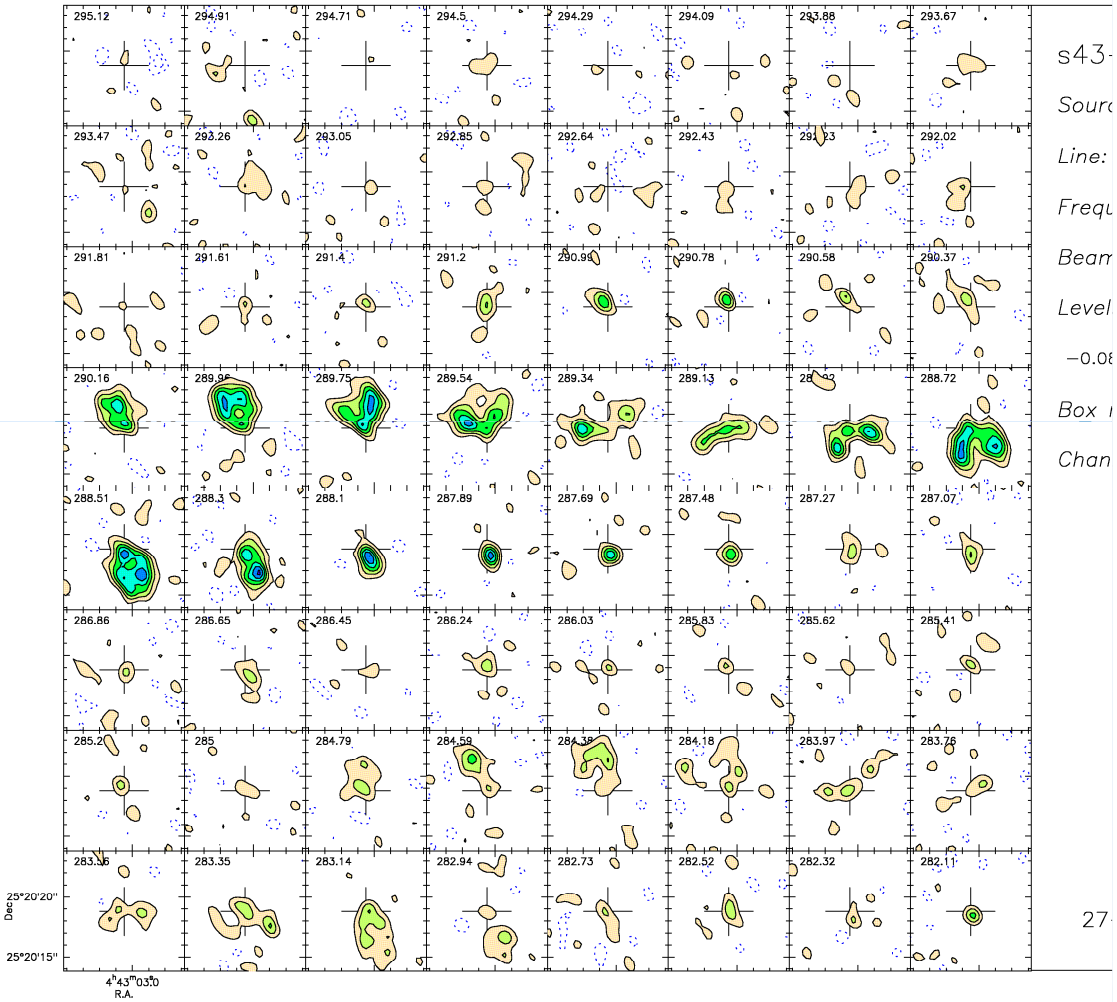
H_2D^+ (Chapillon et al 2011, submitted:
& W Hya)
Sulfur-bearing molecules (Dutrey et al
submitted)

PdBI CN J=2-1 data in GO Tau (DM Tau -like)
One hyperfine component
dv = 0.2 km/s, res~ 1”



→See also presen

- H_2O in Disks with Herschel

Detecte

- **Detection**

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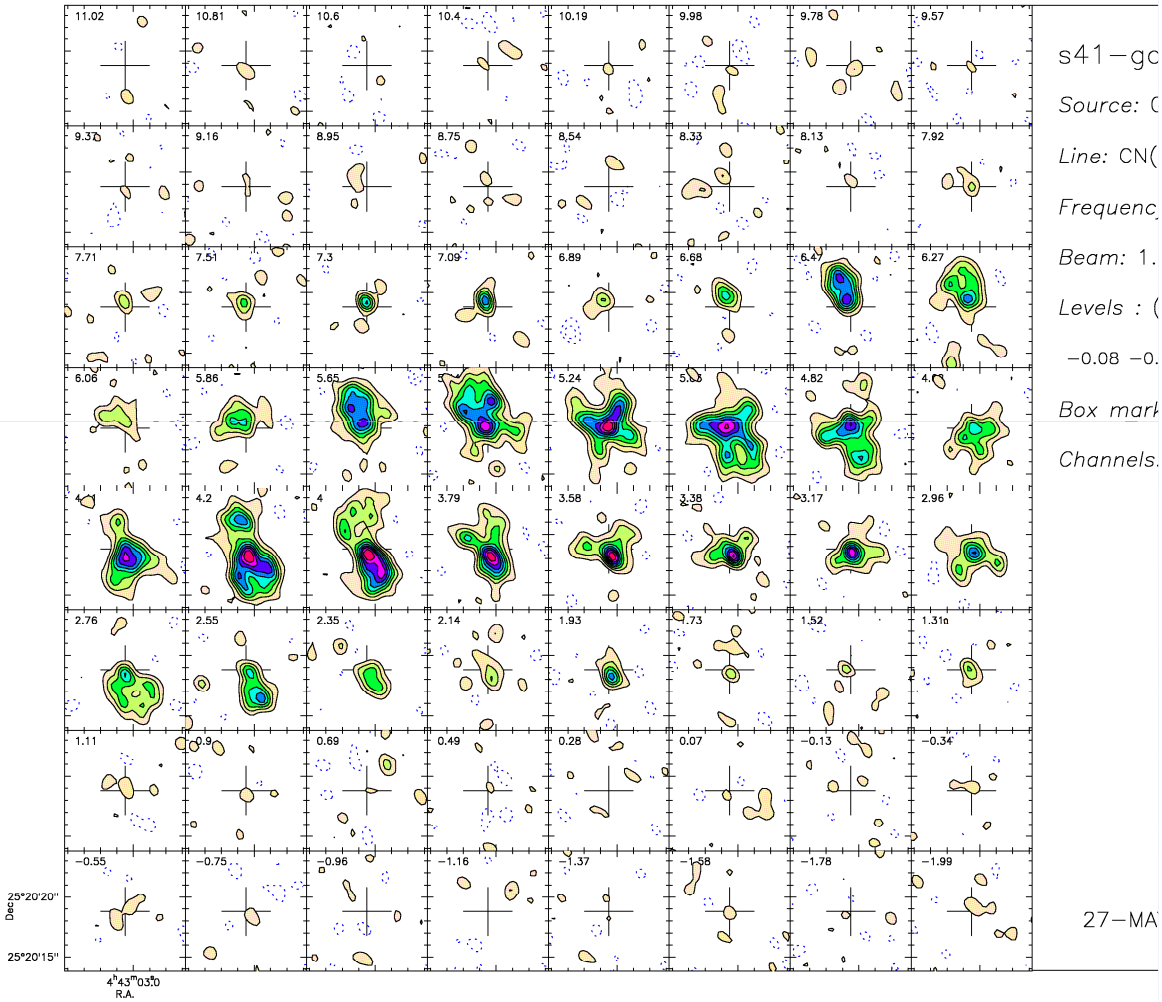


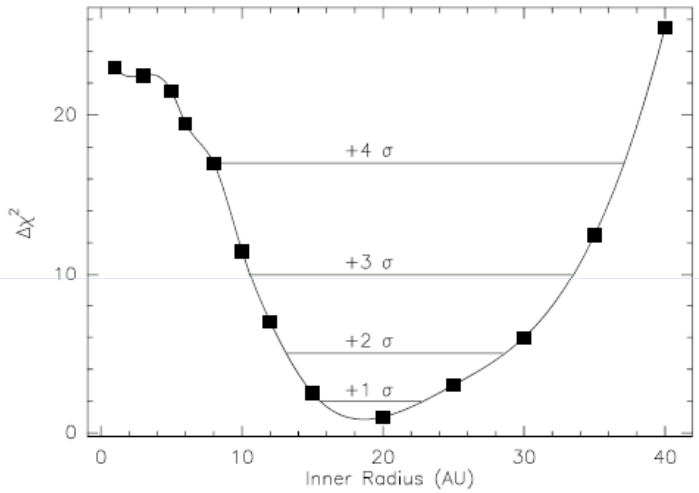
→**See also pres**

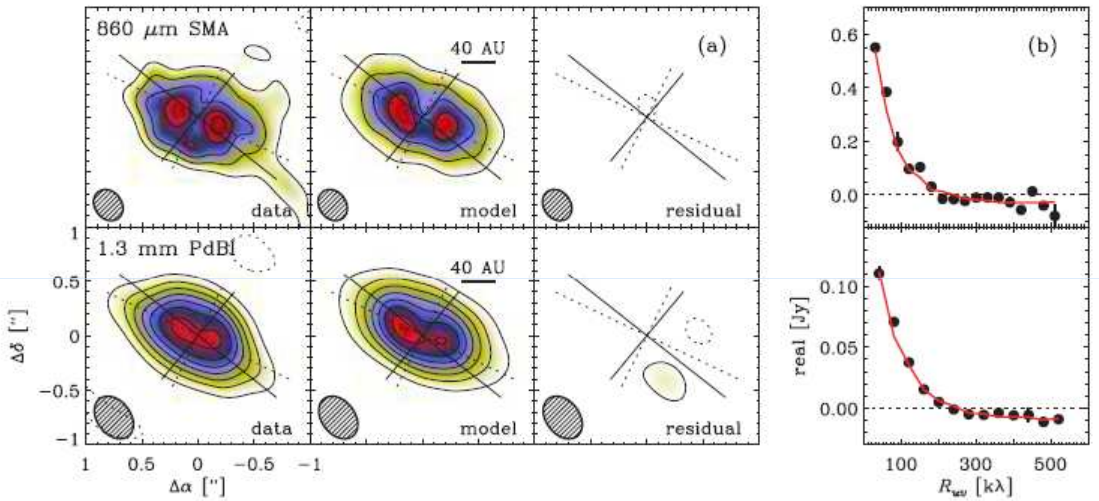
- H_2O in Disks with Herschel

CO: Morphology … The GM Aur case

Dutrey et al., 2008 (CID) → **Rin = 20 AU**
Spectroscopic detection

Hughes et al., 2009 **– same dust inner radius**





Analysis 12CO, 13CO, C18O 1-0, 2-1
PdBI data

The cavity is «devoid » of dust and gas

CO line wings are tidally truncated « super resolution »
→companion: is this a planet ? (mass ~ 5 – 10 Mjup)

Cavity Radius < Pluto's Orbit

DM Tau: the case study
CO analysis

Increasing opacity

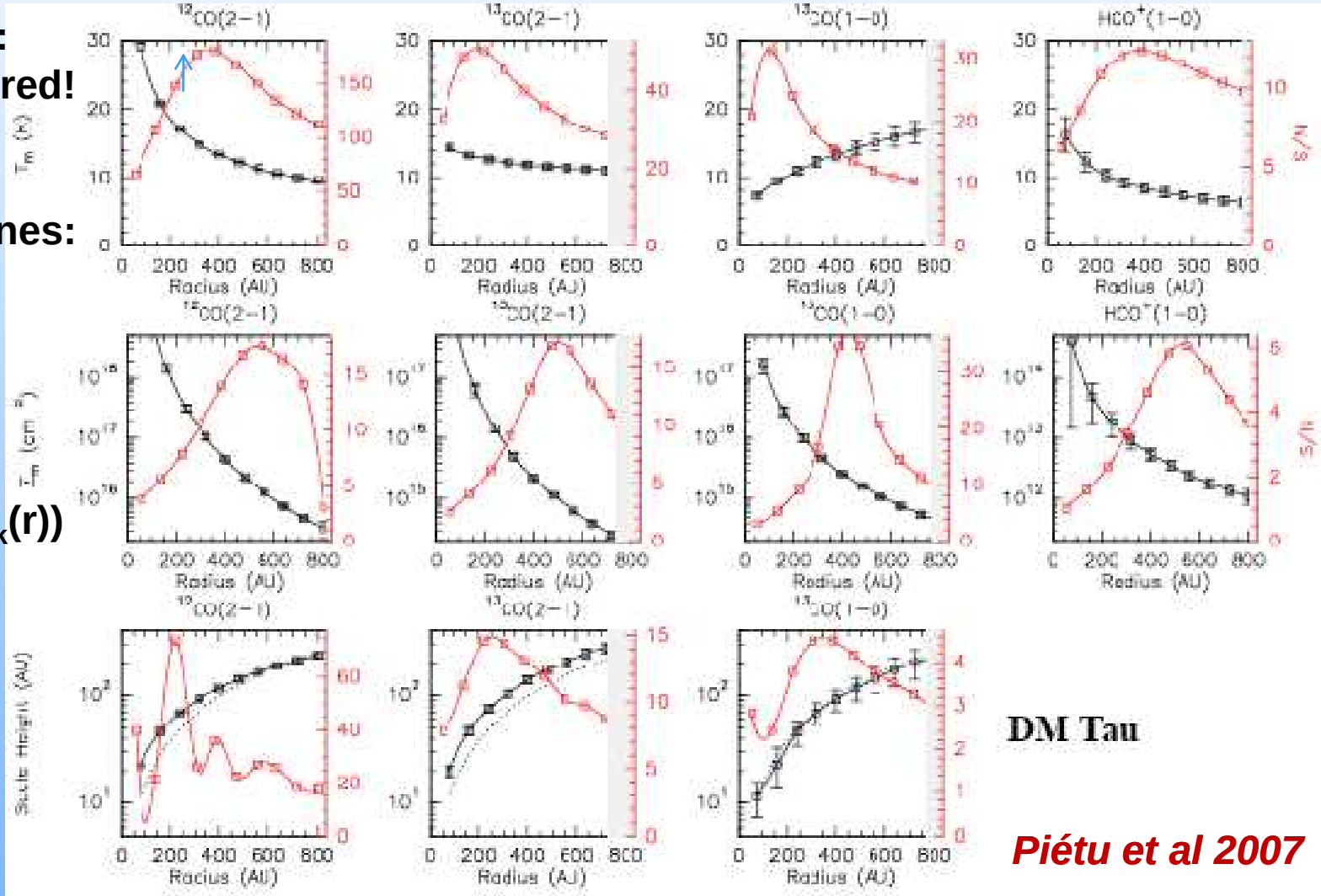
Interferometry:
T_B (r) is measured!

Thermalised lines:

Opt.Thick:
$T_B(r) \propto T_k(r)$

Opt.Thin:
$T_B(r) \propto F(\Sigma(r), T_k(r))$

Subthermal:
$T_k(r) \longrightarrow T_{ex}(r)$



Piétu et al 2007

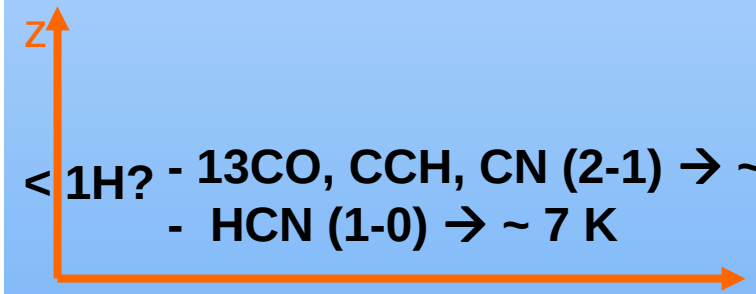
➔ **Compromise angular resol./line opacity: still true with ALMA**

Gas temperature around mid-plane: towards a (partly) cold molecular layer ?

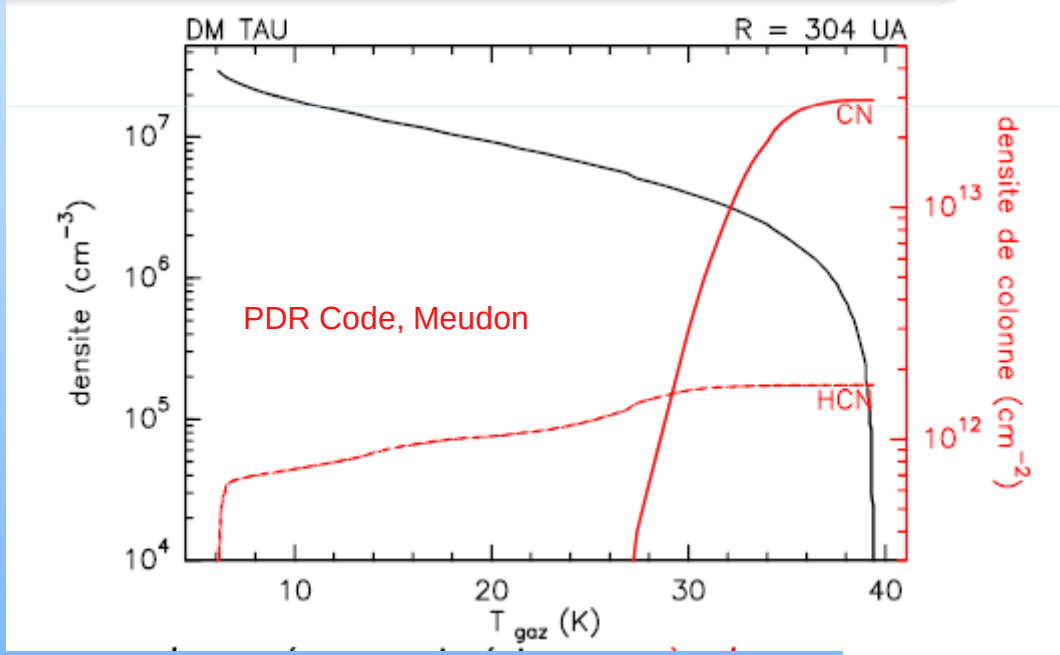
- **CO/^{13}CO PdBI data:** ***Dartois et al 2003***, the outer disk is cold, r ~ 100 AU, Tk~ 10 K confirmed by ***Pietu et al 2007***
- Vertical/Radial mixing: ***Semenov et al., 2006, Aikawa 2007***

- **CCH (CID):** ***Henning et al 2010*** → ~ 8-10K at 100 AU
- **CN/HCN (CID):** ***Chapillon et al., 2011, submitted,*** PdBI data

HAe: MWC 480 – warm (~ 30 K)
TTauri: LkCa15 (as cold as DM Tau)
→ **cold mid-plane or cold molecules**
→ difficult to reconcile with models



< 1H? - 13CO, CCH, CN (2-1) → ~ 9 K
- HCN (1-0) → ~ 7 K



KIDA Kinetic Database for Astrochemistry

Chemistry in Disks

Gas temperature around mid-plane: towards a cold molecular layer ?

Chapillon et al 2011, submitted

Table 2. Results of analysis

Source	Molecule	Σ 10^{12} cm^{-2}	p	R_{out} (AU)	δV (km s^{-1})	T_k (K)	q	R_{int} (AU)	α_d
MWC 480	HCN 1-0	1.1 ± 0.4	2.4 ± 0.4	[550]	0.3 ± 0.2	[30]	[0]		0.0 ± 0.7
	CN 2-1 (high)	11 ± 1	2.1 ± 0.1	540 ± 40	0.25 ± 0.04	33 ± 6	[0]		0.0 ± 0.3
	CN 2-1 (low)	11 ± 1.2	2.1 ± 0.15	550 ± 70	0.26 ± 0.07	33 ± 6	[0]		–
	CN 2-1 (all)	10.4 ± 0.9	2.1 ± 0.1	545 ± 35	0.25 ± 0.04	30 ± 4	[0]		–
LkCa 15	HCN 1-0	10.6 ± 1.5	1.1 ± 0.2	600 ± 40	0.20 ± 0.03	7.0 ± 0.6	0.55 ± 0.25	[30]	0.0 ± 0.8
	CN 2-1 (high)	38 ± 4	2.3 ± 0.2	570 ± 20	0.18 ± 0.02	10.8 ± 0.7	0.20 ± 0.07	[30]	0.15 ± 0.17
	CN 2-1 (low)	115 ± 18	0.2 ± 0.2	690 ± 20	0.26 ± 0.03	6.6 ± 0.3	0.80 ± 0.07	[30]	–
	CN 2-1 (all)	58 ± 5	0.8 ± 0.1	630 ± 35	0.18 ± 0.01	8.8 ± 0.3	0.95 ± 0.05	[30]	–
DM Tau	HCN 1-0	6.5 ± 0.9	1.0 ± 0.3	660 ± 20	0.18 ± 0.01	6.0 ± 0.4	0.00 ± 0.12		0.0 ± 0.5
	CN 2-1 (high)	26 ± 4	2.1 ± 0.15	650 ± 20	0.16 ± 0.01	8.6 ± 0.5	0.05 ± 0.05		0.0 ± 0.3
	CN 2-1 (low)	46 ± 9	0.7 ± 0.15	550 ± 25	0.20 ± 0.01	6.5 ± 0.5	0.50 ± 0.08		0.0 ± 0.3
	CN 2-1 (all)	35 ± 9	0.6 ± 0.06	620 ± 15	0.17 ± 0.01	7.5 ± 0.3	0.60 ± 0.05		0.0 ± 0.3

α_d is the depletion scale height (see text). All values are referred to 300 AU.

- **Should be thermalised (n ~ a few 10^6 cm^{-3})**
- **T = 8 K for DM Tau & LkCa 15, 30 K for MWC 480**
- **But CN is expected mostly close to the warm PDR**

PDR: HCN + hv → CN + H (high amount of HCN)

N + CH → CN + H (upper in the disk)
N + C2 → CN + C

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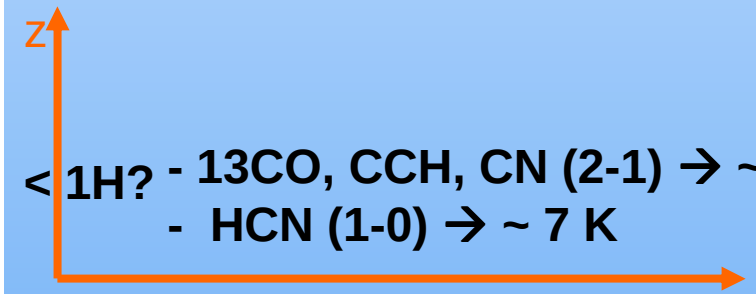

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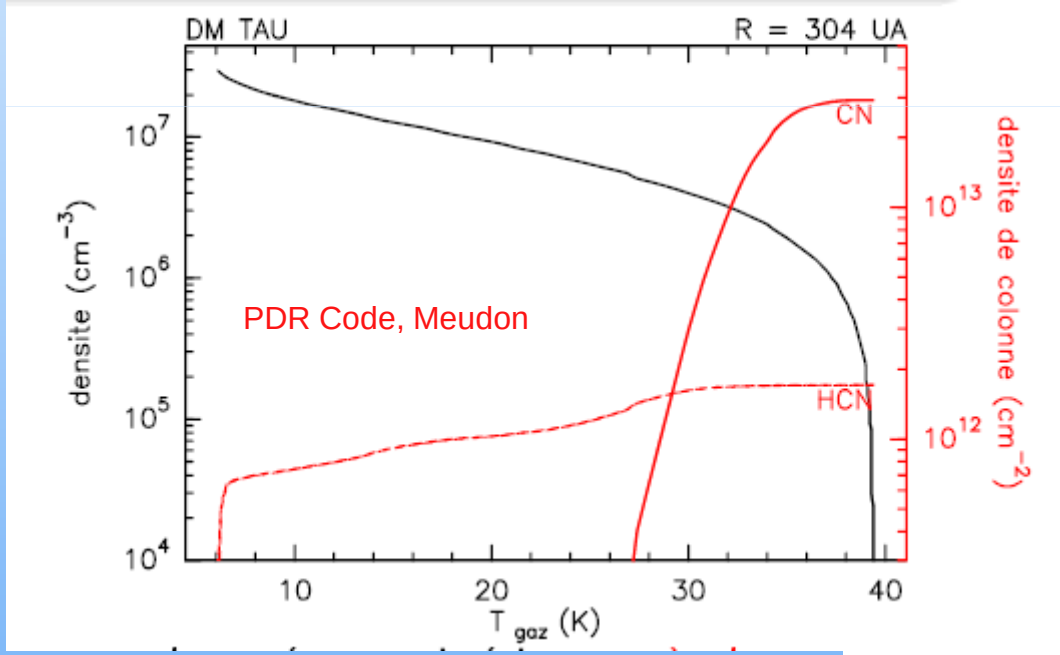


Mid-plane: is H_2D^+ a good tracer ?

Chapillon et al 2011, submitted JCMT/ APEX data on DM Tau & TW Hya

O - H_2D^+ ($1_{1,1}$-$1_{1,0}$) 372 GHz

•H_2D^+ formed in gas phase at low temperature, easily destroyed by CO, N_2
→should be abundant in the cold depleted mid-plane

•No detection (3x better than previous data) → significantly lower than expected

•Analysis: chemical model from Parise et al 2011

- Several disk structures (Σ, Tk, R_{out})
- No UV (mid-plane)
- Several CR rates (10^{-17} – 3.10^{-17} – 10^{-16} s^{-1})
- Several grain sizes (a = 0.1 – 1 – 10 µm)
- Several CO abundance (10^{-4} – 10^{-5} – 10^{-6})

• Results on DM Tau: only excludes
-X(CO) = 10^{-6} and a = 0.1 µm
- If X(CO) = 10^{-5} , all grain sizes ok

ALMA detection
→ not so easy

	H_2 density								Temperature			
	Model 1				Model 2				Case L		Case H	
	$\Sigma_0^{H_2}$ (cm^{-2})	p	R_0 (AU)	R_{out} (AU)	$\Sigma_0^{H_2}$ (cm^{-2})	p	R_0 (AU)	R_c (AU)	T_{100} (K)	q	T_{100} (K)	q
DM Tau	8.4×10^{23}	0.85	45	700	9.6×10^{23}	0.45	45	180	15	0.4	30	0.63
TW Hya	4.3×10^{23}	1.0	45	200	3.3×10^{23}	0.7	45	30	30	0.5	40	0.2

Turbulence versus radius in disks derived from molecular lines ?

Dartois et al 2003, Pietu et al 2007 – PdBI data, DMT au, MWC480, LKCa15

- **Turbulence → Amplitude of the local velocity fluctuations**

- **Spectrum local line-width given by DV = $\sqrt{(v_{th}^2 + v_{turb}^2)}$**

- **Link to α (viscosity parameter) depends on the nature of the turbulence of the order of ≈ $\sqrt{\alpha}.c_s$ - $\alpha.c_s$, with sound speed c_s such as H(r) ≈ c_s /Ω**

→If the molecular disk is spatially,spectrally resolved → DV(r)
→Since lines have different opacities → DV(z)

ALMA: DV(r,z)
Spec.&.Ang. Resol

- **So far, CO and isotopologues (^{13}CO, C^{18}O)**

→Subsonic broadening DV ~ 0.1 – 0.4 km/s < c_s

- **Well suited for ALMA sensitivity and angular, spectral resolution**

→If the thermal structure is properly constrained, linked to line opacity, density structure … etc…

→Will remain the main uncertainty, even with ALMA

See also Hughes et al 2011: TW Hya, HD163296

Ionisation in Disks

- **N_2H^+** has been observed at PdBI (CID "Chemistry In Disks) ***Dutrey et al., 2007***

5σ detection LkCa15 and DM Tau, upper limit on MWC480

- **Main results:**

HCO^+ remains the most abundant molecular ion in disk

$[N_2H^+]/[HCO^+]$ ~ 0.02- 0.05 (similar to dense cores)

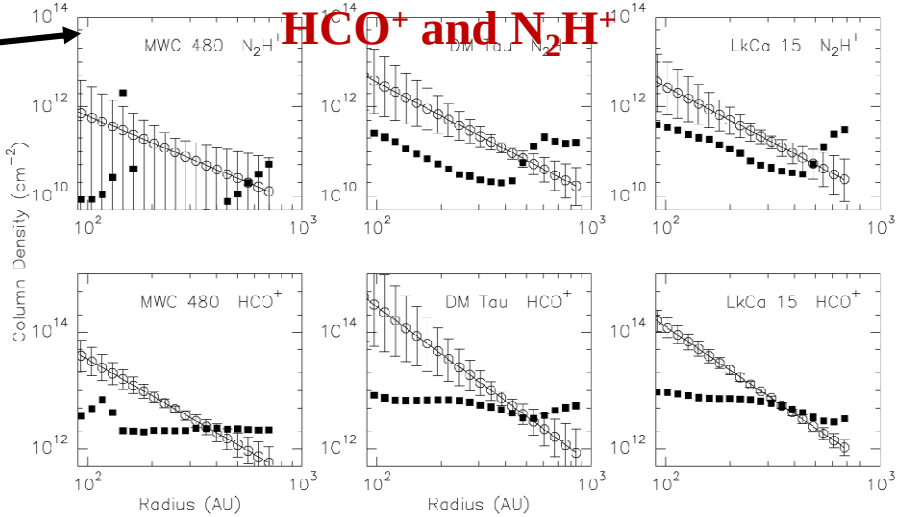
- **DCO^+/HCO^+** in TW Hya

Qi et al., 2008

$[e] = n(e)/n(H_2) \sim 10^{-7}$ in the disk layer where the molecules are present (following Caselli 2002)

- **Less HCO^+ in Herbig Ae Disks ?**
- AB Auriga: ***Schreyer et al 2009 (CID)***
- MWC480: ***Dutrey et al 2007 (CID)***

HCO^+ and N_2H^+



~~Good agreement, but the slope p is not yet properly reproduced !

$N_2H^+ + CO \rightarrow HCO^+ + N_2$

Towards more complex molecules ?
Sulfur-bearing molecules in TTauri Disks

Dutrey et al 2011 (CID), submitted – IRAM 30-m - DM Tau, LkCa15 & MWC480

→ So far, molecules observed in disks are the most abundant seen in cold clouds

•**Deep search** for Sulfur-bearing molecules: **CS, SO, H_2S**

•CS detected, significant upper limits on SO, H_2S (~7x better - Dutrey et al 2000)

•**Results:** (outer) disk chemical modeling (Nautilus, Hersant et al 2009)

- Grains 0.1µm
- full network, inc. surface chemistry

→**H_2S modelling incompatible with upper limit …**

locked onto grains, form other species → no desorption

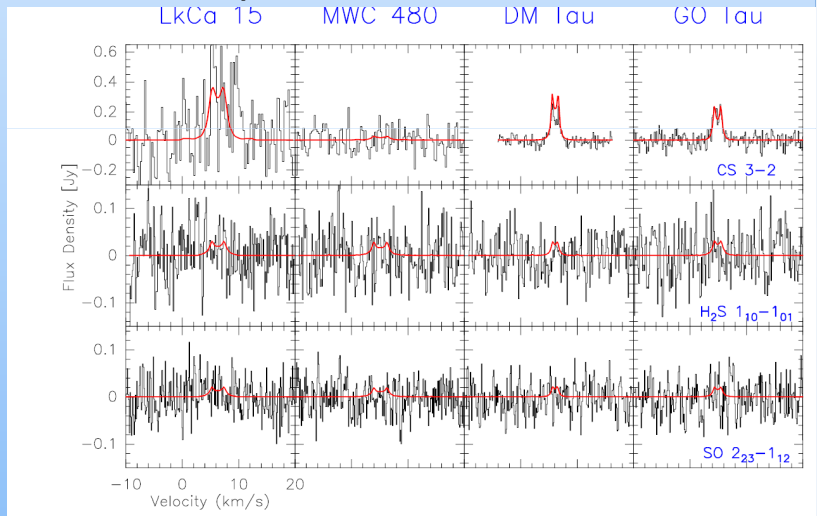


Fig. 1. Observations of SO $2_{23} - 1_{12}$, H_2S $1_{10} - 1_{01}$ and CS 3-2 in the four disks. For CS J=3-2, the best models have been superimposed sources. For SO and H_2S, the models always correspond to the 3σ upper limits.

→**Need for a proper chemistry at grain surface**

Large temperature gradients (10-100 K) on small spatial scales (H ~ 20 AU at r= 20-50 AU)

• **Importance of the physical structure (current observations not accurate enough)**

•Weakness (surface chemistry) of current chemical models!

→ Must be solved for ALMA data interpretation!

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LkCa 15 MWC 480 DM Tau GO Tau

Table 3. Sulfur-bearing Molecules: detections and 3σ upper limits.

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

Notes. Sulfur-bearing molecules surface densities (cm^{-2}) at 300 AU (modeled as $\Sigma(r) = \Sigma_{300}(r/300\text{AU})^{-1.5}$). The surface densities are derived from the 30-m data (except for CS 3-2 in DM Tau) and the model DISKFIT. See text for details.

Velocity (km/s)

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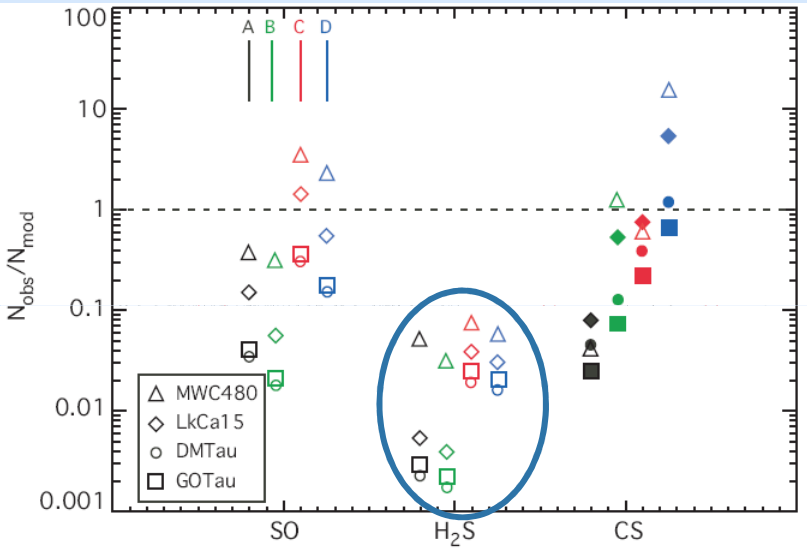

Fig. 3. Ratio between the column densities of SO, CS and H_2S observed in the four protoplanetary disks at 300 AU from the central star and the values computed with NAUTILUS. For SO and H_2S, they corresponds to upper limits. The four models (A, B, C and D) correspond to the elemental abundances given in Table 4 and to the prameters given in Table 5.

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Gas to Dust Ratio ?
The CQ Tau case

Chapillon et al 2008, 2010 – PdBI & APEX data on CQ Tau (A8-F2, ~ 1.5 Msun)

- ***Chapillon et al., 2008***
- **Warm CO disk with depletion ~ 100!**
- 1°either « strong UV fied »
- 2°or weak UV field + low g/d

- ***Chapillon et al., 2010***
- Next step → search for CI
- No detection
- → **CI upper limit is constraining**

- PDR models qualitatively compatible with our CI upper limit **ONLY IF** g/d ≤ 10

-CI surface density sensitive to the UV spectrum shape, (Strong UV field → C^+)

→Suggests that the CQ Tau disk is in a transition phase between a proto-planetary and debris disk

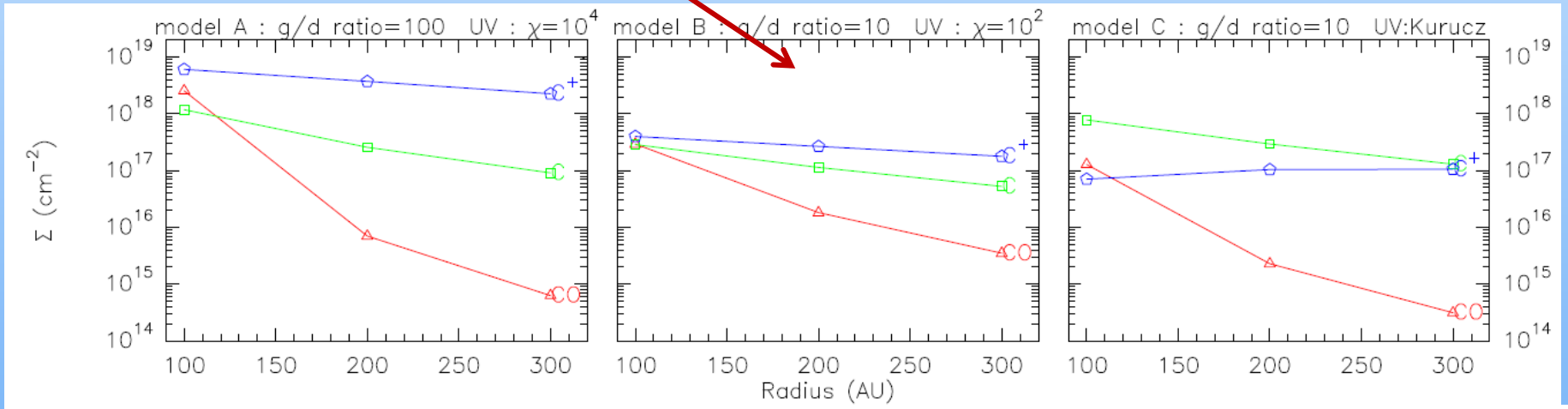


Fig. 3. Radial distribution of the surface density of C^+, C, and CO for three models which are in agreement with the CO observations

Impact of large dust grains on molecular Chemistry

(PdBI data -CO in the disk of CQ Tau)

Edwige Chapillon PhD thesis 12/2008
Chapillon et al., 2008

How to explain a large CO depletion (~100) in a warm (~ 30 K) disk ?

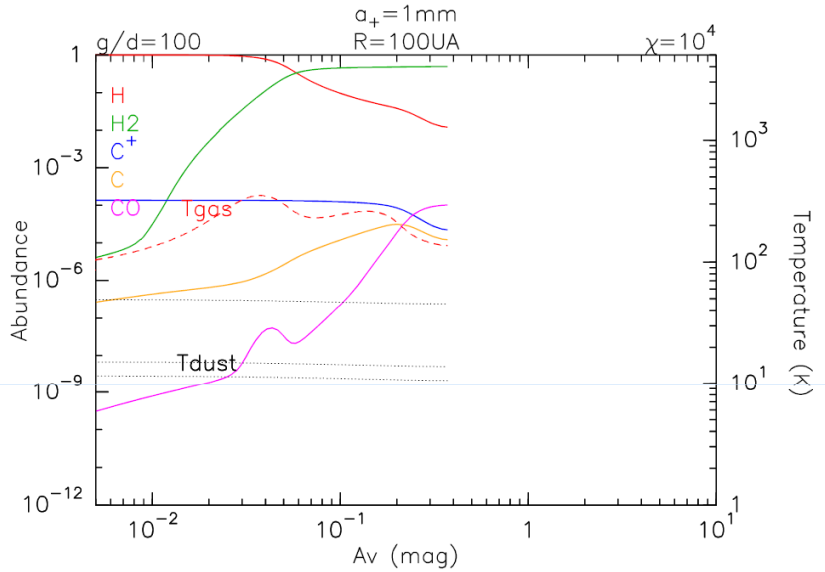
One possibility would be:

1) CO is removed from the gas phase during the cold pre stellar phase by adsorption on small grains.
2) Grains grow, and CO stays stick on larger grains
3) Heating of the gas but large grains still cold enough to retain C,O on grains

Feedback on
Disk Structure (density/temperature)
Surface (and gas phase) chemistry
Disk temporal Evolution

Des gros grains froids ?

Les gros grains peuvent être froids ($T \leq 10\,K$)



→ cumulative effect with dust sedimentation along the mid-plane and possible radial variations …

Impact of Dust Properties on molecular Chemistry II

PdBI data at 2.7 and 1.3mm (best resolution ~ 0.3") - Survey of ~ 20 sources

Guilloteau, Dutrey, Piétu, Boehler 2011

- Analysis: Compare « power laws » and « viscous » models for surface density

$$\Sigma(r) = \Sigma_0 \left(\frac{R_0}{r}\right)^{\gamma} \exp\left(-(r/R_c)^{2-\gamma}\right)$$

- Results:

-In most cases no significant differences between both models BUT

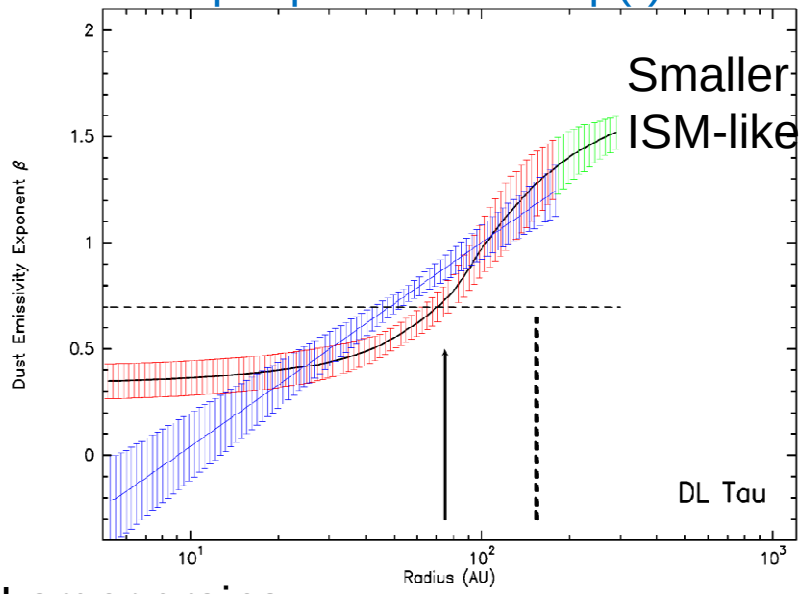
- β, the dust spectral index, varies with radius ! $K_\nu = K_o\ (\nu/230\ \mathrm{GHz})^{\beta(r)}$

Impacts on

- **the local gas/dust ratio, varies in (z,r)**
- **the extinction curve in the UV (z,r)**
- **disk UV field and chemistry**

Red: $0 \le \beta(r) \le 1.7$ (ISM)

Blue: simple power law for β(r)



Smaller grains ISM-like

Larger grains

The ALMA perspective …
« Cuvée » 2011

1) **Temperature determination** → where is the molecular layer , warm versus cold ?
- Large temperature/density changes within a few AU - impact on chemistry?
- How to trace the **« cold » mid-plane** ?

→ **H_2D^+ detection not as easy as expected** (emission should be resolved)

2) **Density distribution** → absolute value of the gas mass ?
- No direct tracer of H_2, X(mol)?

→**CO and isotopologues remain robust to determine the temperature and density gradients** detailed excitation conditions needed

3) **Roles of grains ?**
- Grain size varies with (r,z) – radial and vertical evolution
- UV extinction & G/D variable in (r,z)
- Surface chemistry needed - temperature gradients, vertical mixing…

→ **Should be incorporated in chemical models**

4**) Molecular complexity ? Sensitivity** (ALMA characteristics)

5) **Turbulence DV(r,z)**

- → **ALMA will open a new domain (dynamics)**

KIDA Kinetic Database for Astrochemistry

Chemistry in Disks