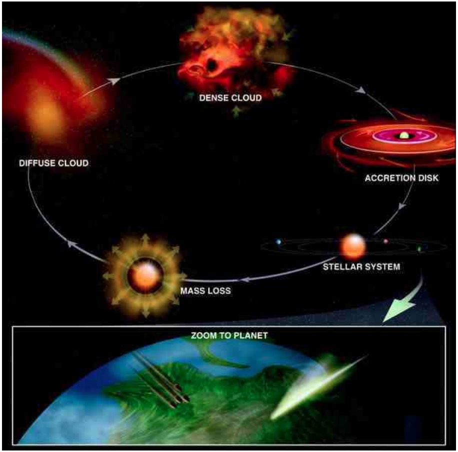
Observations of Disk Chemistry in the ALMA Age

Edwige Chapillon

IRAM/LAB

Protoplanetary disks



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intermediate step between molecular clouds and planetary system

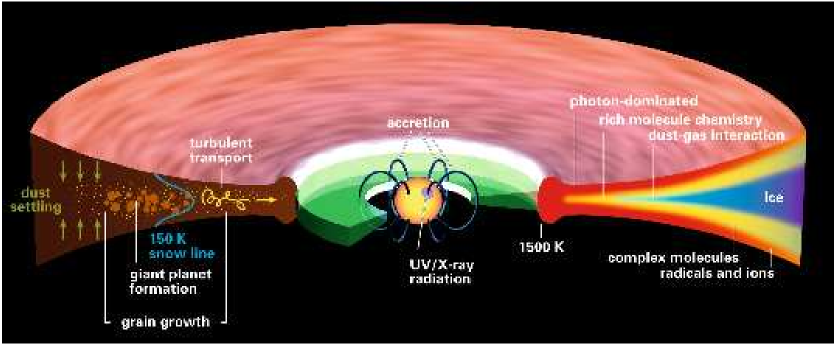
- Protoplanetary disks (gas + dust)
- Debris disks (dust)

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

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

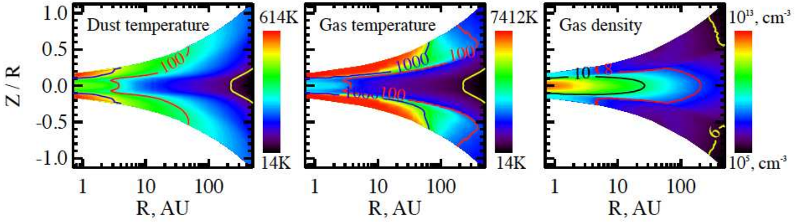
What is a protoplanetary disks ? – State of the art

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



Henning & Semenov 2013

What is a protoplanetary disks ?



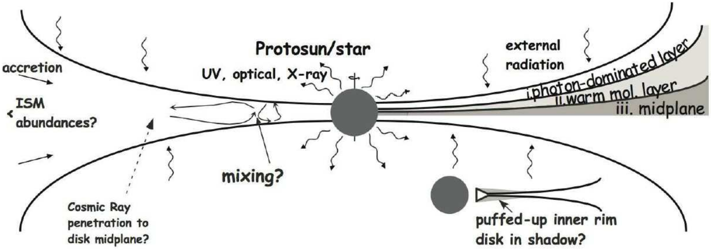
Akimkin et al 2013

- 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 ratio
- molecular content
- ...

Strong gradients in disks → chemistry definitively not homogeneous

Chemistry

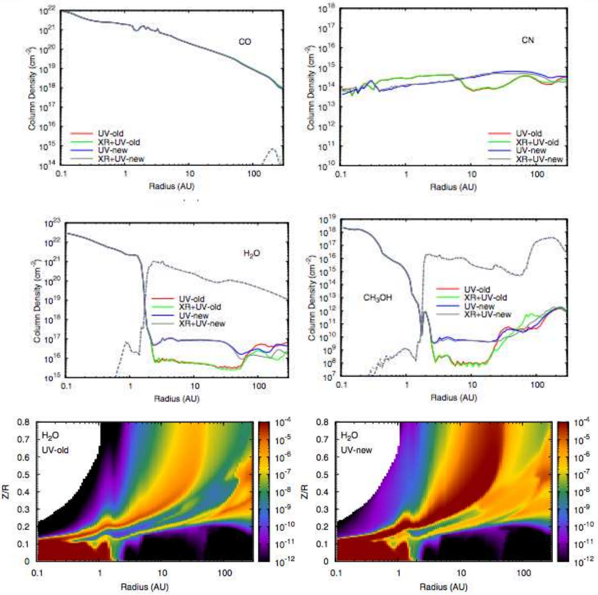
- Surface chemistry (on grains) (need a realistic size distribution)
- Neutral - neutral (low and high T)
- Ion - neutral
- 3 body reactions (?)
- Photodissociation, photoionization by UV
- Interactions with X rays
- Interactions with cosmic rays
- photodesorbtion



Bergin et al. 2007

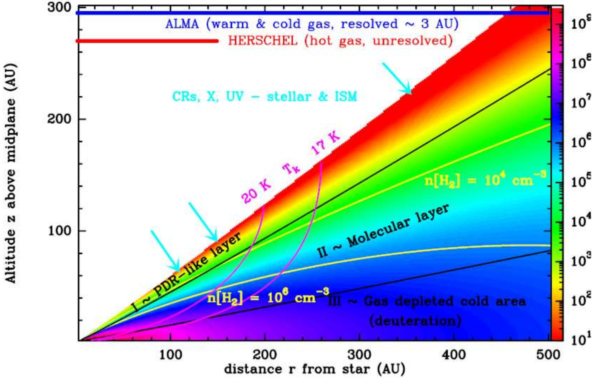
some chemical codes : Nautilus (Hersant et al 2009), ProDiMo (Woitke)...
some disks models : see papers by e.g. Aikawa, Walsh, Fogel, Akimkin, Nomura...

Chemical model results



Walsh et al. 2012

Protoplanetary disks observation



Dutrey et al 2014 PPVI

IR observations

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

mm observations

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

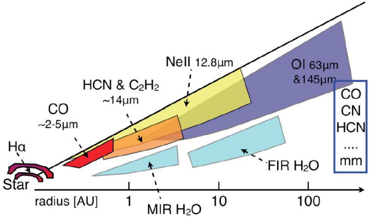
Molecules (and atoms) detected in disks (so far)

- CO, ^{13}CO, C^{18}O
- CN, HCN, HNC, CS, SO, H_2CO, CCH, HC_3N, c-C_3H_2 , CH_3CN (e.g. Dutrey et al 1997, Henning et al 2010, Chapillon et al 2012, Qi et al 2013, Öberg et al. 2015)
- 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 detected in mm

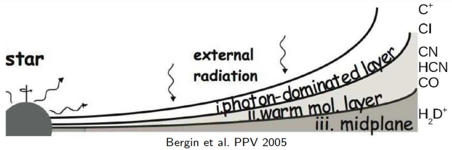
Sampling the disk

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

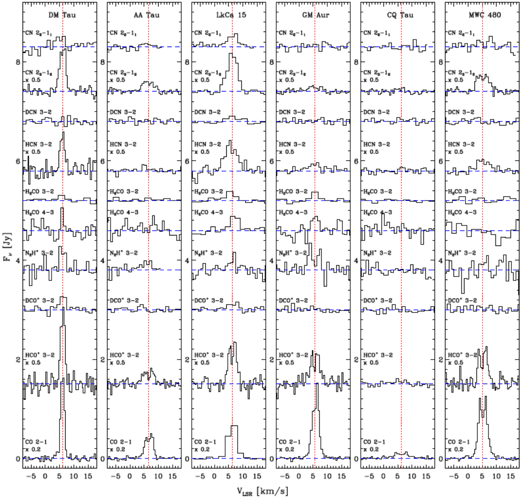
→ bring information on kinematics, density, thermal structure, turbulence...

(sub)millimeters chemical "Survey"

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

General trend :

- no complex molecules detected (pre-ALMA)
- Herbig Ae are poor in molecules.

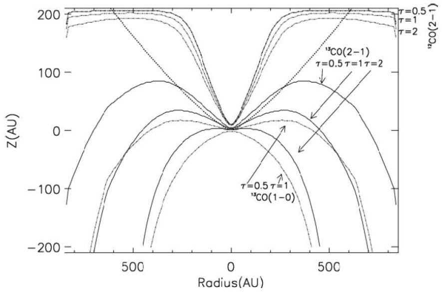


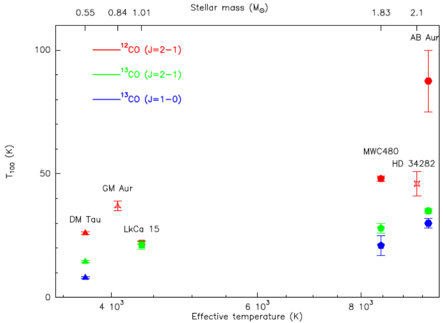
Öberg et al 2010

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 (∼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)
  CCH J=4-3 Kastner et al 2014 (TW Hya, V4046 Sgr)
- CN J=2-1 /HCN J=1-0 Chapillon et al 2012 (DM Tau, LkCa 15)
  CN J=3-2 Kastner et al2014 (TW Hya, V4046 Sgr)
- CS J=3-2 and J=5-4 Guilloteau et al 2012 (DM Tau)

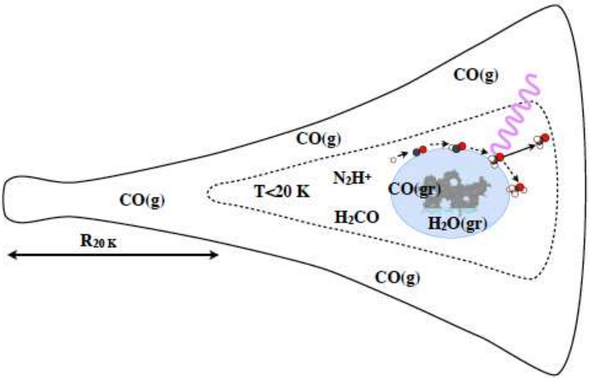
So far, observations cannot be reproduced by chemical models

But warm gas in MWC 480 (Herbig Ae)

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

⇒Surprisingly low temperature for gas phase molecules in T-Tauri
↪ turbulence ? (Aikawa et al 2007)
↪ photodesorption ? (Hersant et al 2009)
⇒Discrepancy T-Tauri / Herbig Ae

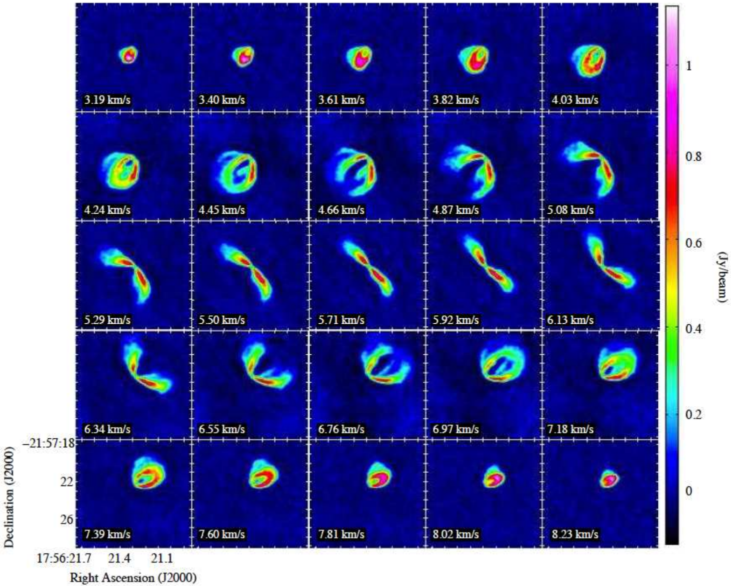
Disk structure



Qi et al 2013

HD 163296 ALMA SV observations

$^{12}CO(3\text{-}2)$ channel map : (De Gregorio et al. 2014, Rosenfeld et al 2013).



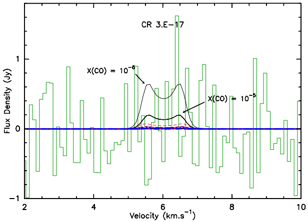
Investigating the disk mid-plane :

Searching for H_2D^+

o-H_2D^+ 372 GHz line

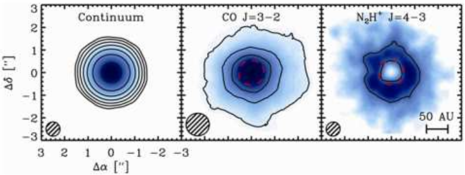
TW Hya (APEX), DM Tau (JCMT)

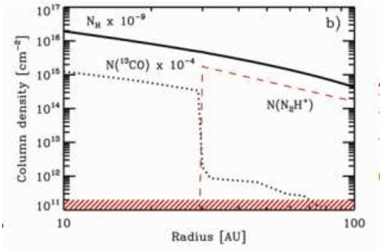
no detection (Chapillon et al 2011)



Tracing the CO snow line : N_2H^+ in TW Hya

Qi, Öberg et al 2013



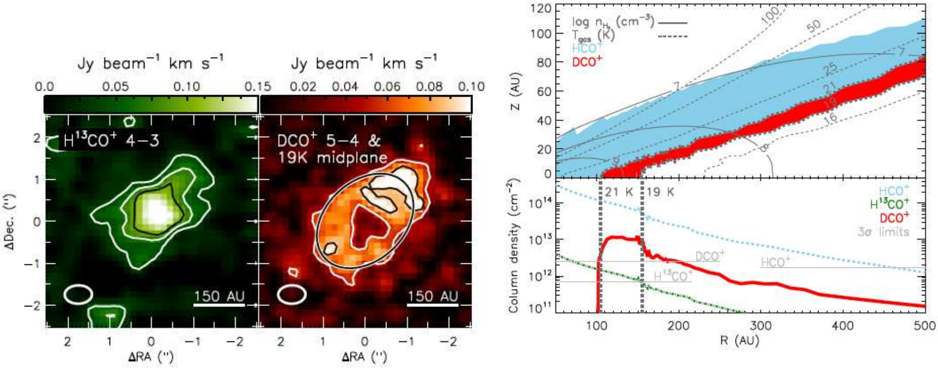


CO snow-line ∼ 30 AU

CO snow-line in HD 163296

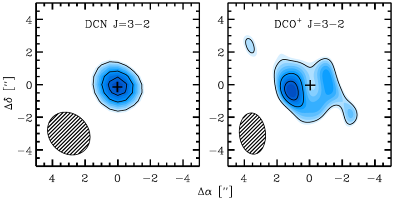
Tracing the CO snow line at R ∼ 155 AU in HD 163296

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



Deuterium chemistry

Multiple pathway to deuteration (Öberg et al 2012)
DCN (ALMA science verification), DCO^+ (SMA) 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^+

DCO^+ detected in

- DM Tau (Guilloteau et al. 2006 ; Oberg et al. 2010, 2011a ; Teague et al. 2015),
- TW Hya (van Dishoeck et al. 2003 ; Qi et al. 2008 ; Oberg et al. 2012)
- HD 163296 (Mathews et al. 2013)
- LkCa 15, IM Lup, AS 09, and V4046 Sgr (Oberg et al. 2010, 2011b)

Teague et al 2015 :

- 50 AU hole in DCO^+ AND HCO^+
- $R_D = \frac{N(HCO^+)}{N(DCO^+)} = 0.1 - 0.2$ for R=50 - 430 AU
- HCO^+ dominant molecular ion

DCO^+, a tracer of the CO snow-line or a probe of ionization ?

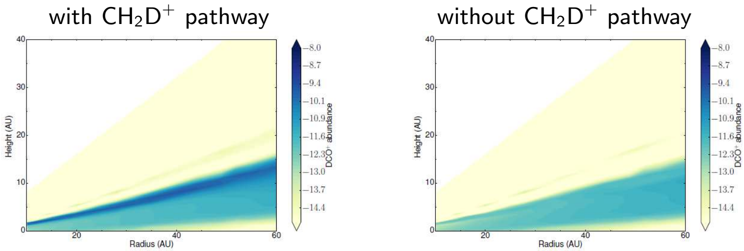
Main formation pathway :

$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 + 232K$ and then, $H_2D^+ + CO \rightarrow DCO^+ + H_2$

$CH_3^+ + HD \rightleftharpoons CH_2D^+ + H_2 + \Delta E$. and then $CH_2D^+ + O \rightarrow DCO^+ + H_2$

Study by Favre et al. 2015

- T-Tauri DM Tau-like model
- update of energy barriers for $CH_2D^+ \rightarrow DCO^+$ reactions (Roueff et al 2013)
- X-ray ionisation and photodesorption Lyα (Fogel et al 2011)

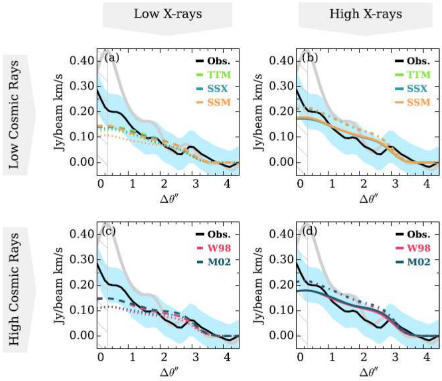


- favor deuteration in warm conditions
- DCO^+ in upper layer where X-ray ionization occurs

Constraint on X-ray and Cosmic-ray ionisation

Cleeves et al 2015

- SMA and ALMA observations of HCO^+ and N_2H_+ in TW Hya
- Test several CR rate and X-Ray



- CR rate in the mid-plane is $< 10^{-19}s^{-1}$
- predict a "low turbulence" dead zone $R < 60au$

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

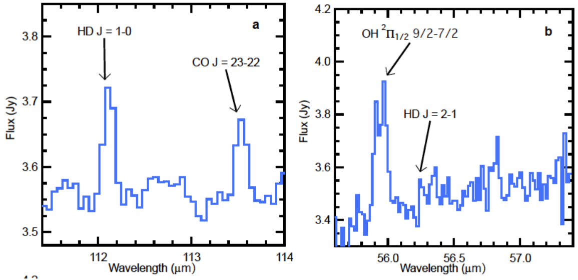
Estimation of the disks masses

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

- from gas emission → need molecular abundaces
- from dust emission → need gas-to-dust ratio

"Direct" measurement

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



⇒ $M_{disk} > 0.05 M_\odot$

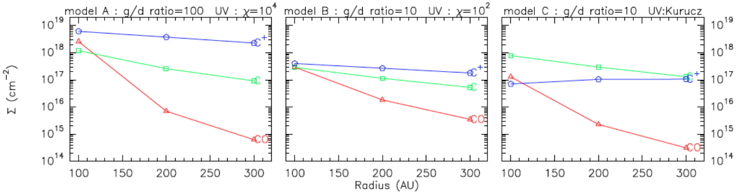
Talk by D. semenov

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)

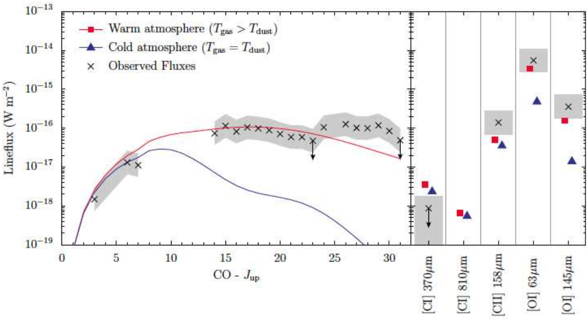
⇒ gas-to-dust-ratio ∼ 10 in CQ Tau



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

Carbon in disks

HD 100546, a Carbon-poor disk ?



Lot 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

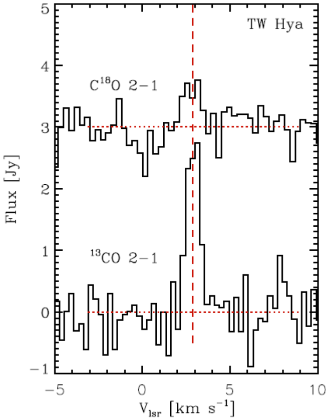
Bruderer et al 2012

Carbon in disks

Carbon active chemistry

- T-Tauri TW Hya
- HD (1-0) and $C^{18}O$ (2-1) Herschel and SMA data
  - CO destroyed in the atmosphere
  - rapid formation of carbon chains
  - freeze out

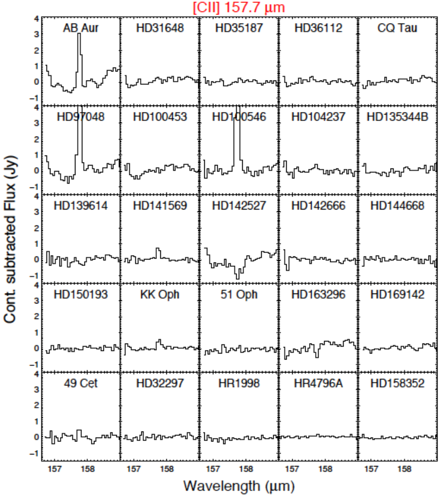
Favre et al. 2013



Carbon in disks

CII detection rate is poor

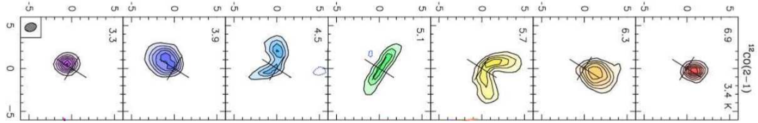
but predicted strong. → Contamination by clouds ?



Meeus et al 2012

Kinematic

Protoplanetary disks are in keplerian rotation :
MWC 480 ^{12}CO J=2-1 Piétu et al 2007

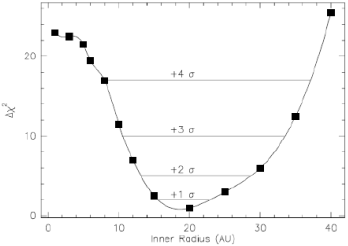


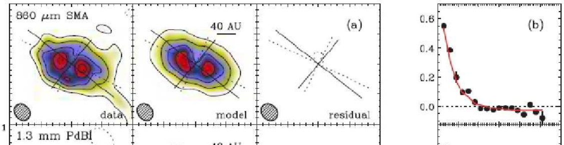
CO cavity in GM Aur

- 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

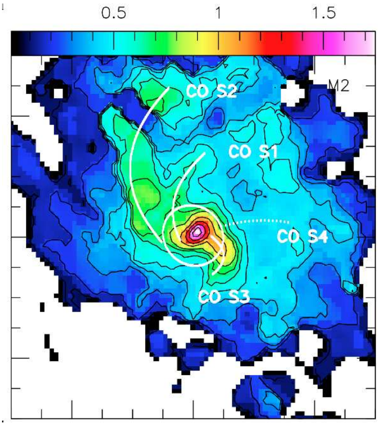
→ planets (5-10 M_{jup}) ?

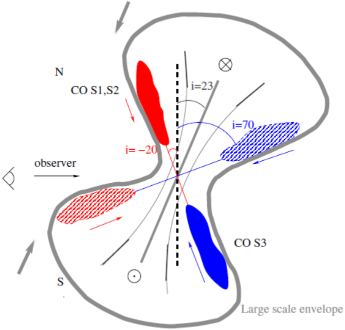




Departure from Keplerian rotation

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, apparent conter-rotation

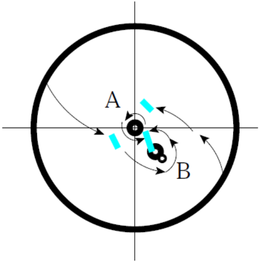




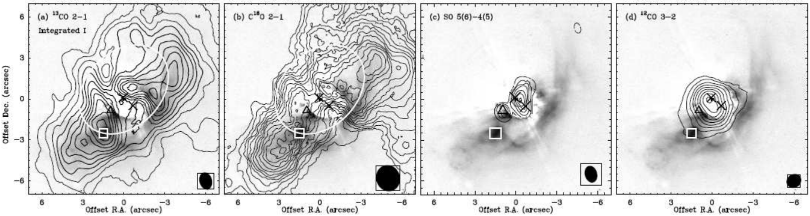
UY Aurigae

Tang et al 2014
PdBI and SMA observation of ^{13}CO(2-1), C^{18}O(2-1), SO 5(6)-4(5) and ^{12}CO(3-2)

- circumbinary disk detected in ^{13}CO and C^{18}O
- streamers from circumbinary disk to circumstellar disks in ^{13}CO and C^{18}O, spitral patern
- SO likely trace accretion shocks on the circumstellar disks.

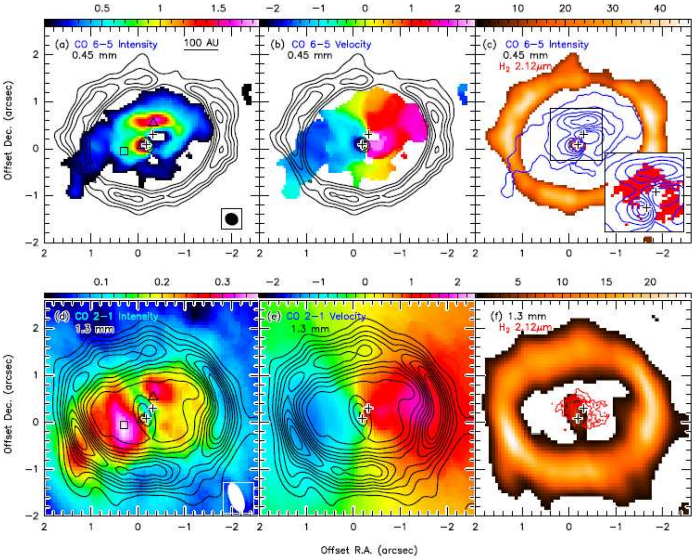


Face–on



GG Tau A

PdBI and ALMA observation of CO (6-5) and CO (3-2)



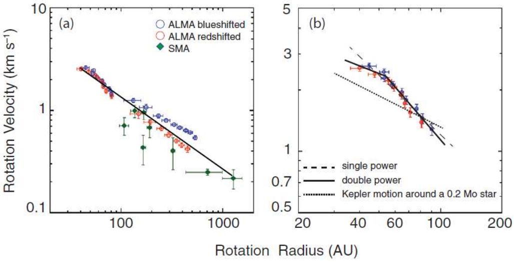
- streamers
- disk arround Aa
- hot spot

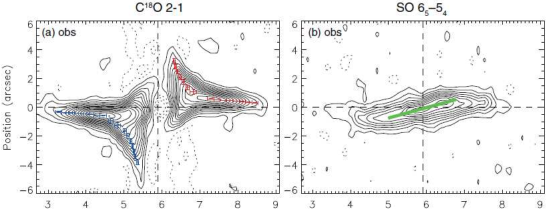
Dutrey et al 2014

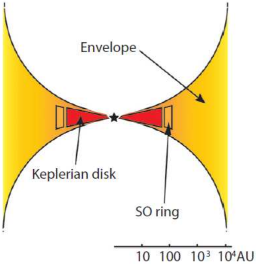
Early phases, the Class 0 L1527 IRS

Class 0 L1527 IRS Ohashi et al 2014

- Class 0 solar type protostar ($0.3\,\mathrm{M}_\odot$).
- ALMA data on $C^{18}O\,(2\text{-}1)$ and $SO\,(6_5 - 5_4)$
- infalling enveloppe traced in $C^{18}O$ solid rotation ($r^{-p}, p \sim 1$)
- inner disk in $C^{18}O$ differential rotation ($p < 1$)
- ring in CS, interaction enveloppe–disk ?

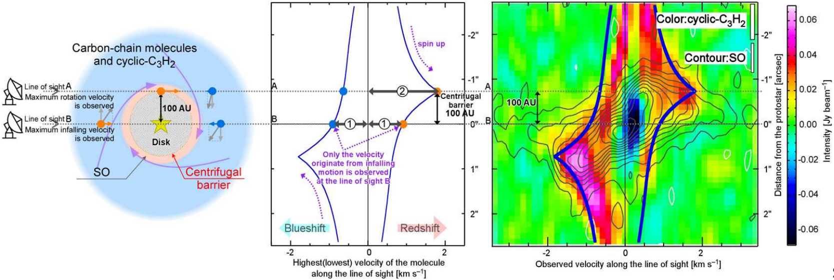






Classe 0 L1527

Sakai et al 2014 Nature



see

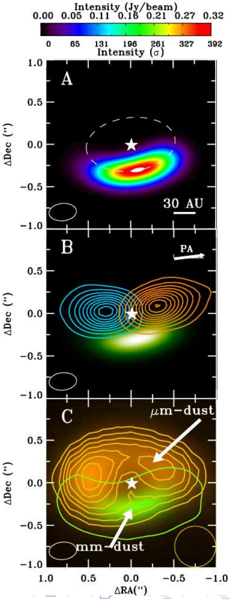
also studies by Linberg et al 2014 (R CrA), Lee et al 2014 (HH 212), Yen et al 2014 (L1489 IRS), Murillo et al 2013 (VLA1623)

Transition disk : Oph IRS 48

Van der Marel 2013

- B9 observation ($0.3 \times 0.2''$) Oph IRS 48 (A)
- strong asymetry in dust (contraste ~ 130)
- ring in CO 6-5 and dust μm
- $\rightarrow$ "dust trap"

see also Bruderer et al 2014



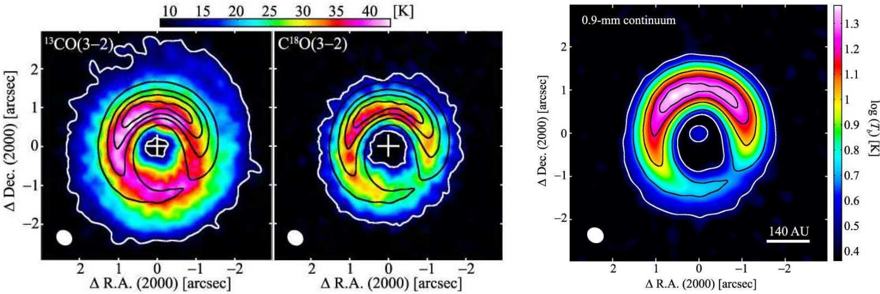
A : continuum 685 GHz. B : CO 6-5,

C : VLT/VISIR 18.7 μm

Asymetries in disks : HD 142527

Fukagawa et al 2013

- continuum + ^{13}CO et C^{18}O 3-2 in HD 142527
- ring (en dust ans gas) + internal disk
- strong assymetry



black levels = continuuum, color = gas continuum

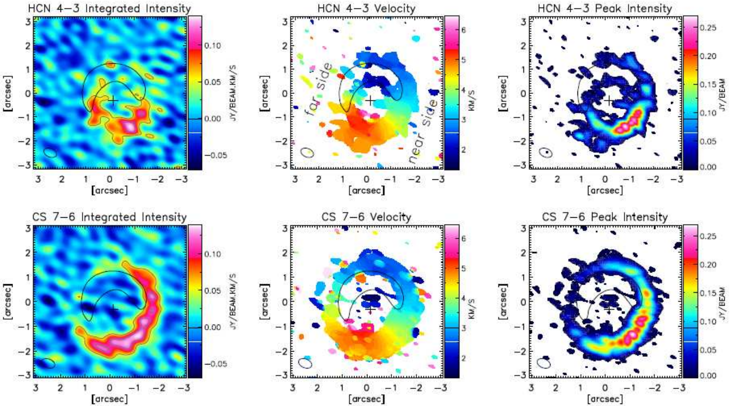
Peak surface density = 28g cm^{-2} → instable

⇒ planetary formation ? see also Casassus et al 2013, Christiaens et al 2014,

Perez et al 2013,2015, van der Plas et al 2014 (detection of HCN and CS)

HCN and CS observation toward HD 142527

van der Plas et al 2014



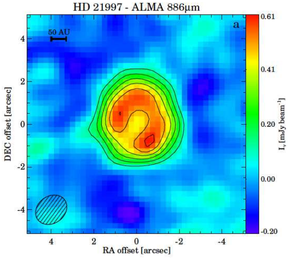
Lack of gas where dust is

- low T dust, then low T gas and fainter emission
- higher dust opcaity : shield part of the emission

HD 21997

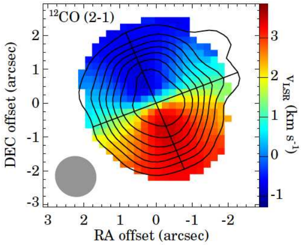
Moor et al 2013 ApJ 777L ; Kospal et al 2013 ApJ 776

CONTINNUM



continuum 886 μm

CO line



- smooth ring',
- $R_{int} \sim 55$AU

- ^{12}CO et ^{13}CO 2-1 et 3-2 + $C^{18}O$ 3-2
- no cavity → internal disk gas-rich, dust-poor

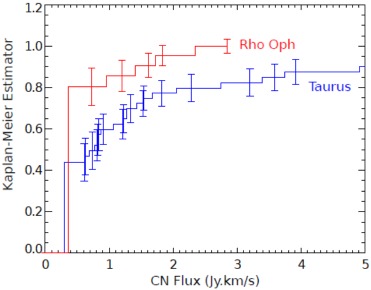
⇒ primordial gas and second generation dust ?

Molecules in disks : Taurus VS ρ-Ophiucus regions

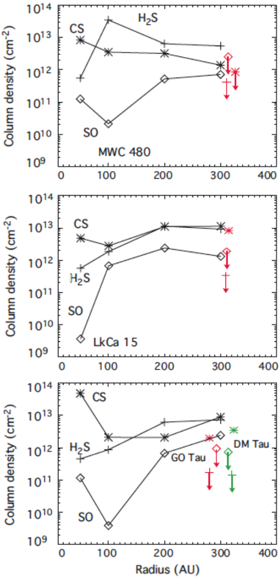
Survey of $^{13}\mathrm{CO}$ CN, H_2CO, and SO with the IRAM 30m telescope

- in Taurus (Guilloteau et la 2013)
- in ρ-Oph and upper Scorpius (Reboussin et al 2015)

- CN is a good tracer of disks in Taurus
- no longer true in ρ-Oph (5 detections on 29 sources)
- high T in ρ-Oph $\rightarrow$ less CN
- emission weaker in ρ-Oph $\rightarrow$ smaller disks ?



Search for S-bearing molecules in Protoplanetary disks



30m IRAM study Dutrey et al 2011

- CS detected
- SO and H_2S : upper limits

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	$\leq 8.9 \times 10^{11}$	$\leq 1.8 \times 10^{11}$	$2.0 \pm 0.16 \times 10^{12}$

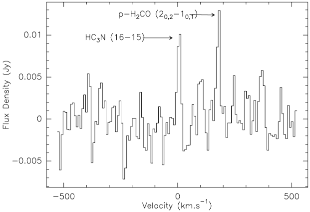
- better agreement with initial C/O = 1.2 (Hincelin et al 2011)
- CS and SO OK
- H_2S failed
  $\rightarrow$ emphasis importance of grain surface chemistry.
  H_2S may be locked into grain mantle

$\Rightarrow$ chemical code to improve

SO detected toward AB Aur by Fuente et al (2011)

Search for CCS and HC_3N

Deep search with the IRAM 30-m and PdBI for heavier molecules.
Chapillon et al 2012



HC_3N in LkCa 15 with PdBI

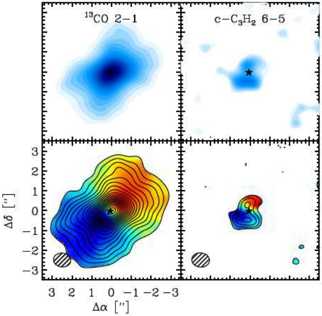
	Σ_{300} (cm^{-2})			
	HC_3N		CCS	
Souce	Derived	Predicted	Derived	Predicted
LkCa 15	$8 \pm 2 \cdot 10^{11}$	$5.2 \cdot 10^{13}$	$\leq 1.4 \cdot 10^{12}$	$2.9 \cdot 10^{11}$
GO Tau	$13 \pm 2 \cdot 10^{11}$	$4.4 \cdot 10^{13}$	$\leq 1.2 \cdot 10^{12}$	$3.7 \cdot 10^{11}$
DM Tau	$\leq 3.5 \cdot 10^{11}$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

Toward molecular complexity

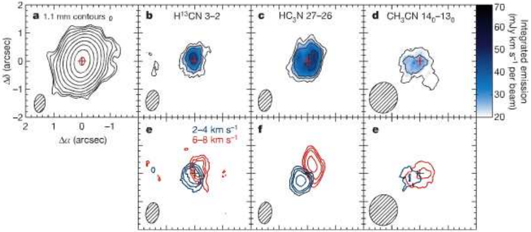
ALMA detection of c-C_3H_2 and CH_3CN (Qi et al 2013, Öberg et al 2015)

c-C_3H_2, SV data HD 163296



ring structure

$H^{13}CN$, HC_3N and CH_3CN in MWC480

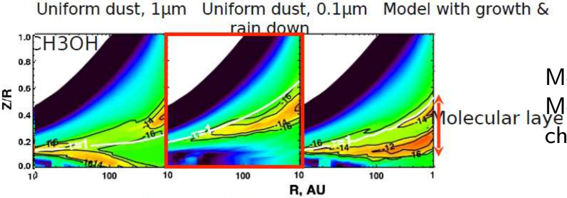


ratio compatible with the one observed in comets

Chemical model

Courtesy D. Semenov

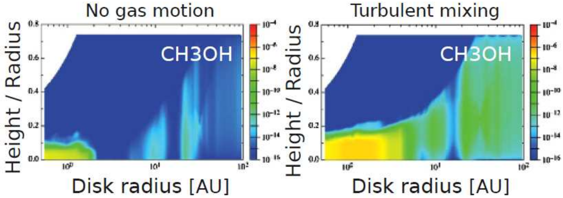
Grain growth



Vasyunin et al. (2011), ApJ 727, 76

Molecules closer to midplane → More dust surface available for chemistry

Transport



- Turbulent mixing enhances H2O, OH, HCN, C2H2, CH3OH,
- Stronger hot/warm lines of water & organics

Heinzeller et al 2011

Importance of grain chemistry, grain evolution and turbulence

Chemistry in Protoplanetary disks

Some success (i.e. CO snow line in HD163296), but still lot of discrepancies

- Current models do not reproduce well 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
- initial conditions
- 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 ?)

Conclusion

Early stages

- Detection of (proto-)disks and accretion toward Class 0 sources.
- Molecular observation is a good to to investigate the structure (kinematic, shocks...)
- need thin tracers

Protoplanetary disks

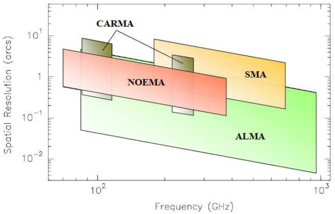
- new detections, complex moelcules detection need integration time
- need more accurate physico-chemical models (for now, few real 3D codes)
- fundamental parameters like disk mass or turbulence are still not well known
- disks are evolving. feedback on the chemistry ? (first attempt Turner et al. 2007, MHD + simple chemistry)

Transition disk

- Still very phenomenological
- Cavities, spirals and asymetries are now observed in dust and gas.
- Gas and dust not always peaks at the same place
- origine of structure, → planet-disk interaction ?
- link to numerous theory models (MRI, dead-zones, planet-disk interactions)

- Protoplanetary disks are complex object, being compact with strong radial and vertical gradient in density and temperature
- Chemistry is a powerfull tool to study protoplanetary disks structure and composition
- But it is complex and need accurate models to analyse the data

With new inteferometers (ALMA, NOEMA, SMA), (together with other wavelenght (IR))



NOEMA :

- 12 15m antennas
- 32 GHz bandwidth
- Dual band observations
- Baselines up to 1.6 km

- Imaging lines that are already detected with much better accuracy
- Imaging of complex molecules, not so easy, requiere integration time
- Study the first stages of disk formation
- Imaging of the older disks
- High spectral resolution (details on the kinematics, turbulence, dead zones ?)

⇒ **observation of gas AND dust**
⇒ **Improve chemical and physical time dependant models**

Thank you !

Appendix

the MAYS programme

Survey of 14 sources in CN (2-1) with the PdBI
spectal type M1-A4

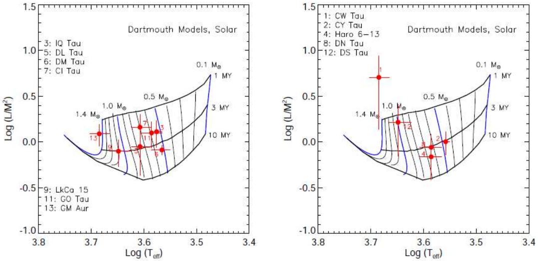


Fig. 7. Stars on the modified, distance-independent, HR diagram L/M^2 *vs* $T_{\rm eff}$ from Dotter et al. (2008) evolutionary tracks. Left: stars with dynamical masses accurate to < 5%, right: other stars.

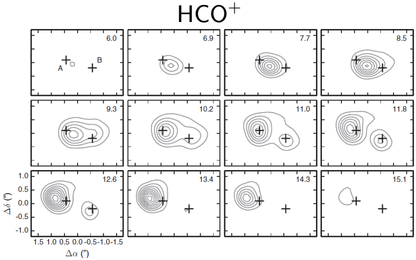
Guilloteau et al. 2014

uncertainties due to inclination
embedded sources difficult

Misaligned binary system

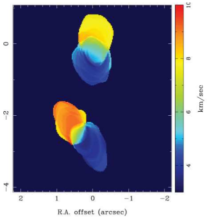
In Orion

A binary system in Orion,
440 au separation,
observed in CO J=3-2,
HCO^+ J=4-3, HCN J=3-2 and
CS J=7-6.
72° between the projected axis
Williams et al. 2014



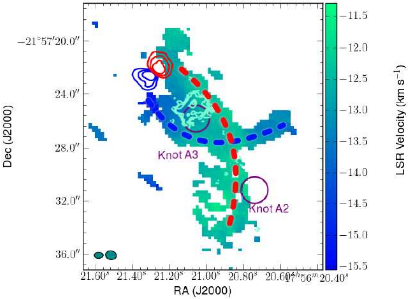
In Taurus : HK Tau system

CO (2-1) and (3-2) ALMA data
separation ∼ 400 au misalignement by
60-68 °
Jensen & Akeson 2014



Outflow : HD 163296

Klaassen et al 2013 A&A



- B6 and B7 observation of HD 163296 (Science Verification)
- outflow / disk wind in CO
- CO 3-2 peaks corresponding to the "knots HH"

ρ-Oph 102

Ricci et al 2012 ApJ 761L

- Observation B3 (100 GHz) et B7 (345 GHZ) continuum + DCO^+
- Resolution $\sim 1.7''$ B3 et $\sim 0.6''$ B9
- disk non-resolved
- $R_{out} \leq$ 40AU
- spectal index $\sim$ 2.3 $\rightarrow$ mm grains
- Detection of a conpact structure in ^{12}CO 3-2 at the star position
- Mass $\sim$ 0.3%–1% of disk