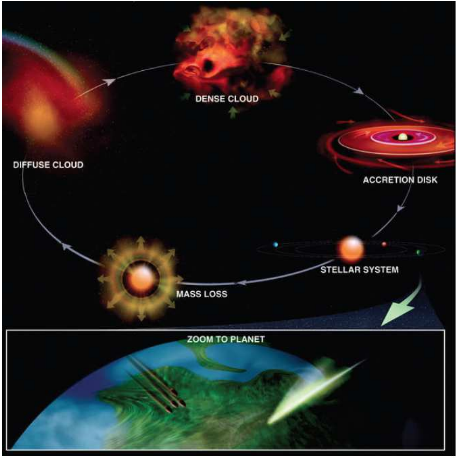
Abundances in (outer) protoplanetary disks

Edwige Chapillon (LAB/IRAM)

Abundance Measurements in Protoplanetary disks



Credit: Bill Saxton, NRAO/AUI/NSF

intermediate step between molecular clouds and planetary system

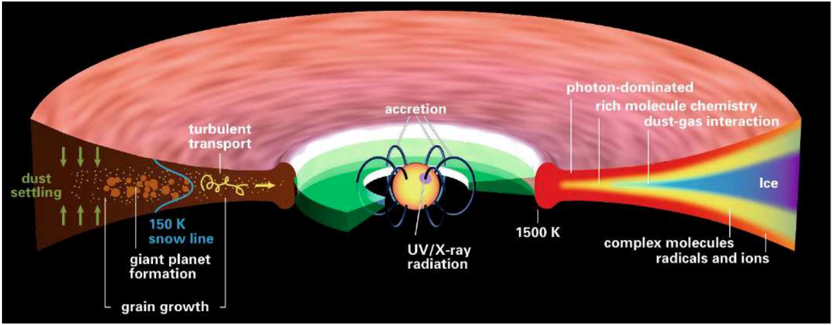
- Protoplanetary disks (gas + dust)
- Debris disks (dust)

- Protoplanetary disks = birth place of planets
- Inheritance of matter
- Initial conditions

- physical conditions ?
- molecular content ? (complexity)
- dust properties ?
- gas/dust ratio ?

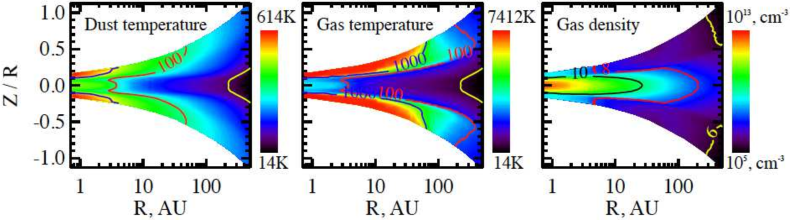
What is a protoplanetary disks ? – State of the art

Disks arround low-mass PMS stars ($\leq 2\,M_\odot$)



Henning & Semenov 2013

What is a protoplanetary disks ?



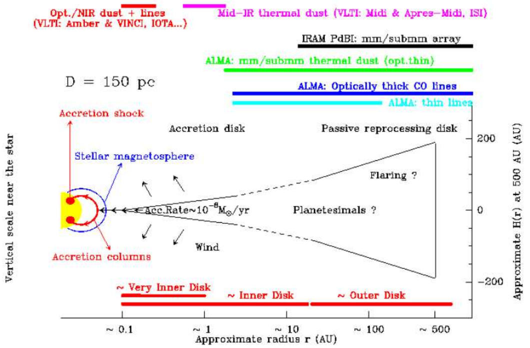
Akimkin et al 2013

- typical disk mass $\sim 10^{-2}\,M_{\odot}$
- small (radius $<$ 1000 AU)
- geometricaly thin
- large gradients in temperature
- large gradients in density
- gradients in velocity (Keplerian)

- dust properties (grain growth, settling...)
- UV, X-ray illumination
- turbulence
- gas/dust ration
- ...

Strong gradients in disks → chemistry deffinitively not homogeneous

Observations



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)

Spectra (single dish) spectro-imaging channel map (interferometer)

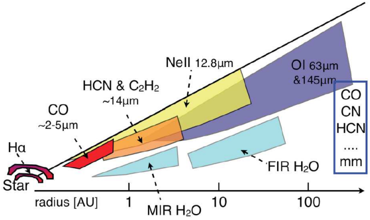
Molecules (and atoms) detected in disks (so far)

- 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)

detected in IR

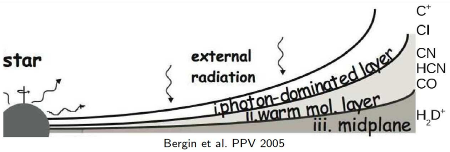
Sampling the disk

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

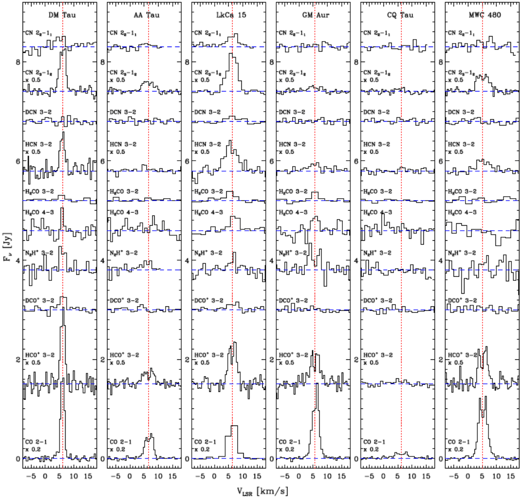
→ need to observe several molecule (isotopologues) and transition to retrieve disk's physical structure
→ bring information on kinematics, density, thermal structure, turbulence...

(sub)millimeters chemical "Survey" of the outer disks

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

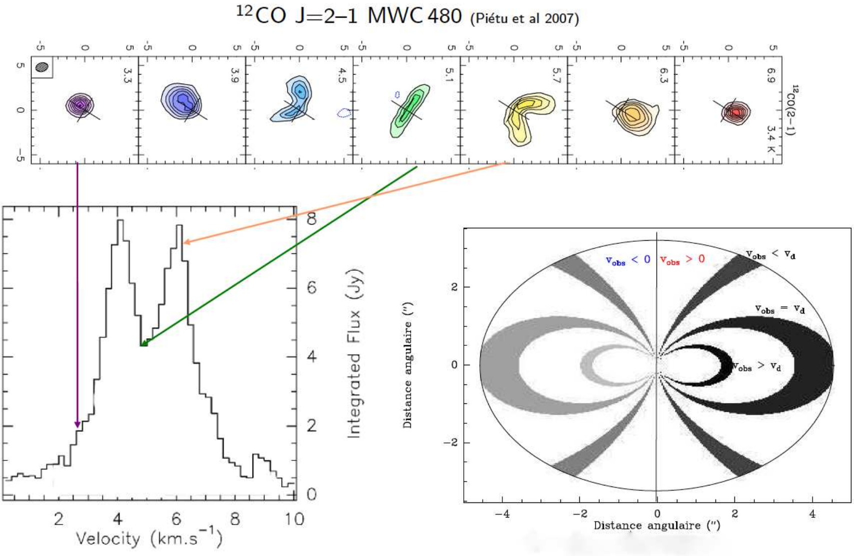
General trends :

- lines are weak (0.1–1 Jy)
- limited source sample
- no complex molecules detected (C_3H_2, HC_3N)
- Herbig Ae are poor in molecules.



Öberg et al. 2010

Line formation and Keplerian rotation



Line analysis

observable = line intensity, what we want = 3D structure (molecular abundances, density, temperature...)
2 methods :

- Forward method
  - compare the observed intensities with results from a physico/chemico models
- Inversion method
  - retrieve the physical parameters (T_{ex}, molecular surface density Σ) and associated error-bars

Hypothesis

- temperature parametric law (gradient in r and z) ; calculated from dust radiative equilibrium modeling
- surface density parametric (power) law ; molecules and total disk
- scale height power law ; calculated from temperature profile
- turbulence Line-width : thermal broading + turbulence $\Delta V = \sqrt{\delta v_{th}^2 + \delta v_{tu}^2}$
- excitation condition ETL (OK for J$\leq$3) ; Non-LTE

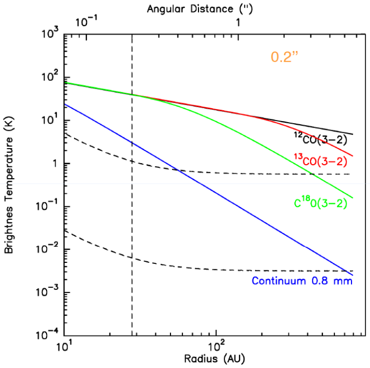
Inversion method

Parametrization of the disk : power law of the radius
(Rotation, temperature, scale height, density, surface density)

Analyse in the *uv*-plane : χ^2 minimization $\rightarrow$ errorbars
Only hypothesis on the physics of the disk : hydrostatic equilibrium

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

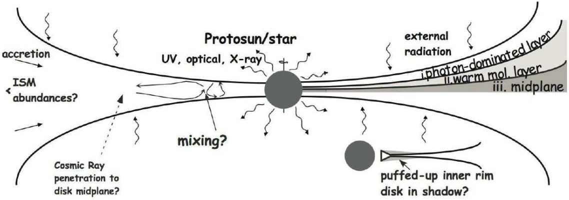
- If optically thick lines $\rightarrow$ $T_B(r) = T(r)$
- If optically thin lines $\rightarrow$ $T_B(r) = \tau T(r) \propto (T, \Sigma)$
  linear molecule, $h\nu << kT$
  - J=1-0 $T_B \propto \Sigma/T$
- if thermalised T = Tk
- if non-LTE T = Tex



Chemical codes

These codes needs

- a density structure (from hydrostatic model or derived from observation)
- a thermal structure
- grain distribution (and grain properties - size)
- chemical network



Bergin et al. 2005

- initial abundance
- Surface chemistry (on grains) (need a realistic size distribution)
- Neutral - neutral (low and high T)
- Ion - neutral
- 3 body reactions (?)

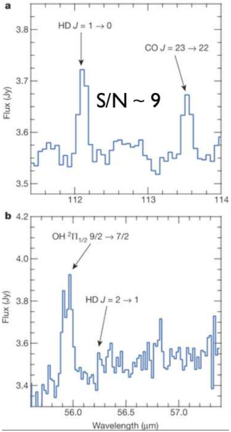
- Photodissociation, photoionization by UV
- Interactions with X rays
- Interactions with cosmic rays
- photodesorbtion
- ...

Different codes make different hypothesis

Total gas mass

H_2 is not observable $\rightarrow$ usual tracer is CO

- $\Sigma(H_2) = \Sigma_{mol} \ / \ X(mol)$
  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

One exeption : HD in TW Hya Bergin et al 2013 (Herschel)
A probe of gas mass : $M_{disk} > 0.05\ M_\odot$
Enough mass to form another solar system

Thermochemical models

Combine calculation of chemistry and physical structure

A few examples

- ANDES (Akimkin et al 2013)
- DENT grid (use MCFOST and ProDiMo (Pint et al 2009, Woitke et al 2009)
- Glassgold et al (2004,2007,2009,2012)
- Nomura et al 2007
- Gorti and Hollenbach 2004, 2008
- ...

Needs

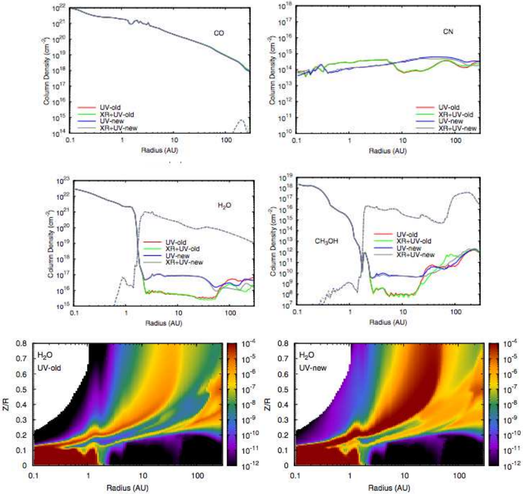
- density structure
- thermal structure
- dust properties
- UV / X-Rays

Radiative transfer codes

- RATRAN Hogerheijde and van der Tak (2000)
- Pavlyuchenkov et al 2007, Semenov et al 2008 : non LTE
- LIME Brinch and Hogerheijde (2010) : 3D inhomogeneous grid (opacity)

Chemical model

⇒ Chemical modeling. Several codes, see work by F. Hersant (Nautilus), P. Woitke (ProDiMo), Akimkin (ANDES), Y. Aikawa, C. Walsh, Fogel, H. Nomura...

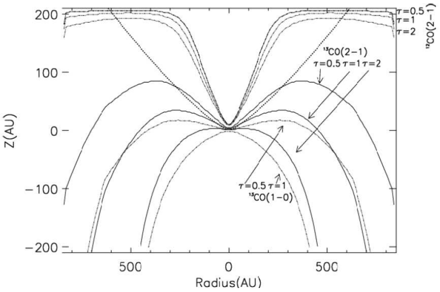


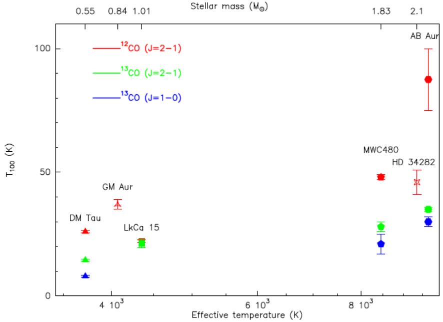
Walsh et al. 2012

Some results (where abundance is not the main point)

Gas temperature and 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

Some results (where abundance is not the main point)

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=2-1Dartois 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 reproduced by chemical models

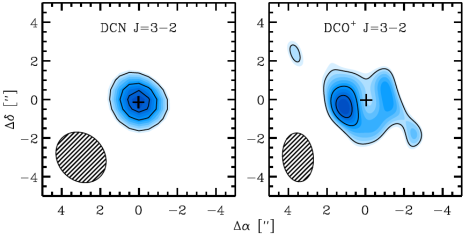
But warm gas in MWC 480 (Herbig Ae)

- $CO/^{13}CO$ T$>$ 20 K Piétu 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

Some results (where abundance is not the main point)

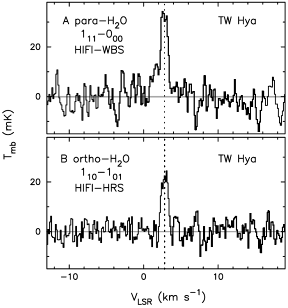
- caracterization of the brighest disks (e.g. DISCS and CID papers)
- cavity in dust in LkCa 15 (Piétu et al 2006) and gas in GM Aur (Dutrey et al 2008
- deuteration (Oberg et al 2012) ring in DCO^+, DCN centrally peaked



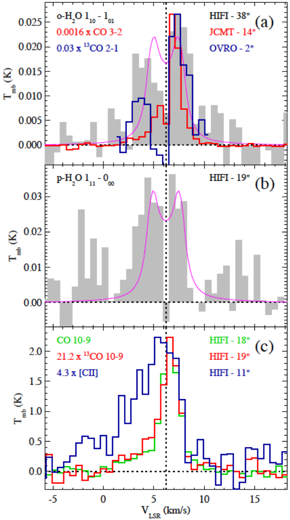
- turbulence (Hughes et al 2011, Guilloteau et al 2012)

H_2O

- tentative detection in DM Tau (Bergin et al 2010)
- detection in TW Hya (Hogerheijde et al 2011) T_{spin}=13,5± 0,5 K, layer of maximum abundance 0.5 - 2. 10^{-7} (/H_2)

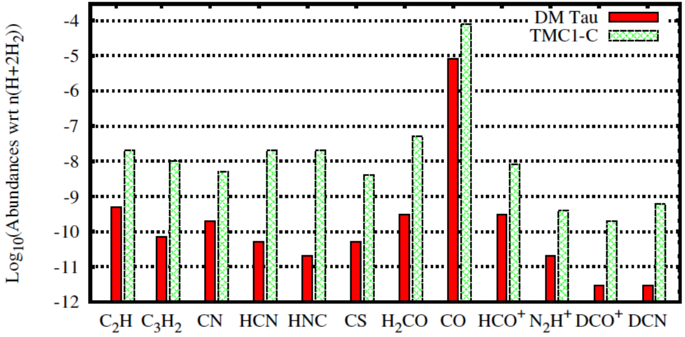


- detection in DG Tau (Podio et al 2013) trace the disk's kinematic strong stellar UV flux, orrigine of water in a super-heated layer.



DG Tau

Abundances



Molecular abundance in DM Tau and TMC-1 Henning & Semenov 2013

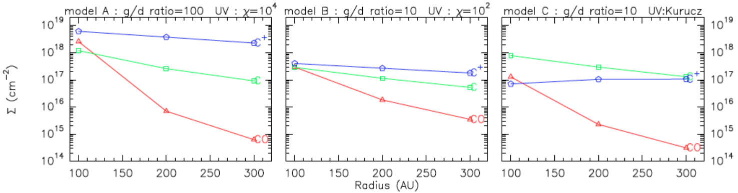
CO abundance in TW Hya revision after HD measurement :
X[CO] = 0.1 - 3 10^{-5}

Example : Carbon abundance in disks

CQ Tau, a gas-poor dusty rich source ?

- 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)

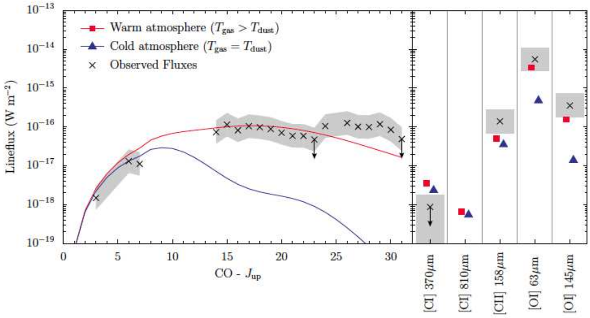
⇒ gas-to-dust-ratio ∼ 10 in CQ Tau



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

Example : Carbon abundance in disks ?

HD 100546, a Carbon-poor disk ?



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

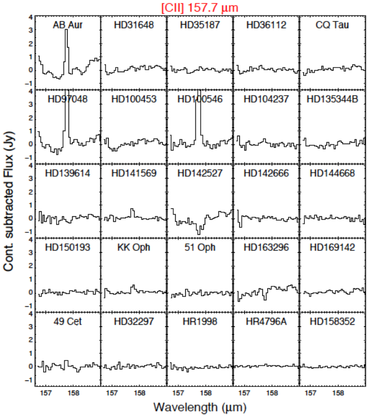
- Warm atmosphere (Tgas > Tdust) needed to reproduce the high-J CO
- Can explain the upper limit of CI together with the CO ladder and OI for high gas-to-dust ratio, but low amount of volatile carbon. But this underproduces CII.
- CII likely affected by cloud emission

Bruderer et al 2012

Example : Carbon abundance in disks

CII detection rate is poor

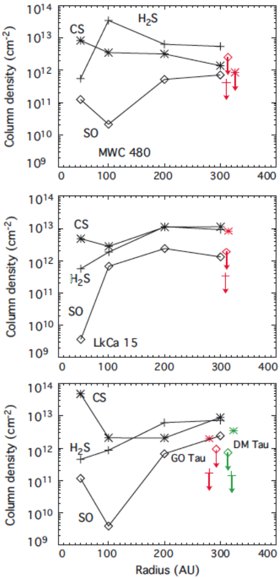
but predicted strong. $\rightarrow$ Contamination by clouds ?



Meeus et al 2012

$\Rightarrow$ Still a lot of uncertainties

Example : S-bearing molecules



- CS detected
- SO and H_2S : upper limits

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

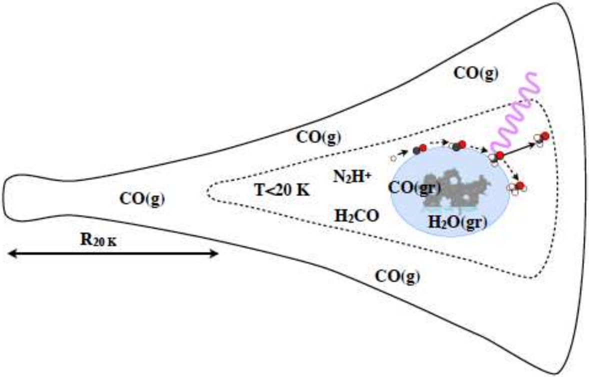
Sources	Σ_{300} (cm^{-2}) SO	H$_2$S	CS
DM Tau	$\leq 7.5{\cdot}10^{11}$	$\leq 1.4{\cdot}10^{11}$	$3.5 \pm 0.1{\cdot}\ 10^{12}$
LkCa15	$\leq 1.9{\cdot}10^{12}$	$\leq 3.6{\cdot}10^{11}$	$8.7 \pm 1.6{\cdot}\ 10^{12}$
MWC480	$\leq 2.5{\cdot}10^{12}$	$\leq 4.1{\cdot}10^{11}$	$\leq 8.4 \cdot 10^{11}$
GO Tau	$\leq 8.9 \cdot 10^{11}$	$\leq 1.8 \cdot 10^{11}$	$2.0 \pm 0.16{\cdot}\ 10^{12}$

Notes. Sulfur-bearing molecules surface densities (cm^{-2}) at 300 AU (modeled as $\Sigma(r) = \Sigma_{300}(r/300\mathrm{AU})^{-1.5}$). 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

ALMA results

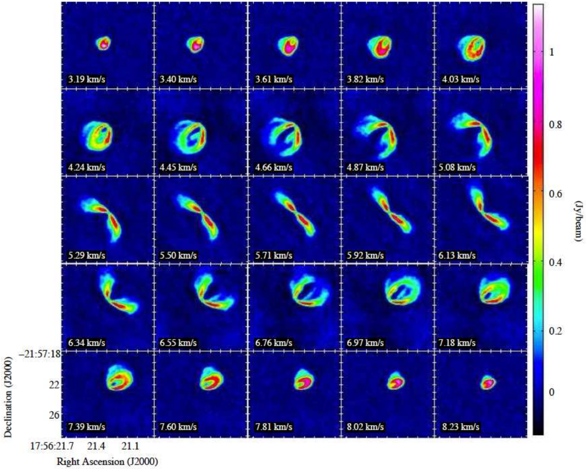


Qi et al 2013

Vertical structure

de Gregorio et al 2013 A&A, Rosenfeld et al. 2013 ApJ

Science Verification HD 163296 (Herbig Ae), B6 et B7, CO and continuum



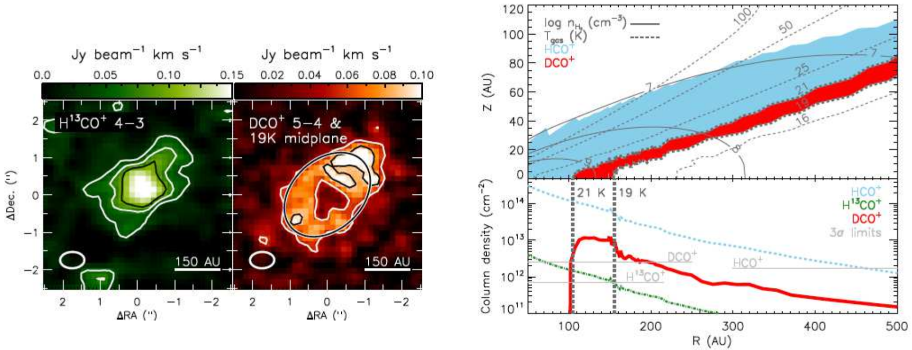
2 CO layers
→ CO depleted in the mid-plane

^{12}CO 3-2 channel map

Radial structure

Mathews et al 2013 A&A

DCO^+ and HCO^+ in HD 163296 (Science Verification)

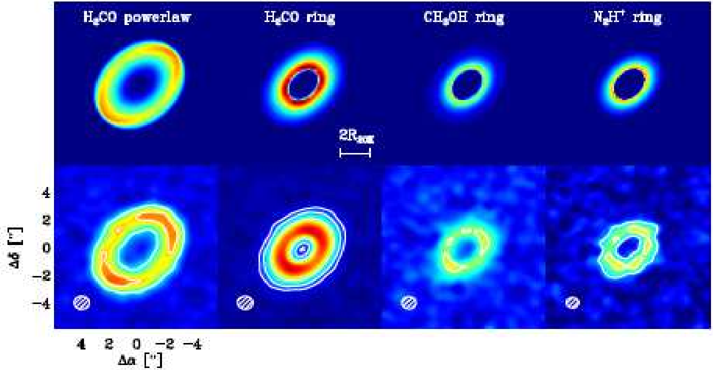


CO snow-line $\sim$ 155 AU

in agreement with previous SMA observations (CO Qi et al 2011 and H_2CO Qi et al 2013)

Radial structure

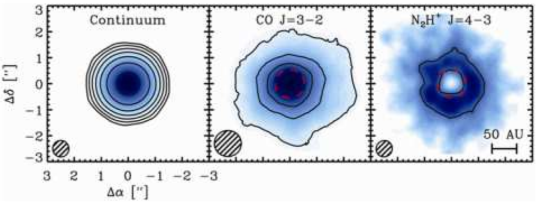
CO snow-lines ALMA pediction in HD 163296

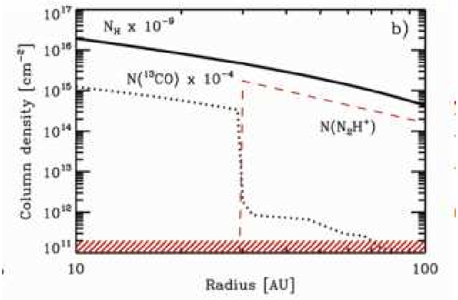


Qi et al 2013

Radial structure

Öberg, Qi et al 2013 N_2H^+ in TW Hya (Science Verification)





CO snow-line ∼ 30 AU

Limitations

We have an idea of the variation of abundance in radius, but not the absolute value.

- poor uv coverage $\rightarrow$ non-linear effect of deconvolution (work in uv-plane). No longer valid with ALMA
- only a handful of molecules are firmly detected in disks so far.
- "real" disk structure in density and temperature not well known (expept for TW Hya ?).
  Assumption on T (derived form CO observation, or from dust modeling)
  LTE ? T at one layer , dust properties ?
- initial abundances ?
- interaction grain-gas
- photodesorption (UV, X-Ray, e.g. Walsh et al 2012)
- reaction rates are not so well known
- turbulence (e.g. Nomura et al. 2009)
- disks are evolving. feedback on the chemistry ? (first attempt Turner et al. 2007, MHD + simple chemistry)
- For now, few real 3D code

Conclusion

- Protoplanetary disks are complex object, being compact with strong radial and vertical gradient in density and temperature
- observables are line intensities, converted to column densities, i.e. quatities integrated over the line of sight
- but, a molecule will exist and emits only in a certain range of physical condition.
- the total gas mass is poorly known
- dust is play a key role in chemistry
- unambiguous interpretation of the observational results necessitates advanced modeling of the disk physical structure and evolution, chemical history, and radiative transfer.

Conclusion

Things will improve with the high sensitivity of ALMA and NOEMA

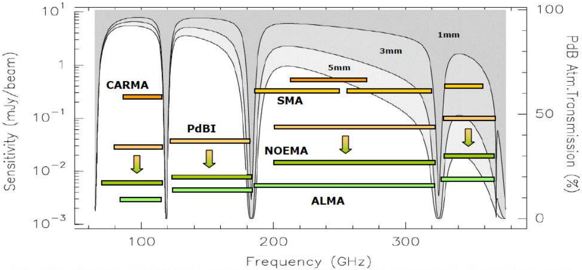


Fig. 1: Point source sensitivity to continuum emission after 8 hrs of current (SMA, CARMA 2008, PdBI 2009) and future millimeter-wave arrays. The calculations assume a mean target elevation of 45°, 8 hrs of integration (70% on-source), and conditions corresponding to a 1mm column of water vapor at 345 GHz, 3mm at 230 GHz and 5mm at 90 and 150 GHz (see also Annexe 1).

AND progress on chemical modeling

Interesting reviews : Bergin et al 2011 (PPV) ; Henning & Semenov 2013 ; Dutrey et al 2014 (PPVI)

Thank you