Chemistry of Protoplanetary Disks at the Dawn of the ALMA Era

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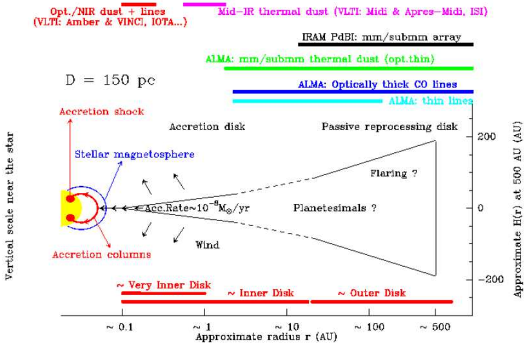
Protoplanetary disks around low-mass PMS stars

Protoplanetary disks : birth place of planets.

- morphology (distribution of density)
- kinematic
- temperature (gas and dust)
- composition of the gas (molecular complexity, deuteration...)
- grains properties
- gas-to-dust ratio

Gas = main component of protoplanetary disks
dissipate during star/planet formation

Protoplanetary disks observation



Dutrey et al. 2004

IR observations

- Sensitive to inner disk
- Optically thick dust emission
- Rotational/vibrational transition of molecules

mm observations

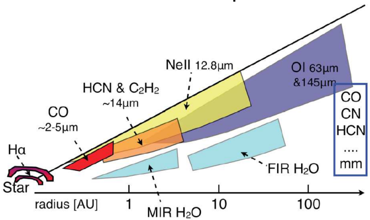
- Sensitive to cold regions (outer disk)
- Optically thin dust emission
- Rotational transitions of molecules
- High spectral resolution
- Sub-arsec resolution (interferometers)

Molecules (and atoms) detected in disks (so far)

- CO, ^{13}CO, $C^{18}O$
- CN, HCN, HNC, CS, SO, H_2CO, CCH, HC_3N, c-C_3H_2 (e.g. Dutrey et al 1997, Henning et al 2010, Chapillon et al 2012, Qi et al 2013)
- C_2H_2, CO_2, OH, HD (e.g. Pontoppidan et al 2010, Thi et al 2011, Bergin et al. 2013)
- ions : HCO^+, $H^{13}CO^+$, N_2H^+, CH^+ (Qi et al 2008, Dutrey et al 2007, Qi et al 2013)
- deuterated : DCO^+, DCN (e.g. van Dishoeck et al 2004, Qi et al 2008)
- H_2O (Bergin et al 2010, Hogerheijde et al 2011, Podio et al 2013)
- CII, OI (e.g. Sturm et al. 2010, Meeus et al 2012)

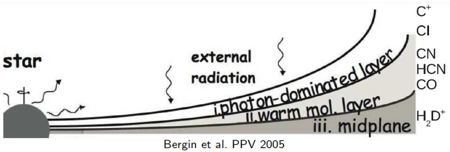
Sampling the disk

Inner part



D. Semenov

Outer part



Bergin et al 2007

Different molecules will trace different regions

- analyse of observational data thanks to radiative transfer codes
- comparison with results from chemical codes

→ bring information on kinematics, density, thermal structure, turbulence...

Radiative transfer

Parametrization of the disk : power law of the radius

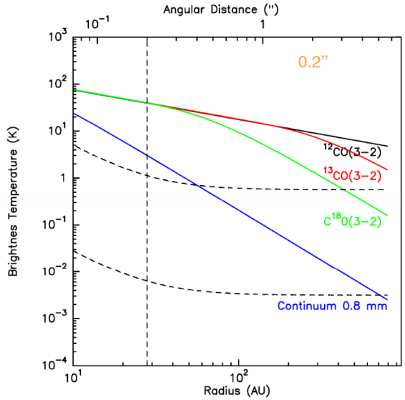
- Rotation : $v(r) = v_0(r/r0)^{-v}$
  Keplerian case : v = 0.5, $v_0 = \sqrt{(GM/r_0)}$ (V is measured)
- temperature : $T(r) = T_0(r/r0)^{-q}$
  if hydrostatic equilibium
- scale height : $h(r) = h_0(R/r0)^{-h}$
- density : $n(r,z) = n(r,0).exp[-(z/h)^2]$
- surface density : $\Sigma(r) = \Sigma_0.(r/r0)^{-p}$ (power law with sharp edge)
  $\Sigma(r) = \Sigma_0.(r/R0)^{-p} exp(-(r/Rc)^{2-p})$ (viscous model)

Analyse in the *uv*-plane : χ^2 minimization $\rightarrow$ errorbars

Brightness temperature

$T_B(r) = (1 - e^{-\tau_\nu}) T(r)$

- If optically thick lines $\rightarrow$ $T_B(r) = T(r)$
- If optically thin lines $\rightarrow$ $T_B(r) = \tau T(r) \propto (T, \Sigma)$
  linear molecule, $h\nu << kT$
  - J=1-0 $T_B \propto \Sigma / T$
- if thermalised T = Tk
- if non-LTE T = Tex



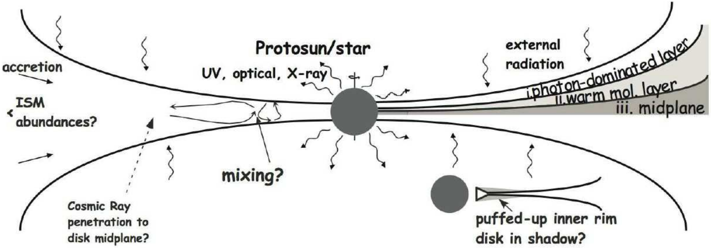
H_2

- $\Sigma(H_2) = \Sigma_{mol}$ / X(mol)
  X(mol) difficult to constrain
- $\Sigma(H_2) = \Sigma_{dust} \times$ g/d
  g/d ?

H_2 mass is not yet well constrained even if distribution is known

Where are the molecules ?

- Surface chemistry (on grains) (need a realistic size distribution)
- Neutral - neutral (low and high T)
- Ion - neutral
- 3 body reactions (?)
- Photodissociation, photoionization by UV
- Interactions with X rays
- Interactions with cosmic rays
- photodesorbtion
- ...



Bergin et al. 2007

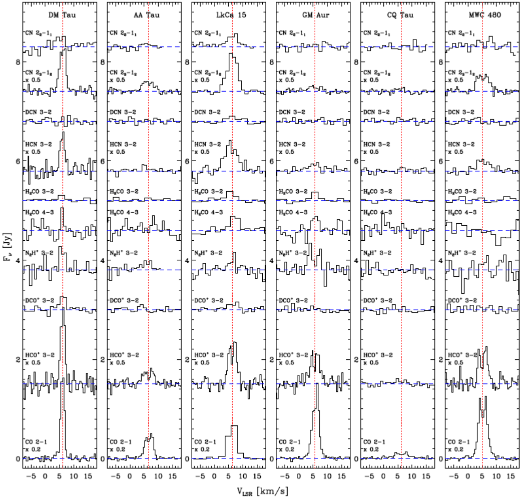
some chemical codes : Nautilus (Hersant et al 2009), ProDiMo (Woitke)...
some disks models : see papers by e.g. Aikawa, Walsh, Fogel...

(sub)millimeters chemical "Survey"

- "Chemistry In Disk" (CID)
- "Disk Imaging Survey of Chemistry with SMA" (DISCS)

General trend :

- no complex molecules detected
- Herbig Ae are poor in molecules.

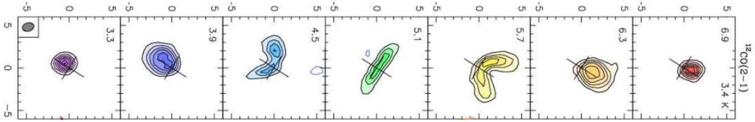


Oberg et al 2010

Kinematic

Protoplanetary disks are in Keplerian rotation :

MWC 480 ^{12}CO J=2-1 Piétu et al 2007



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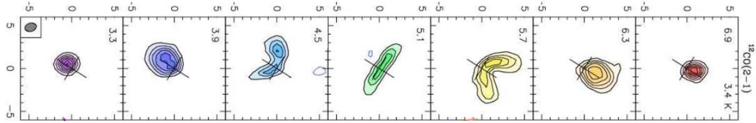
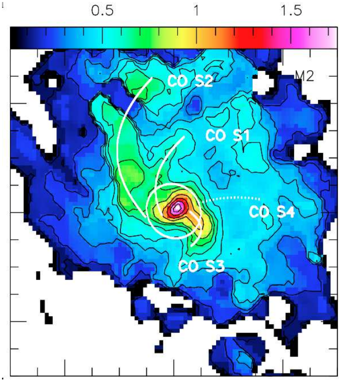


But case of AB Aur : sub-Keplerian rotation (Piétu et al. 2005 ; Lin et al.2006)
Follow-up observation PdBI (1.3mm + ^{12}CO J=2-1) Tang et al 2012
⇒ Infalling material from enveloppe

see also Poster P.42

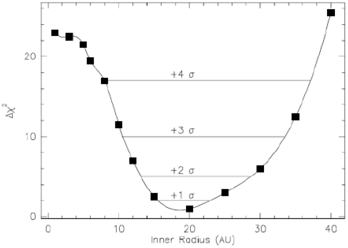


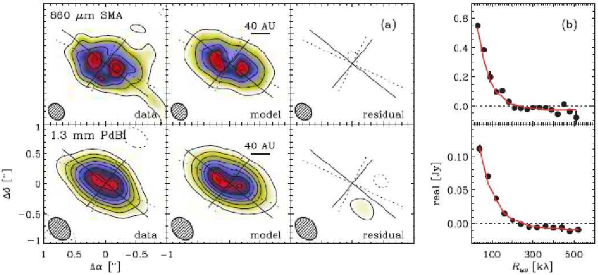
CO cavity : GM Aur

- Dutrey et al 2008 : cavity in CO ($R_{in} = 20$ AU)
- Hughes et al 2009 : similar cavity in dust

  cavity devoided of dust AND gas

→ planets (5-10 M_{jup}) ?

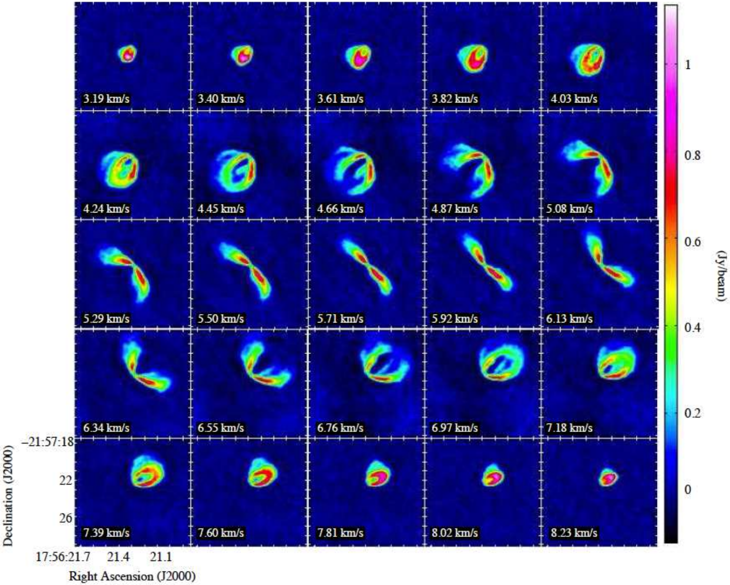




See also poster by S. Bruderer P.4

HD 163296 ALMA SV observations

$^{12}CO(3\text{-}2)$ channel map : (De Gregorio et al. subm.)

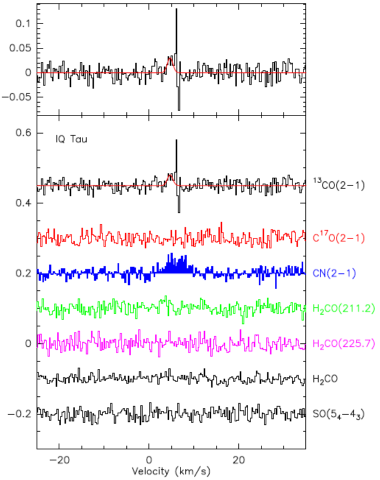


Other disk tracers

Survey with the IRAM 30m
Guilloteau et al 2012

Survey of 42 T-Tauri and Herbig A2 in CN J=2-1, ^{13}CO and $C^{17}O$ J=2-1, H_2CO and SO

- ^{13}CO is strongly affected by confusion,
- CN is a good tracer of disks for stars in the M1-K5 range
- SO is ubiquitously found in outflow-driving, embedded sources, but exceptional in disks (only 1 source).

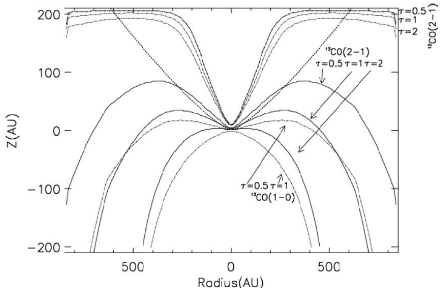


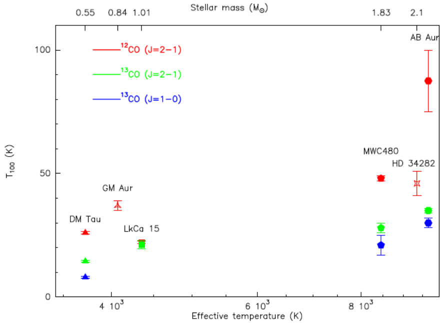
IQ Tau

Gas temperature

Vertical gradient

PdBI observation of CO & ^{13}CO Dartois et al 2003, Piétu et al 2007
see also Akiyama et al 2012





In TTauri disks T can be very low

Cold molecular layer in T-Tauri ?

Observation of molecules at very low temperature ($\sim$10 K at R = 100 AU) in T-Tauri

- CO/^{13}CO J=1-0 and J=2-1 Dartois et al 2003, Piétu et al 2007 (DM Tau)
- CCH J=1-0 and J=2-1 Henning et al 2010 (DM Tau, LkCa 15)
- CN J=2-1 /HCN J=1-0 Chapillon et al 2012 (DM Tau, LkCa 15)
- CS J=3-2 and J=5-4 Guilloteau et al 2012 (DM Tau)

So far, observations cannot be reproduiced by chemical models

But warm gas in MWC 480 (Herbig Ae)

- CO/^{13}CO T$>$ 20 K Pietu et al 2007
- CN T $\sim$ 30 K Chapillon et al 2012

$\Rightarrow$Surprisingly low temperature for gas phase molecules in T-Tauri

$\hookrightarrow$ turbulence ? (Aikawa et al 2007)

$\hookrightarrow$ photodesorption ? (Hersant et al 2009)

$\Rightarrow$Discrepancy T-Tauri / Herbig Ae

Investigating the disk mid-plane :

Searching for H_2D^+

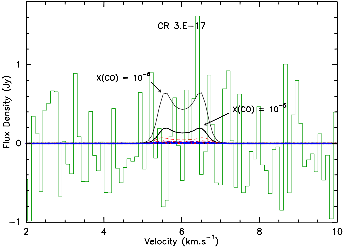
o-H_2D^+ 372 GHz line
TW Hya (APEX), DM Tau (JCMT)
no detection (Chapillon et al 2011)

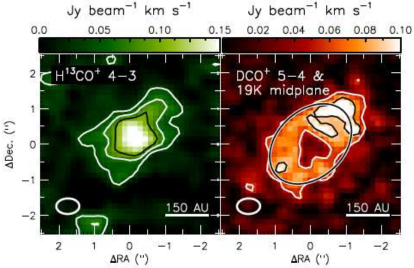
Tracing the CO snow line at

R $\sim$ 155 AU in HD 163296

- from CO isotopologues Qi et al 2011
- from H_2CO Qi et al 2013
- from DCO^+ Mathews et al 2013 subm.

See talks by Mathews and Oberg





Turbulence

Turbulence, important for accretion, grain coagulation...
Line-width : thermal broading + turbulence $\Delta V = \sqrt{\delta v_{th}^2 + \delta v_{tu}^2}$

From CO observation :

- DM Tau : < 0.14 km/s
  Dartois et al 2003,
  Piétu et al 2007
- Hughes et al 2011 :
  TW Hya < 0.04 km/s,
  HD 163296 ~ 0.3 km/s

CS in DM Tau

CS : heavy and still abundant
$\sim 1''$ PdBI data (+30m)

$T_{300AU} = 7 - 10$K
$\delta v_{th} = 0.13 - 0.12$ km/s
Guilloteau et al. 2012 (CID VIII)

Geometric Parameter	Adopted Value	Fitted Value from CS	
Distance (pc)	140		
PA (°)	65	65 ± 2	
i (°)	-35	-35 ± 1	
V_{LSR}	6.08	6.08 ± 0.02	
V_{100} (†)	2.16	2.17 ± 0.10	
M_* ($M_\odot$)	0.54	0.54 ± 0.04	
h	-1.25		
Fitted Value	**Density Model (A) Power Law**	**(B) Tapered Edge**	**Note**
χ^2	2468353	2468336	
H_0 (AU) (a)	[16]	9 ± 1.5	(1)
T_0 (K) (b)	7.2 ± 0.4	8.0 ± 1.3	
q	0.63 ± 0.09	0.60 ± 0.20	
Σ_{CS} (cm^{-2}) (b)	$5.9 \pm 2.5\ 10^{12}$	-	(2)
X_{CS} (b)	-	$4.2 \pm 4.8\ 10^{-10}$	(2)
p_{CS}	0.13 ± 0.20	0.39 ± 0.18	
Σ_d (cm^{-2})	-	$\approx 10^{21.7\pm0.1}$	(3)
R_{out} (AU)	540 ± 10	> 580	
dV_0 (km.s^{-1}) (b)	0.13 ± 0.03	0.12 ± 0.025	
e_V	0.38 ± 0.45	[0.3]	(1)

Notes. (†) Rotation velocity (km.s^{-1}) at 100 AU, which determines the stellar mass M_*. (a) at 100 AU, (b) at 300 AU. (1) a number between brackets [] indicate a fixed parameter. (2) Large errorbar due to strong coupling with temperature. (3) Error bar not symmetric; derivation from covariance matrix inaccurate.

Gas mass estimation

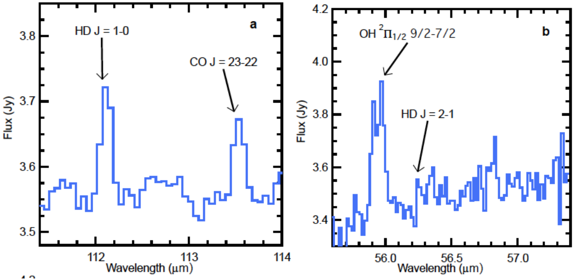
Estimation of the disks masses

Crutial parameter for planetary formation. Very difficult :
Usually from CO

- from gas emission $\rightarrow$ need molecular abundaces
- from dust emission $\rightarrow$ need gas-to-dust ratio

"Direct" measurement

Detection of HD (Bergin et al 2013) in TW Hya

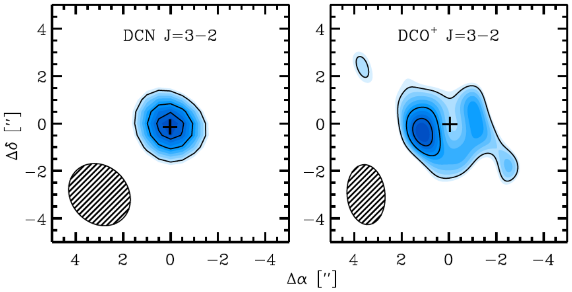


$\Rightarrow$ $M_{disk} > 0.05 M_{\odot}$

Talk by Bergin

DCN and DCO^+

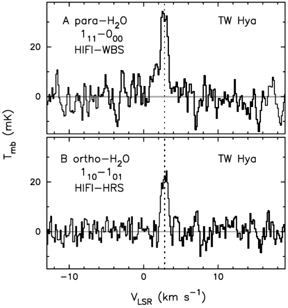
Multiple pathway to deuteration (Oberg et al 2012)
DCN, DCO^+ J=3-2 data



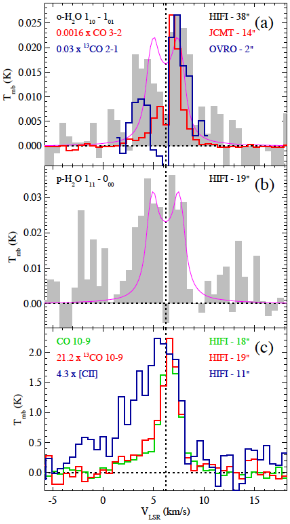
- DCN centraly picked → in the warm region
  additional pathway to formation at $T > 30\,K$ through CH_2D^+
- DCO^+ formed at $T < 30\,K$ through H_2D^+

H_2O

- tentative detection in DM Tau (Bergin et al 2010)
- detection in TW Hya (Hogerheijde et al 2011) T_{spin}=13,5$\pm$ 0,5 K



- detection in DG Tau (Podio et al 2013)
  trace the disk's kinematic
  strong stellar UV flux, orrigine of water in a super-heated layer.

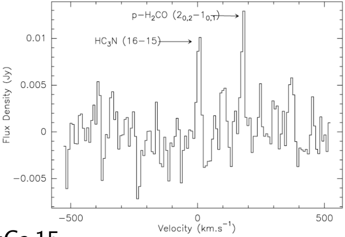


DG Tau

New detection of complexe molecules

H_3CN, deep search with IRAM 30m and PdBI

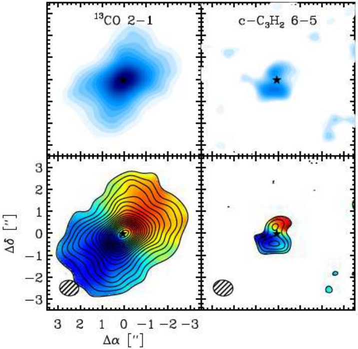
5σ detection in GO Tau LkCa 15 and MWC 480, not detected on DM Tau.



LkCa 15

Chapillon et al 2012

c-C_3H_2, ALMA SV data HD 163296



Qi et al 2013

Search for CCS and HC_3N

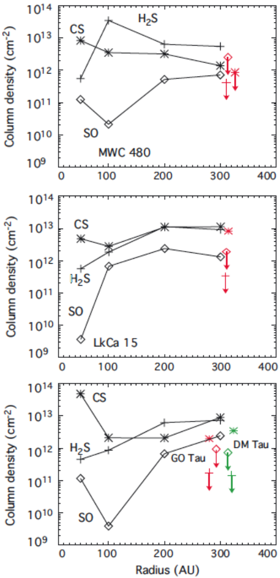
Deep search with the IRAM 30-m and PdBI for heavier molecules.

	Σ_{300} (cm^{-2})			
	HC_3N		CCS	
Souce	Derived	Predicted	Derived	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	$6 \pm 1 \cdot 10^{11}$	$6.4 \cdot 10^{11}$	$\leq 0.9 \cdot 10^{12}$	$3.1 \cdot 10^{11}$

- CCS not detected.
  Upper limit compatible with chemical model
- N(HC_3N) are 2 orders of magnitude lower than predicted
  $\rightarrow$ strong UV field
  $\rightarrow$ grain growth ?
  $\rightarrow$ dust settling ?

Chapillon et al 2012 (CID VII)

Search for S-bearing molecules



- CS detected
- SO and H_2S : upper limits

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

Sources	Σ_{300} (cm^{-2}) SO	H$_2$S	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.

- better agreement with initial $C/O = 1.2$ (Hincelin et al 2011)
- CS and SO OK
- H_2S failed
  $\rightarrow$ emphasis importance of grain surface chemistry.
  H_2S may be locked into grain mantle

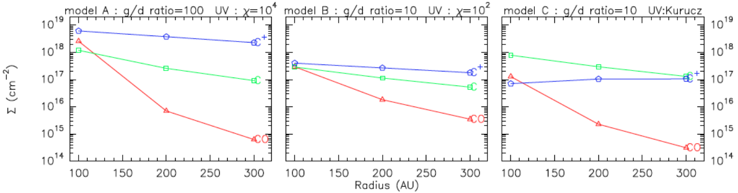
$\Rightarrow$ chemical code to improve
Dutrey et al 2011

Carbon in disks

Gas-poor dusty rich source

- PdBI data on ^{12}CI J=2-1
  CO J=2-1 optically thin + strong continuum
  gas temperature > 50 K Results depletion of factor 100 ? → g/p ∼1 ?
- AND APEX data on CI (upper limits)
- model test grain size, g/p UV field (not well known)

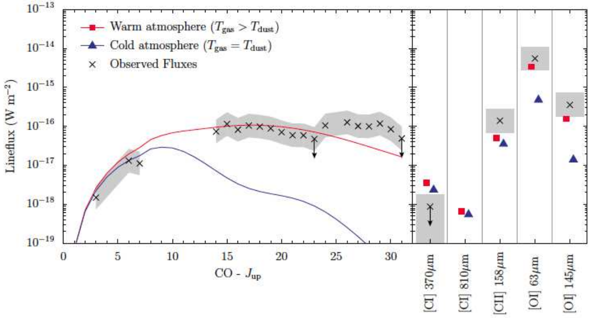
⇒ gas-to-dust-ratio ∼ 10 in CQ Tau



CI is sensitive to the stellar UV profile (“excess”) (Chapillon et al 2008, 2010)

Carbon in disks

HD 100546, a Carbon-poor disk



Lots of CO lines + CII and OI lines and uper limits on CI.

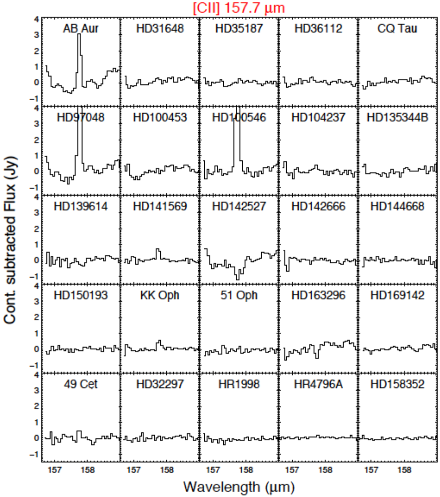
- Warm atmosphere (Tgas > Tdust) needed to reproduce the high-J CO
- Can explain the upper limit of CI together with the CO ladder and OI for high gas-to-dust ratio, but low amount of volatile carbon. But this underproduces CII.
- CII likely affected by cloud emission

Bruderer et al 2012

Carbon in disks

CII detection rate is poor

but predicted strong. → Contamination by clouds ?



Meeus et al 2012

Comparison with current chemical models

Some success (i.e. CO snow line in HD 163296), but still lot of discrepancies

- Current models do not reproduce cold gas-phase molecules in T-Tauri
- Order of magnitude of molecular column densities not reproduced (i.e. HC_3N, H_2S)
- lack of CI and CII
- difference T-Tauri (low mass) / Herbig Ae (intermediate mass)

⇒ We miss something !

- updated reaction rates (KIDA : KInetic Database for Astrochemistry, PI Wakelam)
- initial conditions (better fit with an initial $C/O = 1.2$, Hincelin et al 2011)
- interaction with grains
  - grain surface reactions
  - desorption mechanisms (UV, IR, heatting...)
  - grain growth, sedimentation, radial variation
- Profile of illuminating UV spectrum (e.g. importance of UV excess in the CI prediction)
- X- ray driven chemistry (link to TT/HAe difference ?)

- chemistry is a powerfull tool to study protoplanetary disks structure and composition
- with ALMA,
  - imaging lines that are already detected with much better accuracy
    ↪ allow us to study specific layer in the disk
  - imaging of complex molecules may not be so easy
- we need more accurate chemical modeling
- we need more accurate estimation of the dust content
- we need more accurate estimation of the stellar UV/Xray emission profile
- desorption mechanismes seems important.

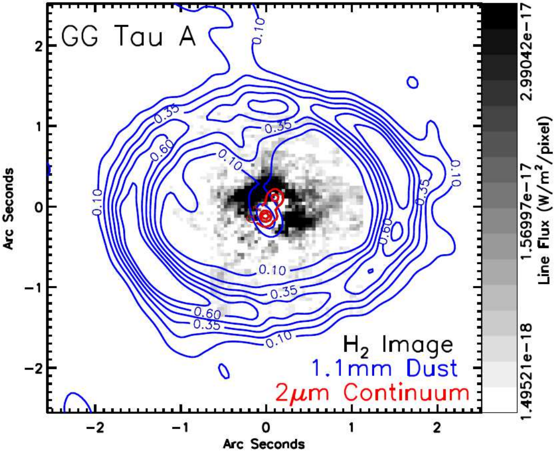
⇒ ALMA observation of gas AND dust ⇒ improve models

THANK YOU !

H_2 emission in GG Tau

GG Tau : circumbinary disks

Severeal lines of H_2 detected (v= 1-0 S(1) and v =2-1)



H_2 emission seems to trace the dust streamer

Beck et al 2012