Molecular and continuum surveys as tools to determine the structure of protoplanetary disks - part I

by Anne Dutrey (LAB, France)

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With inputs from

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Circumstellar Disks around low-mass PMS Stars

- Disks: \( r \sim 100-900 \text{ AU}, \ M \sim 0.001 – 0.1 \text{ Msun (of H}_2\text{ gas)} \)
  - Nearest star forming regions at \( \sim 150 \text{ pc, } 1'' = 150 \text{ AU} \)
  - Planet formation: 1 gap (~5 AU) = 0.03”
  - High angular resolution required

- Mostly cold gas and dust: \( T_k \) 10 to 30 K
  - High sensitivity required
  - (sub)-mm domain well matched (rotation lines, dust emission)

- For \( M_* = 1 \text{ Mo} \), rotation velocities around 2 km/s.
  - Turbulence only around 0.2 km/s.
  - High spectral resolution required

- Large mm and sub-mm arrays are the ideal tools …

  … Geometry, dynamics, temperature, mass distribution …

  – Thermal Dust emission
  – Molecular Rotation Lines such as those of CO (no « easy » detection of \( \text{H}_2 \))

  – Current observations: 0.3” - 0.5” resolution \( \sim 50 – 70 \text{ AU} \)
c), d) Proto-planetary Disks

庞大尘埃 1 μm

含足够气体形成“proto-Jupiter”

总盘质量 ~ 几个 0.01 Msun

大多数盘质量在气态

$G/D \sim 100$ (?)

$H_2$ 不容易检测 (旋转线在 IR，尘埃光学厚)

年龄 ~ 几个 Myr

TTauri stars 0.5 to 2 Msun
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 ?

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

Various Gas $\Sigma(r)$ (G/D = 100) to form our planetary system (from Guillot 2000)

High-mass and low-mass Proto-solar Nebulae

$\Sigma(r)$: a key parameter!

From classes O to III …
### PART I (Anne’s talk)

- What can we learn from CO?
  - \( T_{\text{gas}} \)
  - Gas Surface Density \( \text{(Diskfit)} \)
  - Inner Geometry

- Chemistry & Molecular Surveys:
  - IRAM 30-m
  - CiD project \( \text{(Nautilus,KIDA)} \)
  - Interferometric mapping
  \( \text{(Tgas – ionisation – deuteration)} \)

- Molecular Complexity:
  - \( \text{H}_2\text{CO} \ldots \)
  - What else?

- What about dust?
  - Disk structure
  - Dust Settling

### PART II (Stephane’s talk)

- Dust disks
  - Geometry of inner/outer dust disks
  - \( T_{\text{dust}} \) versus \( T_{\text{gas}} \)
  - Surface density
  - Dust radial and vertical variations
  - Alpha prescription & turbulence

- Impact on Gas Disks
  - Grain growth & UV penetration
  - Role Mixing /turbulence

- Impact on chemistry & G/D?

- How to measure turbulence?

- Stellar Masses?

- Challenges for ALMA
  - A long list …
DM Tau: 
0.5 Msol, Age ~ 5 Myrs

CO J=1-0, pdBI data

Guilloteau & Dutrey 1998

- Keplerian Rotation
  (stellar mass measurement: see Part II)

- Determination of the physical parameters (eg temperature, density, turbulence...) versus r and z.
Dust and Gas Modeling – Diskfit
Dutrey et al., 1994 – Guilloteau et Dutrey 1998 – Piétu et al., 2007

- Power law distributions (or viscous law – see Stephane’s talk):
  - $T(r) = T_0 \cdot (r/r_0)^{-q}$
  - $\Sigma(r) = \Sigma_0 \cdot (r/r_0)^{-p}$
  - $h(r) = h_0 \cdot (R/r_0)^{h}$. - or - $h(r) = \sqrt{(2kT(r)/(\mu m_H))r/v(r)}$
  - $n(r,z) = n(r,0) \cdot \exp[-(z/h)^2]$
  - Kappa($\nu$) = $K_0(\nu/10^{12} \text{ Hz})^\beta$ (Beckwith prescription, Boehler et al 2012...)

- Rotation: $v(r) = v_0 \cdot (r/r_0)^{-v}$
  - Keplerian case: $v = 0.5$, $v_0 = (G.M/r_0)^{1/2}$ (V is measured)

- Line-width: thermal + turbulent
- LTE / non-LTE
- Prédiction of $T_b(r)$ - “ray tracing”

- Minimization in the Fourier plane (not necessary with ALMA)

\[ \chi^2 = \sum_n \sum_i \left( Re(mod_{i,n} - Re(obs_{i,n}))^2 \times W_i + \sum_n \sum_i (Im(mod_{i,n} - Im(obs_{i,n}))^2 \times W_i \right) \]

Benchmark of Diskfit (CiD): Pavlyuchenkov et al., 2007
**CO line distributions**

- If disks are resolved \( \rightarrow \) \( T_b(r) \)
- If optically thick thermalized lines
  \( \rightarrow T_b(r) = T_k(r) \)
- If optically thin thermalized lines
  \( \rightarrow T_b(r) \sim \Sigma \text{mol}(r)/T_k(r) \) for \( J=1-0 \)
- \( \Sigma(H_2) = \Sigma_{\text{mol}} / X(\text{mol}) \)
  \( \rightarrow X(\text{mol}) \) difficult to constrain

\( (\Sigma(H_2) = \Sigma_{\text{dust}} \times G/D) \)

- \( H_2 \) mass is not yet well constrained even if distribution \( \sim \) known
- Non-LTE \( \rightarrow \) replace \( T_k \) by \( T_{\text{ex}} \) …
- \( CO \) \( J=3-2 \) and higher lines are not thermalized everywhere

Dartois et al 2003

DM TAU PdBI data

Dutrey, Guilloteau, Ho, 2007 - PPV
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: $T_k(r) \rightarrow T_{ex}(r)$

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

Piétu et al 2007
**CO: Inner Cavities ... 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*
Current arrays are for 50-100 AU resolution

- For SMA J=3-2
- For PdBI J=2-1

Only outer disks (> 30 AU) studied so far…
Making predictions is not enough

Inversion mandatory with a step by step approach to remove at best degeneracies. Otherwise, you don’t prove anything…

CO in the ALMA era → Disk Gas Structure
Molecular abundances referenced to CO?
• **Detection**
  
  CO, $^{13}$CO, C$^{18}$O (many papers)

  HCO$^+$, CN, HCN, HNC, CS, H$_2$CO and C$_2$H (Dutrey et al 1997: DM Tau & GG Tau, Henning et al 2010, **CID**, Chapillon et al 2011, **CID**: MWC480, DM Tau, LkCa15)


  N$_2$H$^+$ (Dutrey et al 2007, DM Tau, LkCa 15, **CID**)

  DCN (Qi et al 2008: TW Hya)

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

  H$_2$O (Herschel, Bergin et al 2010, Hogerheijde et al 2011)

• **Deep Search**

  H$_2$D$^+$ (Chapillon et al 2011 in DM Tau & TW Hya) - no detection

  Sulfur-bearing molecules (Dutrey et al 2011, **CID**) – only CS

  HC$_3$N, CCS (Chapillon et al 2012 in DM Tau, GO Tau, MWC480 and LkCa15, **CID**)
CiD: Chemistry In Disks

A french-german collaboration
→ started in 2004,
co-leaders: A.Dutrey & Th.Henning

PdBI:
Best angular resolution → 0,35” ≡ 50 AU @ D=140 pc

ALMA: International collab. in 2010
« cycle 0 » Chapillon et al., CN proposal
→ 7 papers written + several satellites

Let’s discuss the CN paradigm, first ...
→ Need for a chemical model including the disk physics
Molecular Disk "Ingredients"

What we need to mimic a disk:

- Surface chemistry (on grains)
  (need for 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

Z
- Surface (3-5H): XDR/PDR Chemistry
- Molecular layer (1-3H)
- Mid-plane (0-1H) with a cold dense cloud chemistry

molecules also observed in the mid-plane or at very cold T~7 K !!!
NAUTILUS – developed in LAB / AMOR

1D code developed in Bordeaux by F. Hersant and V. Wakelam (originally from the Eric Herbst’s team, Ohio State University)

Chemistry:
- full gas-phase network (~4000 reactions, ~400 species): osu_03_2008
- surface chemistry (rate equation approach, ~2000 reactions, ~200 species)
- gas-grain interactions (sticking, thermic and non-thermic desorption, photo-processes)
- UV penetration (1D geometry)

Physics:
- 1D Vertical dimension (Av, T and n)
- z diffusion

Future:
- improve gas-phase network for high temperature
- include 3-body reactions
- study the importance of grain size

- DM Tau structure (Piétu et al., 2007)
- CO photo-desorption (Oberg et al., 2007)

R=300 AU

(team AMOR = Astrochimie Moleculaire et ORigines des systemes planetaires)
• Bordeaux versus Heidelberg chemical models
• osu_2008_03 ratefile
• Accretion / Desorption
• Surface Chemistry: Surface reactions on 0.1μm olivine grains
• ‘TMC1’, ‘Hot core’, ‘DM Tau disk’

Semenov, Hersant, Wakelam, Dutrey et al 2010
ALMA next steps: channel per channel molecular maps

On going ...

- Accretion / Desorption
- Surface Chemistry: Surface reactions on 0.1μm olivine grains
- ‘TMC1’, ‘Hot core’, ‘DM Tau disk’

Semenov, Hersant, Wakelam, Dutrey et al 2010
PdBI CN J=2-1 data in GO Tau (DM Tau -like)
One hyperfine component - dv = 0.2 km/s, res~ 1’’
PdBI CN J=2-1 data in GO Tau (DM Tau -like)
Main hyperfine component $dv = 0.2$ km/s , $res \sim 1''$
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, \( r \sim 100 \) AU, \( T_k \sim 10 \) K, confirmed by *Pietu et al 2007*

- Vertical/Radial mixing: *Semenov et al., 2006, Aikawa 2007, Hersant 2009*

- CCH (CID): *Henning et al 2010* \( \rightarrow \sim 8\text{-}10\) K at 100 AU

- CN/HCN (CID): *Chapillon et al., 2011* PdBI data

  - HAe: MWC 480 – warm \( \sim 30 \) K
  - TTauri: LkCa15 (as cold as DM Tau)

  \( \rightarrow \) cold mid-plane or cold molecules
  \( \rightarrow \) difficult to reconcile with models

\(< 1\)H?

- \(^{13}\)CO, CCH, CN (2-1) \( \rightarrow \sim 9 \) K
- HCN (1-0) \( \rightarrow \sim 7 \) K
**Gas temperature around mid-plane: towards a cold molecular layer?**

Chapillon et al. 2011

**Table 2. Results of analysis**

<table>
<thead>
<tr>
<th>Source</th>
<th>Molecule</th>
<th>( \Sigma ) ( \times 10^{12} ) cm(^{-2} )</th>
<th>( p )</th>
<th>( R_{\text{out}} ) (AU)</th>
<th>( \delta V ) (km s(^{-1} ))</th>
<th>( T_k ) (K)</th>
<th>( q )</th>
<th>( R_{\text{int}} ) (AU)</th>
<th>( \alpha_d )</th>
</tr>
</thead>
<tbody>
<tr>
<td>MWC 480</td>
<td>HCN 1-0</td>
<td>( 1.1 \pm 0.4 )</td>
<td>( 2.4 \pm 0.4 )</td>
<td>[550]</td>
<td>( 0.3 \pm 0.2 )</td>
<td>[30]</td>
<td>[0]</td>
<td>0.0 ± 0.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (high)</td>
<td>( 11 \pm 1 )</td>
<td>( 2.1 \pm 0.1 )</td>
<td>( 540 \pm 40 )</td>
<td>( 0.25 \pm 0.04 )</td>
<td>( 33 \pm 6 )</td>
<td>[0]</td>
<td>0.0 ± 0.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (low)</td>
<td>( 11 \pm 1.2 )</td>
<td>( 2.1 \pm 0.15 )</td>
<td>( 550 \pm 70 )</td>
<td>( 0.26 \pm 0.07 )</td>
<td>( 33 \pm 6 )</td>
<td>[0]</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (all)</td>
<td>( 10.4 \pm 0.9 )</td>
<td>( 2.1 \pm 0.1 )</td>
<td>( 545 \pm 35 )</td>
<td>( 0.25 \pm 0.04 )</td>
<td>( 30 \pm 4 )</td>
<td>[0]</td>
<td>–</td>
<td></td>
</tr>
<tr>
<td>LkCa 15</td>
<td>HCN 1-0</td>
<td>( 10.6 \pm 1.5 )</td>
<td>( 1.1 \pm 0.2 )</td>
<td>( 600 \pm 40 )</td>
<td>( 0.20 \pm 0.03 )</td>
<td>( 7.0 \pm 0.6 )</td>
<td>( 0.55 \pm 0.25 )</td>
<td>[30]</td>
<td>0.0 ± 0.8</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (high)</td>
<td>( 38 \pm 4 )</td>
<td>( 2.3 \pm 0.2 )</td>
<td>( 570 \pm 20 )</td>
<td>( 0.18 \pm 0.02 )</td>
<td>( 10.8 \pm 0.7 )</td>
<td>( 0.20 \pm 0.07 )</td>
<td>[30]</td>
<td>0.15 ± 0.17</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (low)</td>
<td>( 115 \pm 18 )</td>
<td>( 0.2 \pm 0.2 )</td>
<td>( 690 \pm 20 )</td>
<td>( 0.24 \pm 0.03 )</td>
<td>( 6.6 \pm 0.3 )</td>
<td>( 0.80 \pm 0.07 )</td>
<td>[30]</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (all)</td>
<td>( 58 \pm 5 )</td>
<td>( 0.8 \pm 0.1 )</td>
<td>( 630 \pm 35 )</td>
<td>( 0.18 \pm 0.01 )</td>
<td>( 8.8 \pm 0.3 )</td>
<td>( 0.95 \pm 0.05 )</td>
<td>[30]</td>
<td>–</td>
</tr>
<tr>
<td>DM Tau</td>
<td>HCN 1-0</td>
<td>( 6.5 \pm 0.9 )</td>
<td>( 1.0 \pm 0.3 )</td>
<td>( 660 \pm 20 )</td>
<td>( 0.18 \pm 0.01 )</td>
<td>( 6.0 \pm 0.4 )</td>
<td>( 0.00 \pm 0.12 )</td>
<td>[30]</td>
<td>0.0 ± 0.5</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (high)</td>
<td>( 26 \pm 4 )</td>
<td>( 2.1 \pm 0.15 )</td>
<td>( 650 \pm 20 )</td>
<td>( 0.16 \pm 0.01 )</td>
<td>( 8.6 \pm 0.5 )</td>
<td>( 0.05 \pm 0.05 )</td>
<td>–</td>
<td>0.0 ± 0.3</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (low)</td>
<td>( 46 \pm 9 )</td>
<td>( 0.7 \pm 0.15 )</td>
<td>( 550 \pm 25 )</td>
<td>( 0.20 \pm 0.01 )</td>
<td>( 6.5 \pm 0.5 )</td>
<td>( 0.50 \pm 0.08 )</td>
<td>–</td>
<td>0.0 ± 0.3</td>
</tr>
<tr>
<td></td>
<td>CN 2-1 (all)</td>
<td>( 35 \pm 9 )</td>
<td>( 0.6 \pm 0.06 )</td>
<td>( 620 \pm 15 )</td>
<td>( 0.17 \pm 0.01 )</td>
<td>( 7.5 \pm 0.3 )</td>
<td>( 0.60 \pm 0.05 )</td>
<td>–</td>
<td>0.0 ± 0.3</td>
</tr>
</tbody>
</table>

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

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

**PDR:** \( \text{HCN} + \text{hv} \rightarrow \text{CN} + \text{H} \) (high amount of HCN)

\( \text{N} + \text{CH} \rightarrow \text{CN} + \text{H} \) (upper in the disk)

\( \text{N} + \text{C2} \rightarrow \text{CN} + \text{C} \)
Gas temperature around mid-plane: towards a (partly) cold molecular layer?

- CO/\(^{13}\)CO
  - the outer disk is cold, \(r \sim 100\) AU, \(T_k \sim 10\) K, confirmed by Pietu et al. 2007

- Vertical/Radial mixing:
  - Semenov et al., 2006, Aikawa 2007, Hersant 2009

- CCH (CID):
  - Henning et al. 2010
  - \(\sim 8-10\) K at 100 AU

- CN/HCN (CID):
  - Chapillon et al., 2011

Gas temperature around mid-plane:

- \(^{13}\)CO, CCH, CN (2-1) \(\rightarrow\) \(\sim 9\) K
- HCN (1-0) \(\rightarrow\) \(\sim 7\) K

\(< 1\) H? - cold mid-plane or cold molecules

\(\rightarrow\) difficult to reconcile with models
Revisiting the gas-phase kinetic of Nitrogen-bearing species

- New experiments for the measurements of $N + NO$ (Bergeat et al. 2009), $N + OH$ (Daranlot et al. 2011) and $N + CN$ reactions (Daranlot et al. submitted)

- Update of gas-phase reactions involving N-bearing species from KIDA experts (Wakelam et al. in prep)

- Less $N_2$, more $NH_3$ on grains

Simulations of the chemical evolution of a cold dense cloud using Nautilus

![Graph showing chemical evolution](image)

http://kida.obs.u-bordeaux1.fr
Administrator: V. Wakelam (kida@obs.u-bordeaux1.fr)
→ Subscribe to the newsletter

Nautilus: grains of 0.1µm, No UV, $Tk = 10K$, $n(H_2) = 10^4 \text{ cm}^{-3}$
How to trace the disk mid-plane?

→ Wait for CN 3-2 from ALMA …

• \( \text{H}_2\text{D}^+ \) formed in gas phase only at low temperature, easily destroyed by CO, \( \text{N}_2 \)

\[
\text{H}_3^+ + \text{HD} \rightarrow \text{H}_2\text{D}^+ + \text{H}_2 \quad \text{//} \quad \text{H}_2\text{D}^+ + \text{CO} \rightarrow \text{DCO}^+ + \text{H}_2 \quad \text{-} \quad \text{H}_2\text{D}^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{HD}
\]

→ should be abundant in the cold depleted mid-plane

• No detection, so far …

Chapillon et al 2011

→ JCMT (10hrs) - DM Tau
→ APEX (4hrs) - TW Hya

\( \text{O} - \text{H}_2\text{D}^+ (1_{1,1}-1_{1,0}) \) at 372 GHz

• 3x more sensitive than previous data → \( \text{H}_2\text{D}^+ \) still not detected!

• Analysis: chemical model from Parise et al 2011
Mid-plane: is $H_2D^+$ a good tracer?

**Chapillon et al 2011 -** JCMT/ APEX data on DM Tau & TW Hya
O - $H_2D^+$ $(1_{1,1}-1_{1,0})$ 372 GHz

→ Check several disk structures ($\Sigma$, $T_k$, $R_{out}$)

- No UV (mid-plane)
- Several CR rates ($10^{-17} - 3.10^{-17} - 10^{-16}$ s$^{-1}$)
- Several grain sizes ($a = 0.1 - 1 - 10 \mu$m)
- Several CO abundance ($10^{-4} - 10^{-5} - 10^{-6}$)

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

ALMA detection may be not so easy

**Table:**

<table>
<thead>
<tr>
<th>Disk</th>
<th>$\Sigma_0$ (cm$^{-2}$)</th>
<th>$p$</th>
<th>$R_0$ (AU)</th>
<th>$R_{out}$ (AU)</th>
<th>$\Sigma_{H_2}$ (cm$^{-2}$)</th>
<th>$p$</th>
<th>$R_0$ (AU)</th>
<th>$R_e$ (AU)</th>
<th>$T_{100}$ (K)</th>
<th>$q$</th>
<th>$T_{100}$ (K)</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DM Tau</td>
<td>$8.4 \times 10^{23}$</td>
<td>0.85</td>
<td>45</td>
<td>700</td>
<td>$9.6 \times 10^{23}$</td>
<td>0.45</td>
<td>45</td>
<td>180</td>
<td>15</td>
<td>0.4</td>
<td>30</td>
<td>0.63</td>
</tr>
<tr>
<td>TW Hya</td>
<td>$4.3 \times 10^{23}$</td>
<td>1.0</td>
<td>45</td>
<td>200</td>
<td>$3.3 \times 10^{23}$</td>
<td>0.7</td>
<td>45</td>
<td>30</td>
<td>30</td>
<td>0.5</td>
<td>40</td>
<td>0.2</td>
</tr>
</tbody>
</table>
• $\text{N}_2\text{H}^+$ has been observed at PdBI CID, *Dutrey et al., 2007*

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

• Main results:

$\text{HCO}^+$ remains the most abundant molecular ion in disk

$[\text{N}_2\text{H}^+]/[\text{HCO}^+] \sim 0.02$-$0.05$ (similar to dense cores)

• $\text{DCO}^+/\text{HCO}^+$ in TW Hya
  *Qi et al., 2008*

$[\epsilon] = n(\epsilon)/n(\text{H}_2) \sim 10^{-7}$ in the disk layer where the molecules are present (following Caselli 2002)

• Less $\text{HCO}^+$ in Herbig Ae Disks?

  - AB Auriga: *Schreyer et al 2009 (CID)*
  - MWC480: *Dutrey et al 2007 (CID)*

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

$\text{N}_2\text{H}^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{N}_2$
→ So far, molecules observed in disks are the most abundant seen in cold clouds.

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

• Deep search for Sulfur-bearing molecules: **CS, SO, H$_2$S**

• CS detected, significant upper limits on SO, H$_2$S (~7x better than in Dutrey et al 2000)

*Fig. 1.* Observations of SO $2_{23}-1_{22}$, H$_2$S $1_{10}-1_{01}$ and CS 3-2 in the four disks. For CS $J$=3-2, the best models have been superimposed for all sources. For SO and H$_2$S, the models always correspond to the 3σ upper limits.
So far, molecules observed in disks are the most abundant seen in cold clouds.

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

- **Deep search** for Sulfur-bearing molecules: **CS, SO, H$_2$S**
- CS detected, significant upper limits on SO, H$_2$S (~7x better - Dutrey et al 2000)

<table>
<thead>
<tr>
<th>Sources</th>
<th>SO</th>
<th>$\Sigma_{300}$ (cm$^{-2}$)</th>
<th>CS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>H$_2$S</td>
<td></td>
</tr>
<tr>
<td>DM Tau</td>
<td>$\leq 7.5 \cdot 10^{11}$</td>
<td>$\leq 1.4 \cdot 10^{11}$</td>
<td>$3.5 \pm 0.1 \cdot 10^{12}$</td>
</tr>
<tr>
<td>LkCa15</td>
<td>$\leq 1.9 \cdot 10^{12}$</td>
<td>$\leq 3.6 \cdot 10^{11}$</td>
<td>$8.7 \pm 1.6 \cdot 10^{12}$</td>
</tr>
<tr>
<td>MWC480</td>
<td>$\leq 2.5 \cdot 10^{12}$</td>
<td>$\leq 4.1 \cdot 10^{11}$</td>
<td>$\leq 8.4 \cdot 10^{11}$</td>
</tr>
<tr>
<td>GO Tau</td>
<td>$\leq 8.9 \cdot 10^{11}$</td>
<td>$\leq 1.8 \cdot 10^{11}$</td>
<td>$2.0 \pm 0.16 \cdot 10^{12}$</td>
</tr>
</tbody>
</table>

**Notes.** Sulfur-bearing molecules surface densities (cm$^{-2}$) at 300 AU (modeled as $\Sigma(r) = \Sigma_{300}(r/300$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.
Towards more complex molecules? Sulfur-bearing molecules in TTauri Disks

Dutrey et al 2011 (CID)

• Results: (outer) disk chemical modeling (Nautilus, Hersant et al 2009)
  - Grains 0.1µm
  - full network, inc. surface chemistry

→ $\text{H}_2\text{S}$ modeling incompatible with upper limit ... locked onto grains, form other species → no desorption

Experiments from Garozzo et al 2010: sulfur mostly in the form of a rich residuum (polymers, aggregates).

→ 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), inc. UV field

→ Weakness (surface chemistry) of current chemical models!

→ Must be solved for ALMA data interpretation!
What Else?
CCS & HC$_3$N in Disks

Chapillon et al 2012 (CID)

– IRAM 30-m – (EMIR+FTS)

DM Tau, LkCa15, MWC480 & GO Tau

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

• Deep search for heavier molecules in disk
  • CCS, HC$_3$N …

• Results: see future Edwige’s talk …

- Our 3σ upper limits on CCS are in very good agreement with the best modeling of sulfur-bearing molecules from Dutrey et al 2011 and rejects the other models.
Molecular Disk “Ingredients”

What we need to mimic a gas disk: We need Grains.

- Disk temperature governed by grains: dust absorbs the UV & visible light
In most of the disk (< 3-4 Hgas): Tgas = Tdust, by collisions

- Surface chemistry (on grains), need for a realistic (vertical, radial) size distribution

Impact on G/D(z), UV penetration…

z

- Surface (3-5H): XDR/PDR Chemistry
- Molecular layer (1-3H)
- Mid-plane (0-1H) with a cold -dense cloud chemistry
  → Most of the dust << 1H

Dust settling & grain growth – a major ingredient of disk physics and chemistry
First steps: ALMA predictions and inversion of dust vertical structure…
Dust Settling seen by ALMA


Settling controlled by the product:

\[ \Omega \times \tau \]

\( \tau = \frac{\rho_d a}{\rho C_s} \)

- \( \Omega \tau < 1 \) dust coupled to gas
- \( \Omega \tau > 1 \) dust settles toward mid-plane

\[ \frac{H_d}{H} \alpha \left( \left( \Omega \tau \right)_0 \right)^{-\alpha} \]

Small grains: \( \alpha = 0 - \alpha = 0.05 \) (Pinte et al., 2008)

Big grains: Dubrulle et al., 1995, Cabadillo et al., 2006
\( \alpha = 0.5 \)

MRI induced MHD turbulence
(from Fromang et Nelson 2009 simulations)
used to parametrize \( \Omega \tau \)
Dust Settling seen by ALMA

Boehler PhD these, dec. 2011, Boehler et al 2012

- Some Diskfit improvements

- Realistic dust properties
  - $a_{\text{min}} = 0.01 \ \mu\text{m}$
  - $a_{\text{max}} = 3 \text{mm}, \ a_{\text{max}} = 10 \text{cm}$

$\Rightarrow H(\text{dust}) << H(\text{gas})$

$z$

- Surface(3-5H):
  - XDR/PDR Chemistry

- Molecular layer (1-3H)

- Mid-plane (0-1H) with a cold dense cloud chemistry $\Rightarrow$

Most of the dust $<< 1H$
Some Diskfit improvements …

- Realistic dust properties
  - $a_{\text{min}} = 0.01 \ \mu\text{m}$
  - $a_{\text{max}} = 3\text{mm}, \ a_{\text{max}} = 10\text{cm}$

$H_{\text{dust}} \ll H_{\text{gas}}$

Surface (3-5H):
- XDR/PDR Chemistry

Molecular layer (1-3H)

Mid-plane (0-1H) with a cold dense cloud chemistry → Most of the dust $\ll 1H$
Dust Settling: methodology

Inversion is mandatory to estimate the accuracy on derived parameters

Several steps:

- 1) Make both homogeneous & settled disk pseudo observations

- 2) Inversion by an homogeneous one with realistic thermal noise

- 3) Add phase noise

Boehler et al 2012
Dust Settling

Disks: DM Tau-like with Rout = 100 AU
- sharp Rout

homogeneous & settled disk models have the same dust mass

- ALMA simulation at 0.5mm (670 GHz) with Bmax = 2.5km

→ Dust settling visible up to 75 degrees

**Next steps:**

- Several wavelengths: 3mm, 1.3mm, 0.8mm and 0.5mm

- Inversion with noise (inc. Phase noise)
- Results of the inversion by an homogenous model of grains when adding thermal + phase noises

  → Tdust is properly recovered & Hdust is low <<< Hgas(Tdust=Tgas)

  → Phase noise < 40 degrees

Errorbars increase but it does not prevent to observe settling!

→ NEXT STEPS:

  → Define the optimum ALMA observational strategy and quantify settling with ALMA

Boehler et al 2012
Many pending questions

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$_2$D$^+$ detection not as easy as expected** (emission should be resolved by ALMA)

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) **Molecular complexity**?
   Which level of complexity can be reached? **depends on** ALMA final characteristics

4) **Dust settling** should be observable by ALMA!
   Need to be properly incorporated in disk models (thermal eq. & chemistry)

5) **Roles of grains** → See stephane’s talk next week …
   - 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**