Observational Properties of Protoplanetary Disks

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- Today:
  - Molecular specroscopy basics
  - Molecular abundances
  - Molecular line observations of disks: kinematics, turbulence, mass

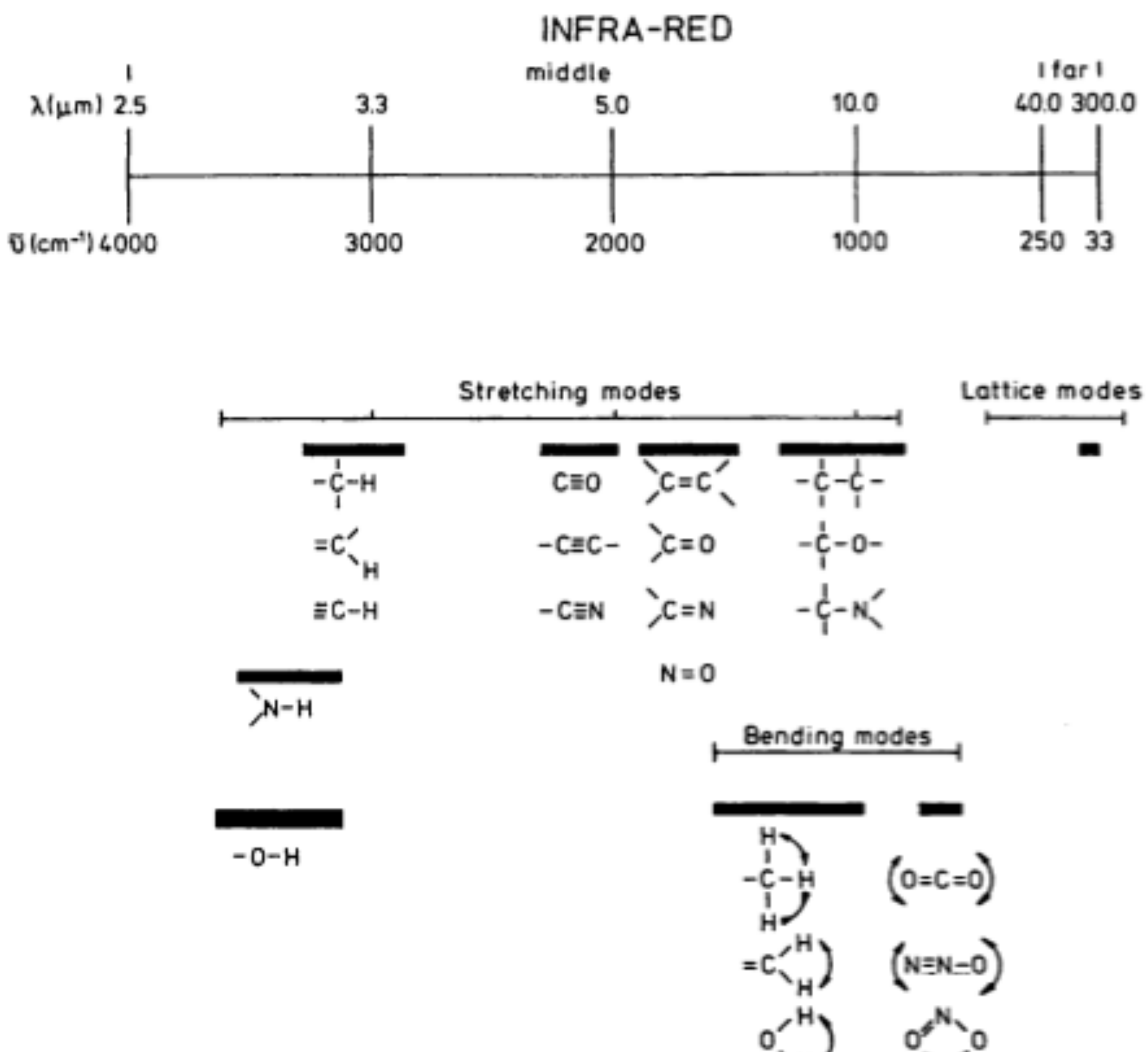
Questions from yesterday

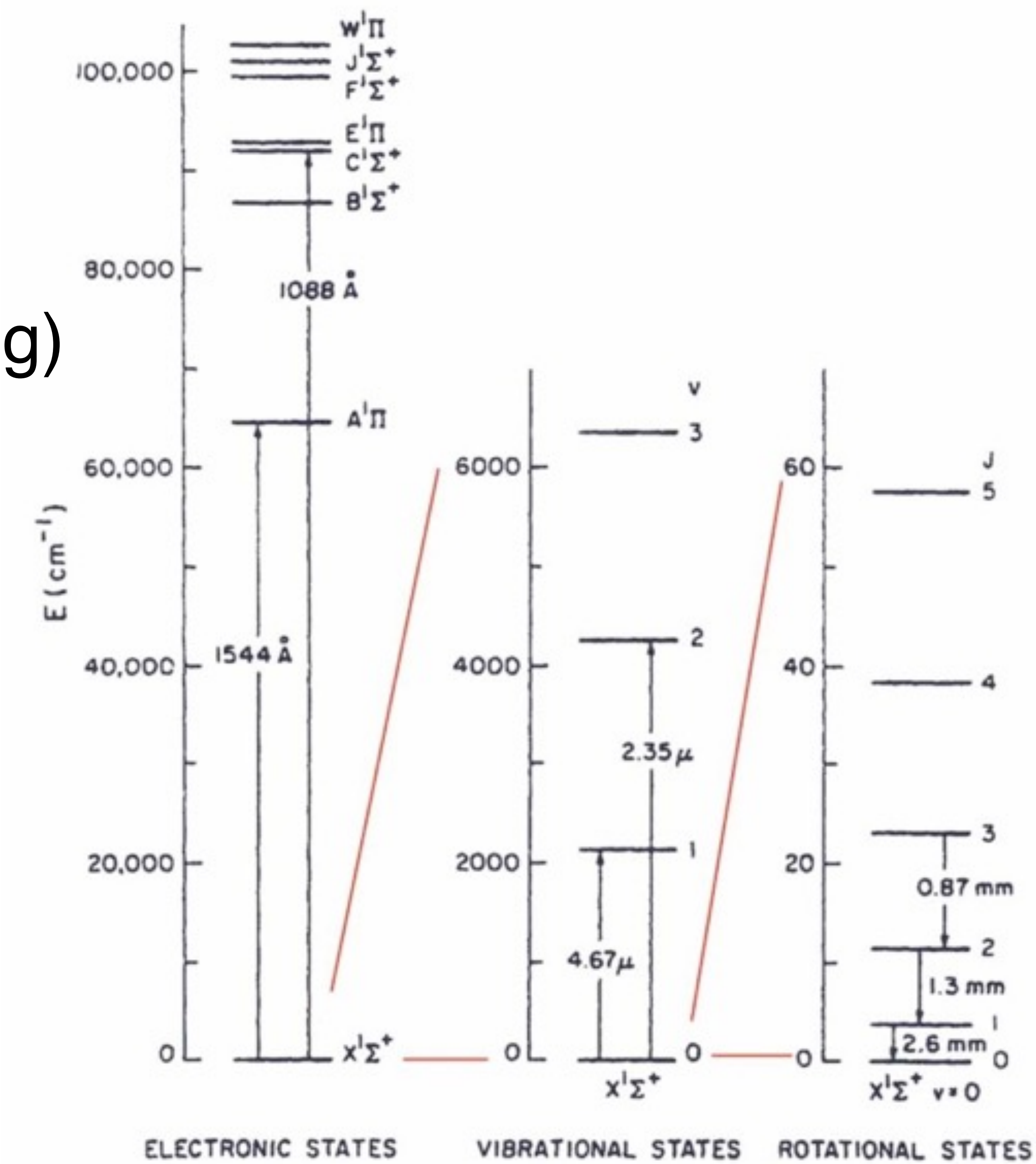
- More on dust traps
  - Just heard from Phil, more this afternoon
- More on Lab Experiments
  - See Testi et al. 2014 PPVI review
  - Specific on laboratory experiments: Blum & Wurm 2008, ARAA

Part VIII
Molecular Spectroscopy

molecular spectroscopy

- Molecular lines:
  - Rotation
  - Vib (Stretching and Bending)
  - Electronic





Molecular rotational lines

- Molecular lines:
  - Rotational spectra of molecules (simplified)

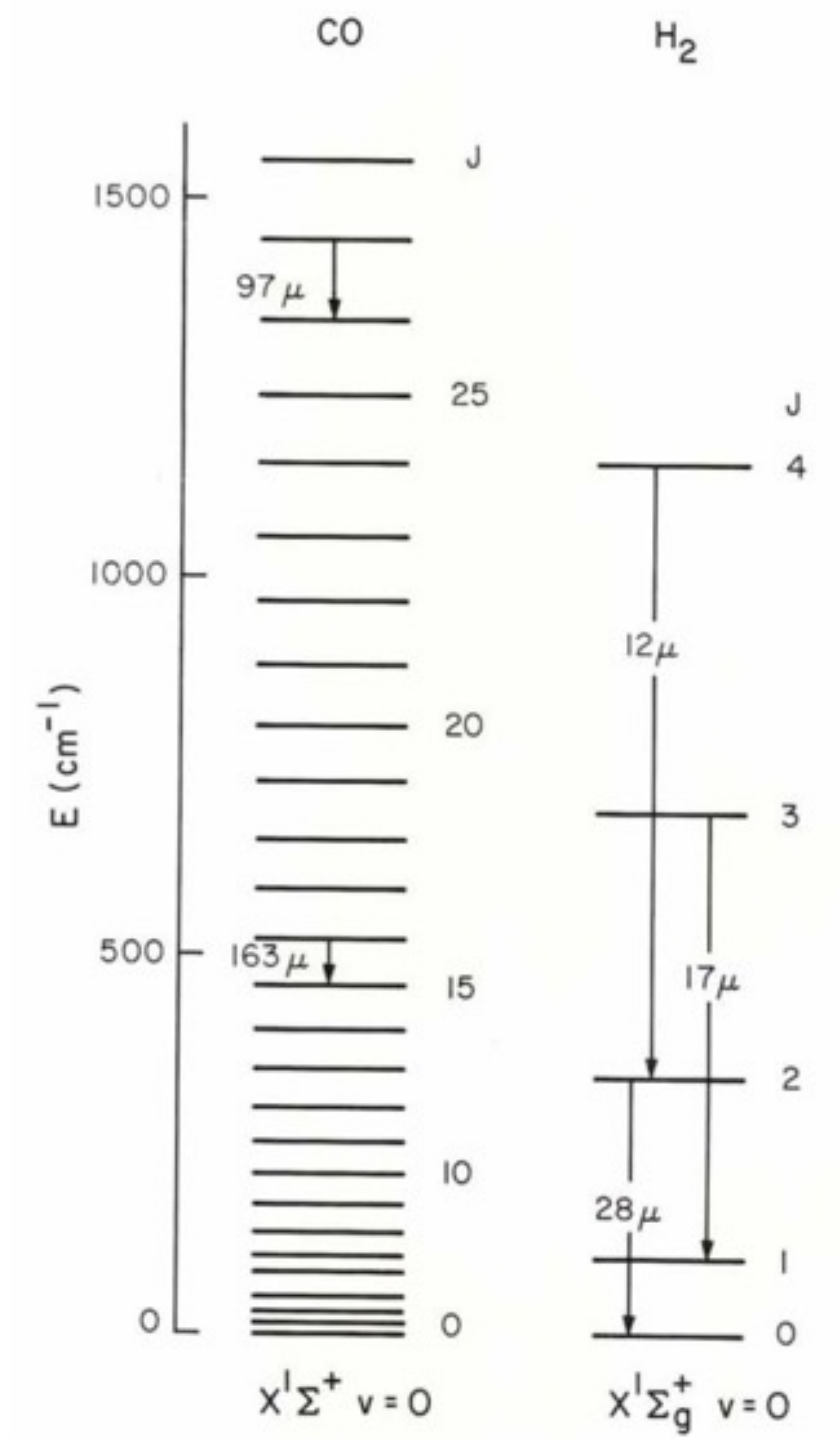
$$E^{rot} = \frac{\hbar^2}{2\mu R_e^2} J(J+1) = B_e J(J+1) \qquad B_e = \frac{\hbar^2}{2\mu R_e^2}$$

$$\Delta E^{rot}(J) = 2B_e(J+1) \qquad J=0,1,2... \qquad m=m_1*m_2/(m_1+m_2)$$

- Selection rules:
  - Permanent dipole moment (H_2, C_2, O_2, CH_4, C_2H_2 not ok)
  - DJ=1 (only adjacent levels)
  - Symmetric molecules => quadrupole transitions (DJ=2)

Molecular rotational lines

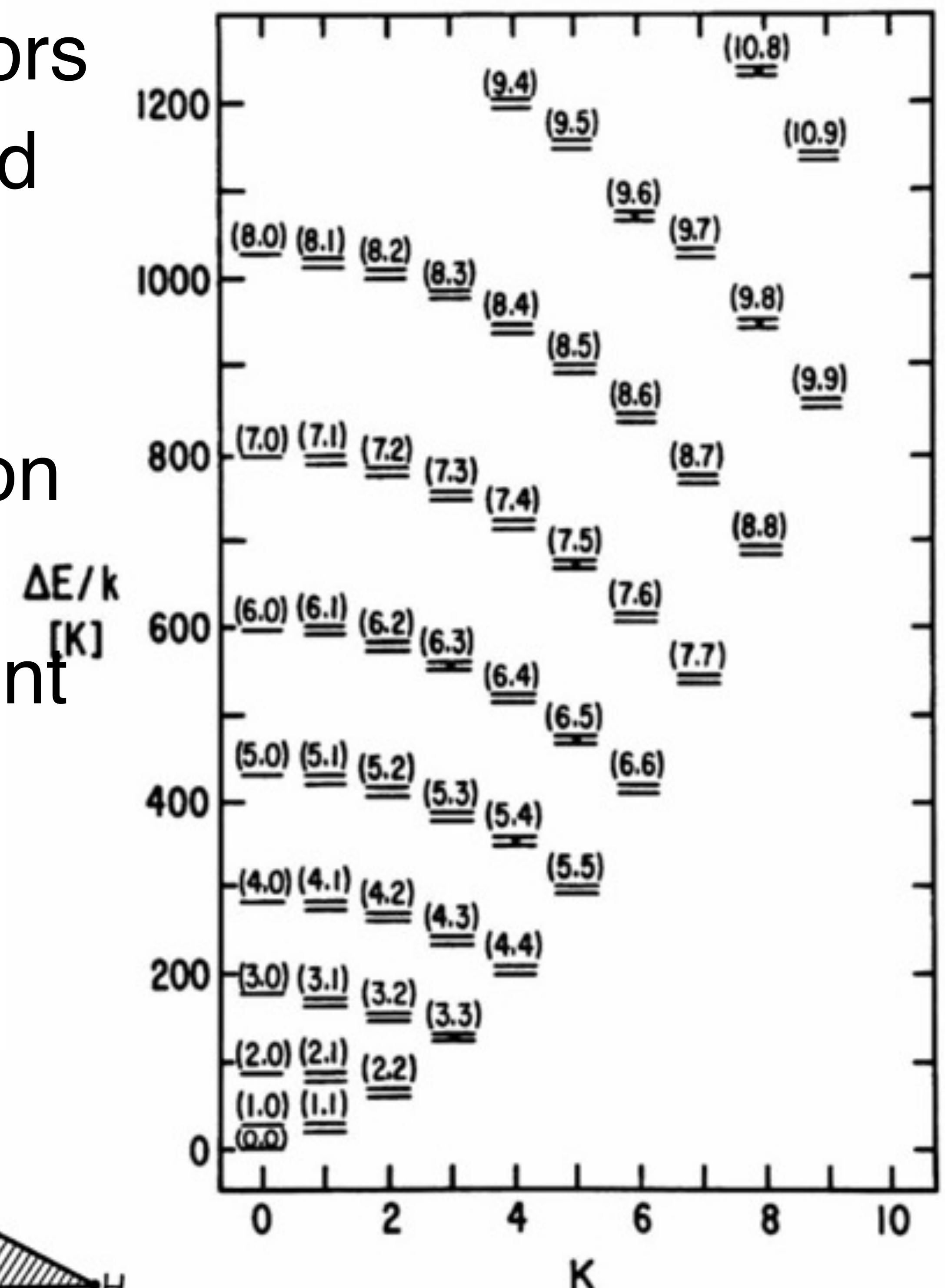
- Examples of diatomic molecules: CO (m=7) and H_2 (m=0.5)

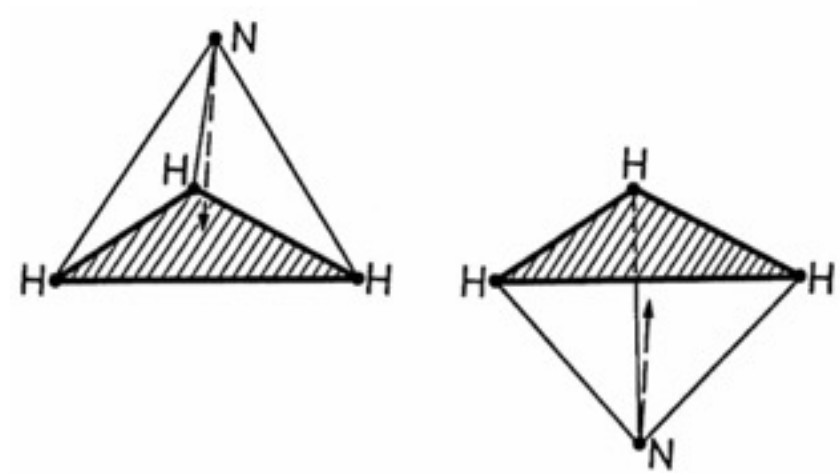


- CO levels are closely spaced
  - Smaller DE => long wavelength transitions, low excitation
  - J=1-0 -> n=115GHz, l=2.7mm
  - J=2-1 -> n=230GHz, l=1.3mm
  - J=3-2 -> n=345GHz, l=0.87mm
- H2 levels are further away, only quadrupole transitions allowed
  - MIR, high excitation lines

Molecular rotational lines

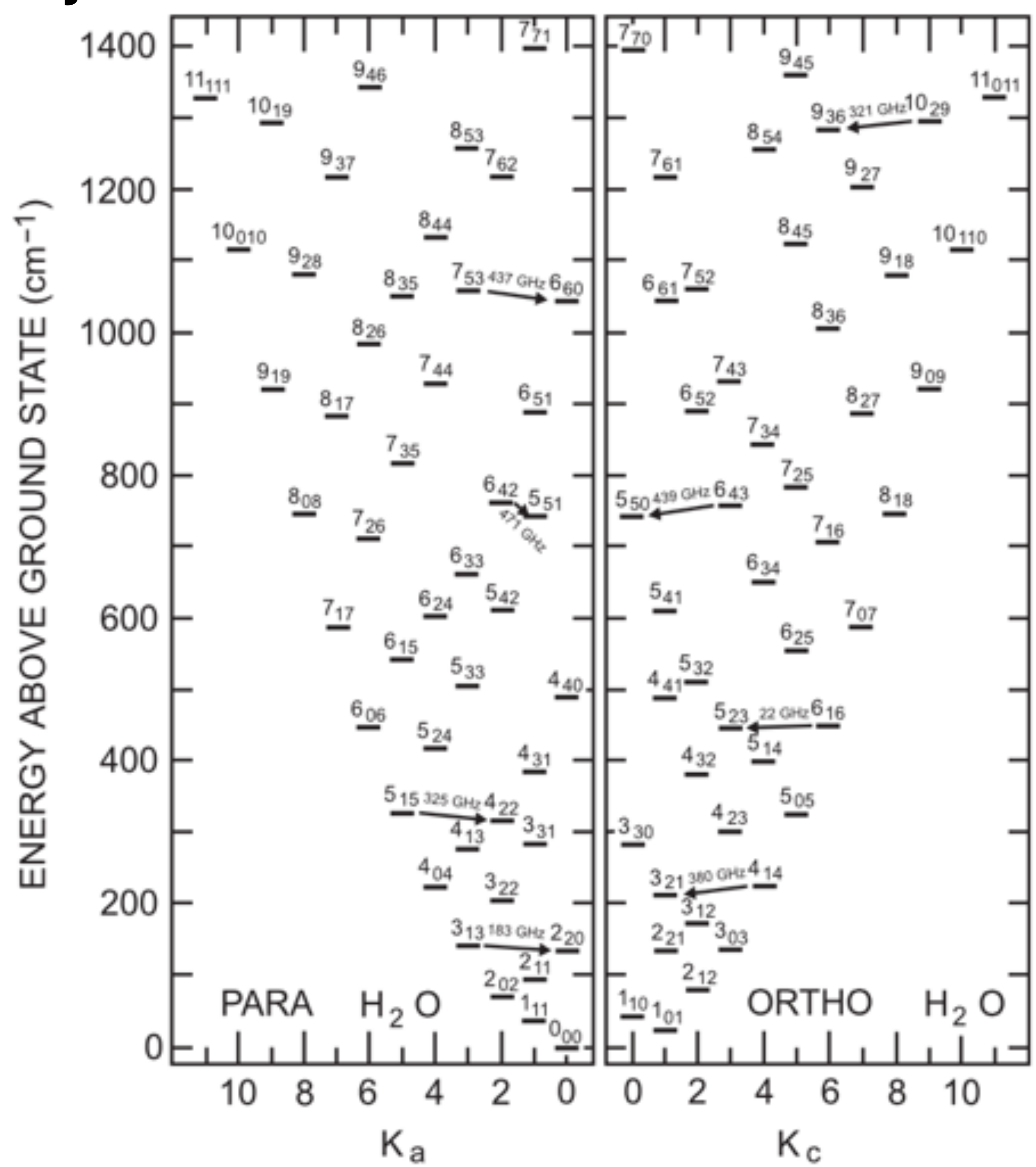
- Molecular lines: symmetric top rotators
  - Molecules with an axis of three-fold or higher symmetry
  - Examples: NH_3,CH_3CN,CH_3CCH
  - Quantum numbers: J and projection on axis K (K<=J)
  - Selection rules: DJ=1 (only adjacent levels), DK=0
  - K=J levels are metastable
  - Example: ammonia inversion transitions





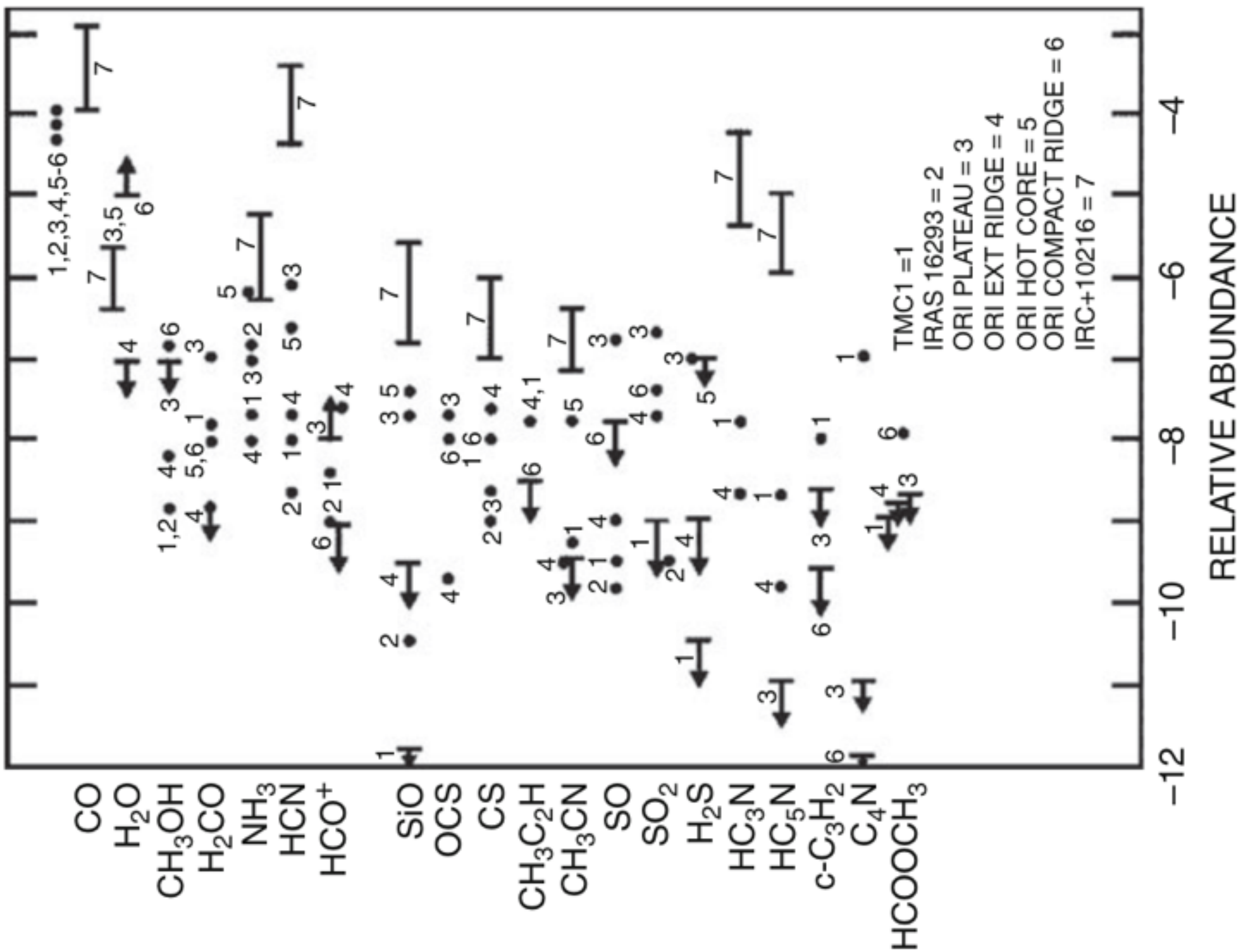
Molecular rotational lines

- Molecular lines: asymmetric rotators
  - Quantum numbers: J and projections on two axes K_- and K_+
  - Complicated spectra
  - Example: H_2O



Molecular abundances

- ✦ Molecular abundances in molecular clouds and YSOs



Part IX
Molecular gas in disks

Molecular gas

- Gas has to dominate the disk mass
  - From geometry : **H/R ~ 0.1 at 1 AU**

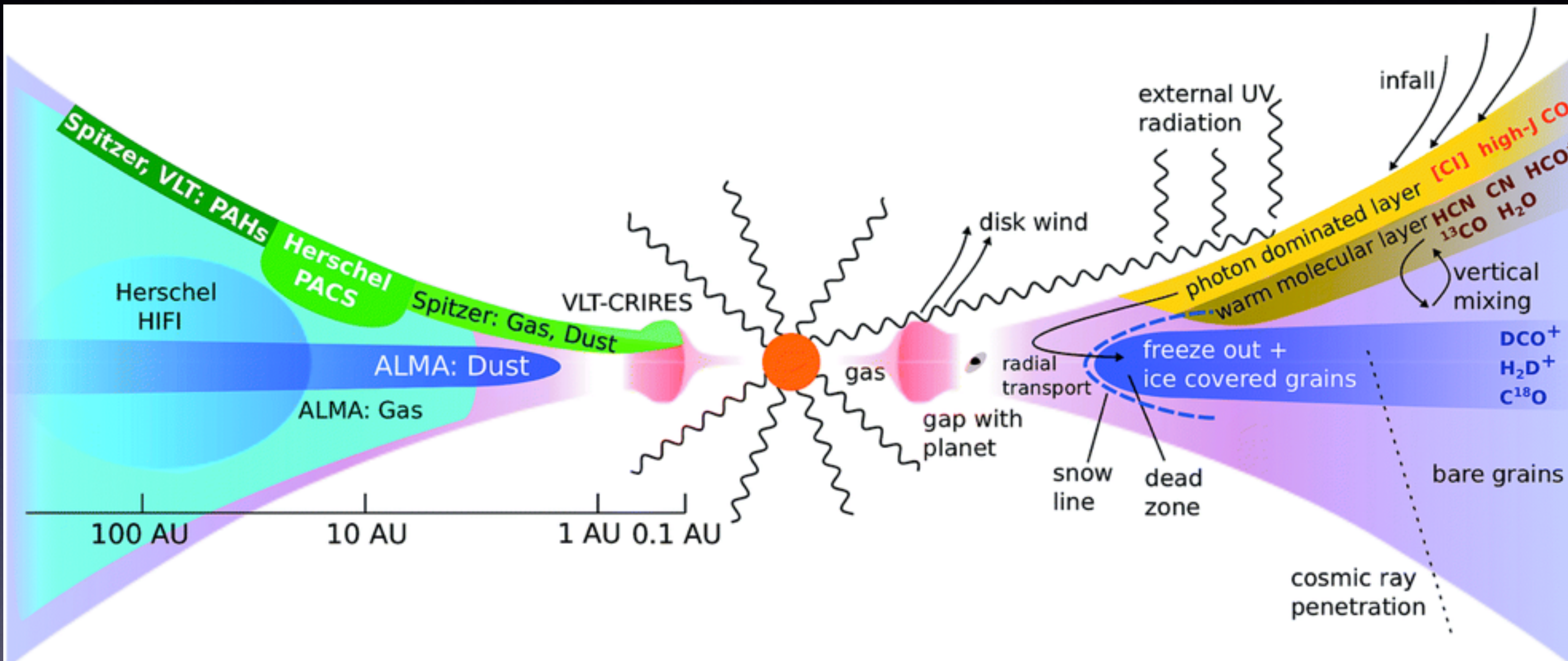
$$\frac{1}{\rho}\frac{\partial p}{\partial z} \sim \frac{p}{\rho z} = -\frac{GM_* z}{R^3}$$

$$\rho(z) = \rho(0)\ exp(-z^2/2H^2)$$

$$H/R = (T_d/T_g)^{1/2}\ (R/R_*)^{1/2}$$

- Direct measurements:
  - Cold gas CO, … (outer disk)
  - Warm gas H_2, CO, H_2O (inner disk)
  - Indirect: Accretion and Jets

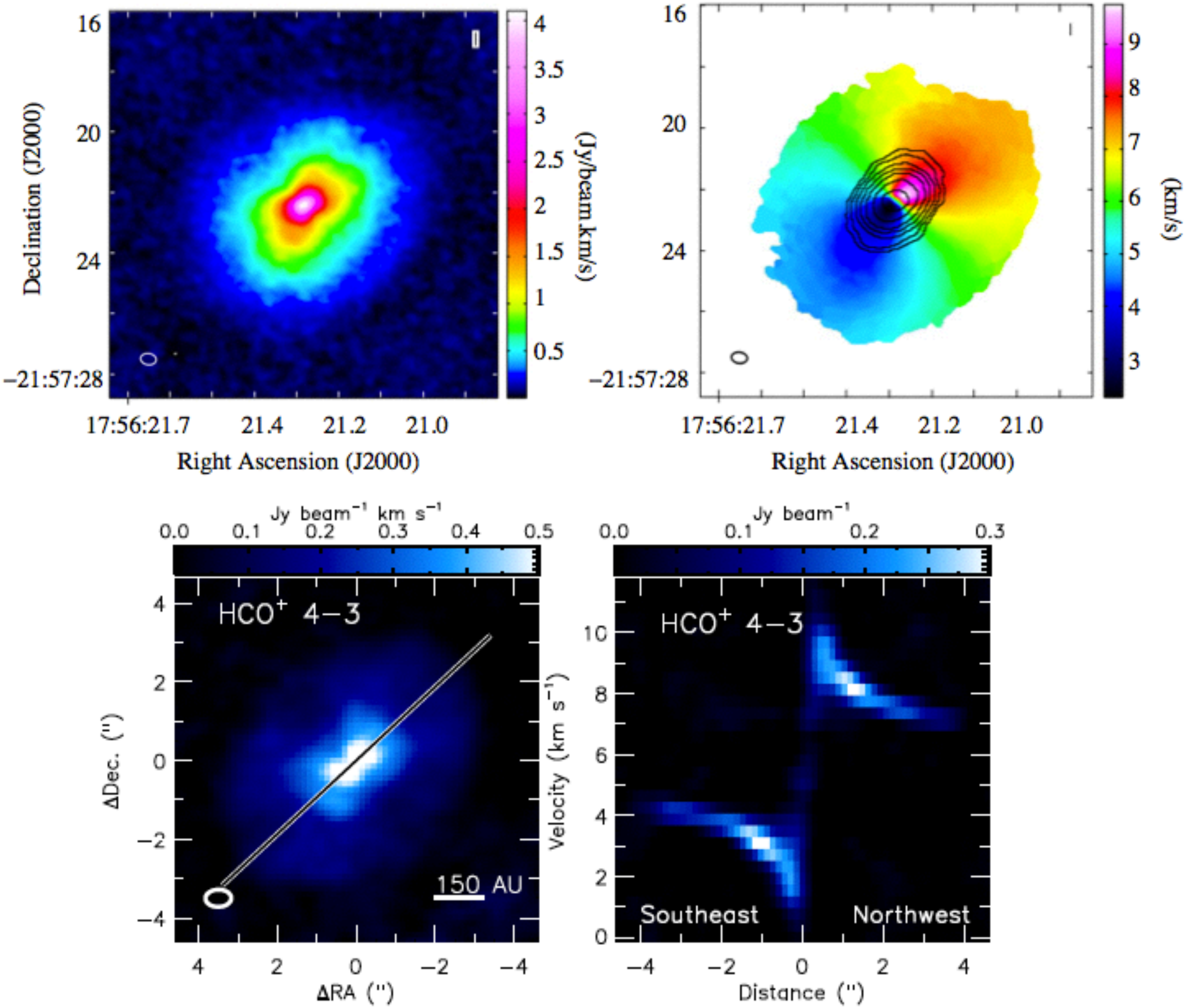
Gas in protoplanetary disks



(van Dishoeck 2014)

Outer disks structure and kinematics

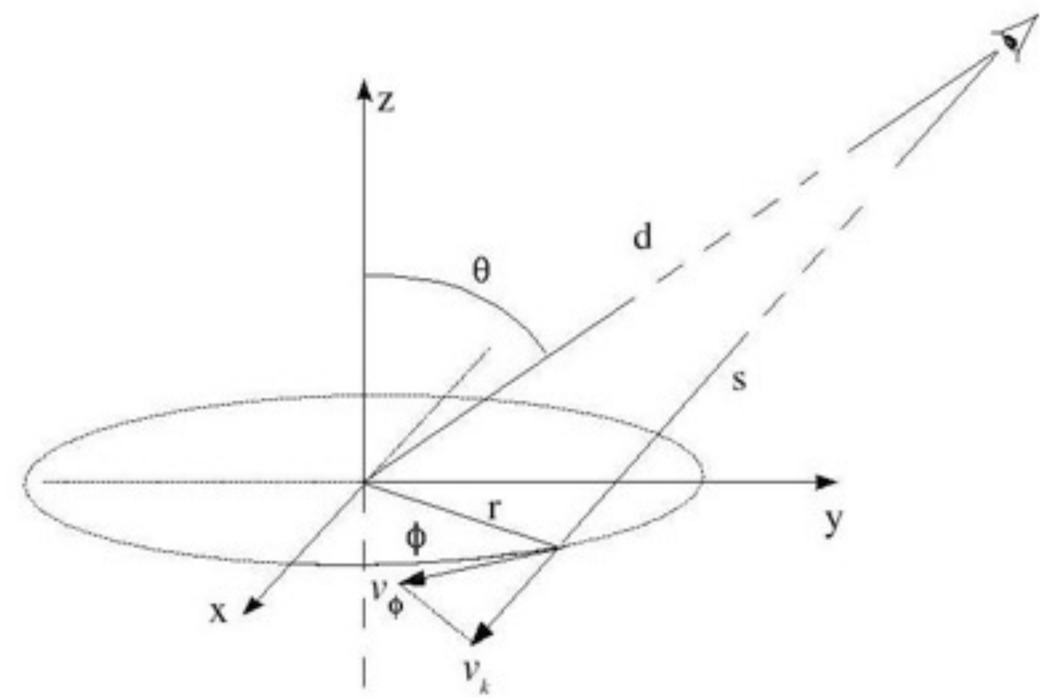
HD163296



(de Gregorio Monsalvo+2013;Mathews+2013)

Molecular gas

- Calculation of the CO emission assuming thermalised gas



$$I_\nu = \int_0^\infty S_\nu(s) e^{-\tau_\nu}(s) K_\nu(s) ds$$

$$\tau_\nu(s) = \int_0^s K_\nu(s')ds' \qquad K_\nu^d(s) = \rho(s) \cdot k_\nu \qquad K_\nu^{CO}(s) = n_l(s) \cdot \sigma_\nu(s)$$

$$n_l(s) = \chi_{CO} \frac{\rho(s)}{m_0} \cdot \frac{g_l\, e^{-E_l/\mathrm{k}T_{CO}(s)}}{Z(T_{CO}(s))}$$

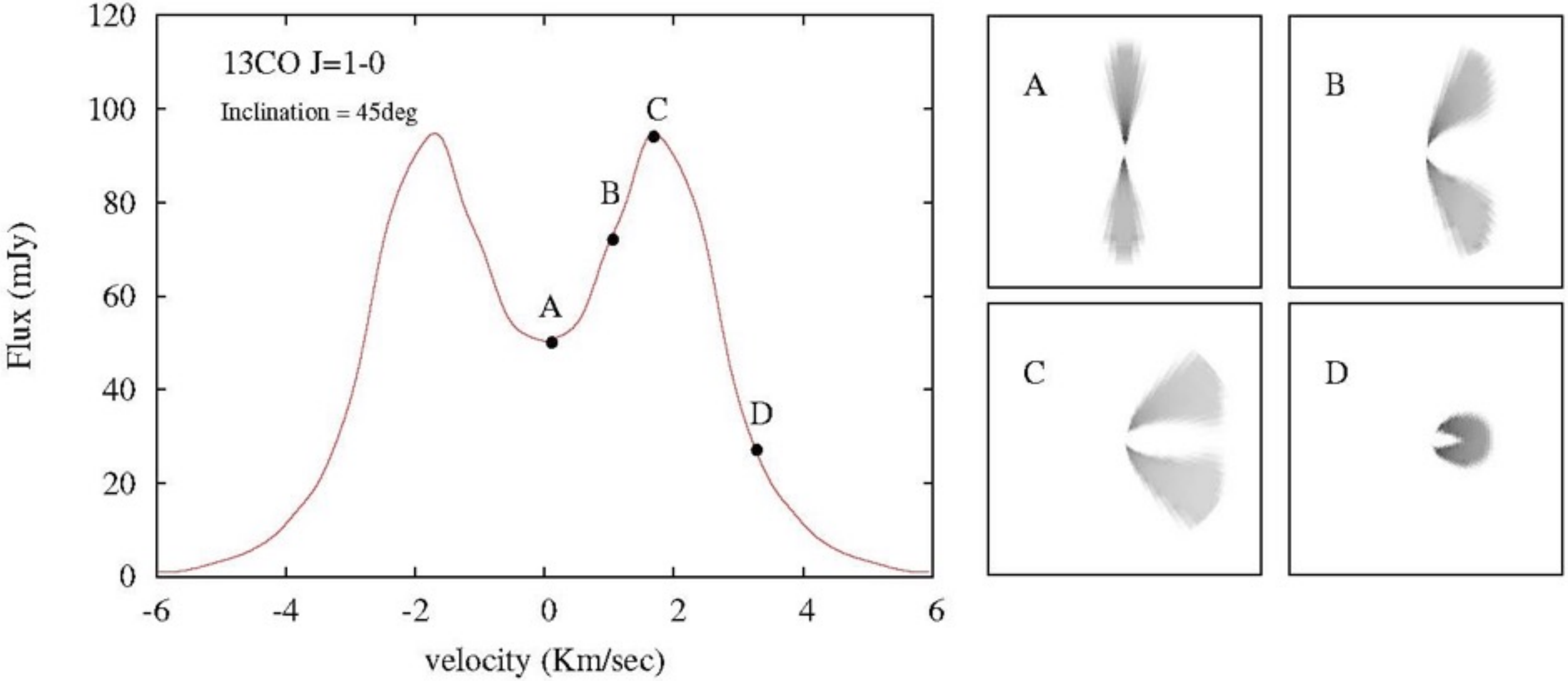
$$S_\nu(s) = B_\nu(T_{CO}(s)) = \frac{2\mathrm{h}\nu^3}{\mathrm{c}^2} \frac{1}{\exp(\mathrm{h}\nu/\mathrm{k}T_{CO}(s)) - 1}$$

$$T_{CO}(r) = T_{CO}(r_0)(r/r_0)^{-q}$$

(Isella et al. 2007)

Molecular gas

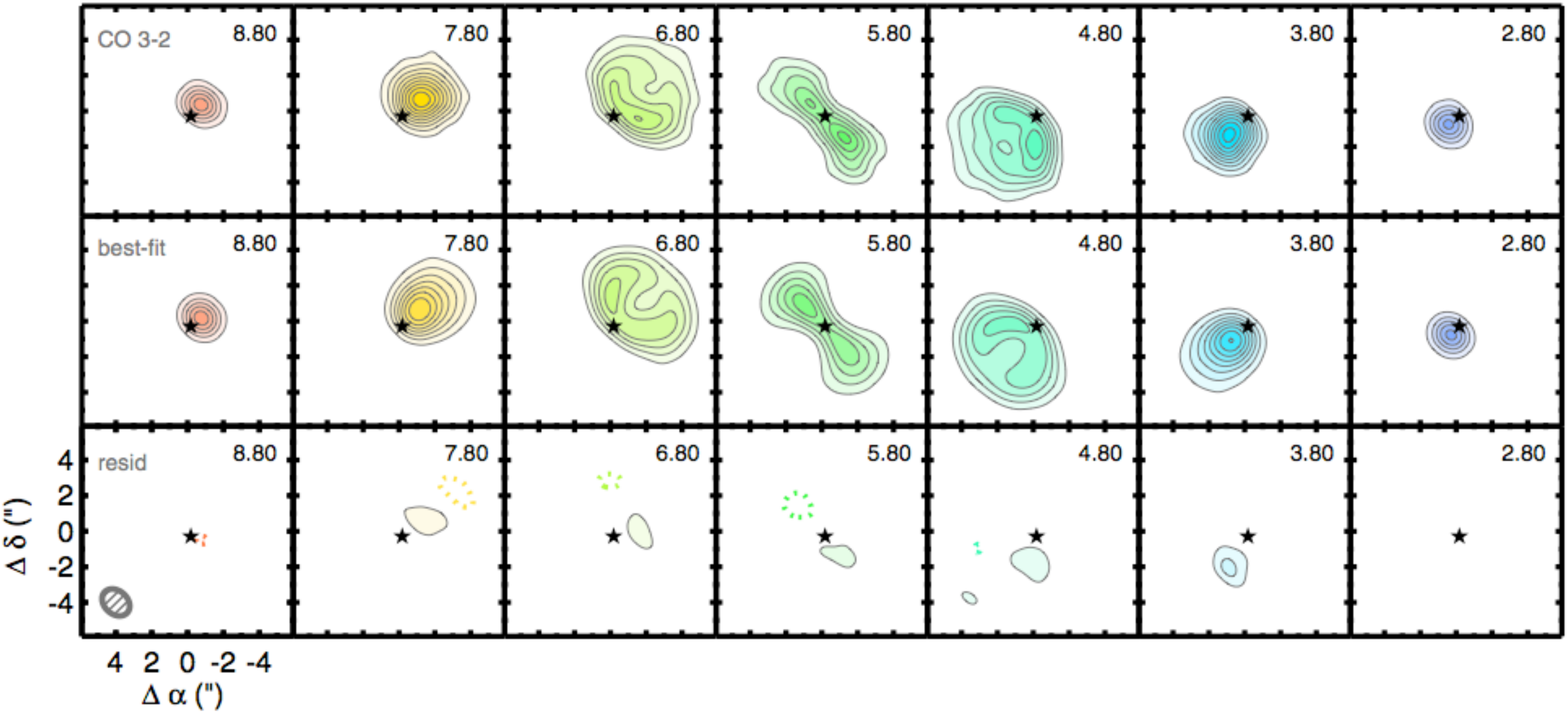
- Simulated CO profiles and maps



(Isella et al. 2007)

Outer disks structure and kinematics

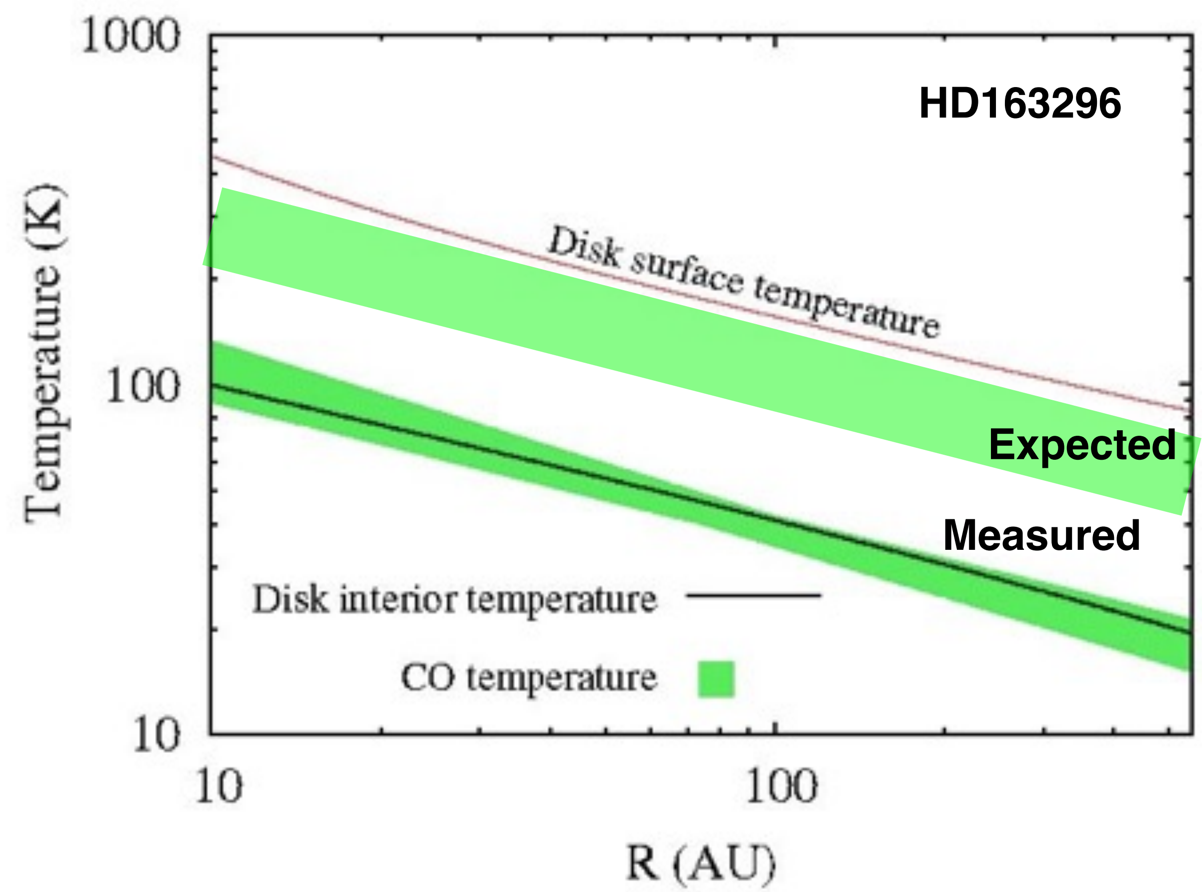
HD163296



(Qi et al. 2012)

Gas properties and evolution

- Kinematics
  - Disk-outflow interaction
  - Possible evidence for non keplerian motions
- Physical properties
  - Temperature, density structure
  - Abundance, gas to dust ratio
- Chemical properties
  - Formation of complex molecules
  - Chemical differentiation in different regions of the disk

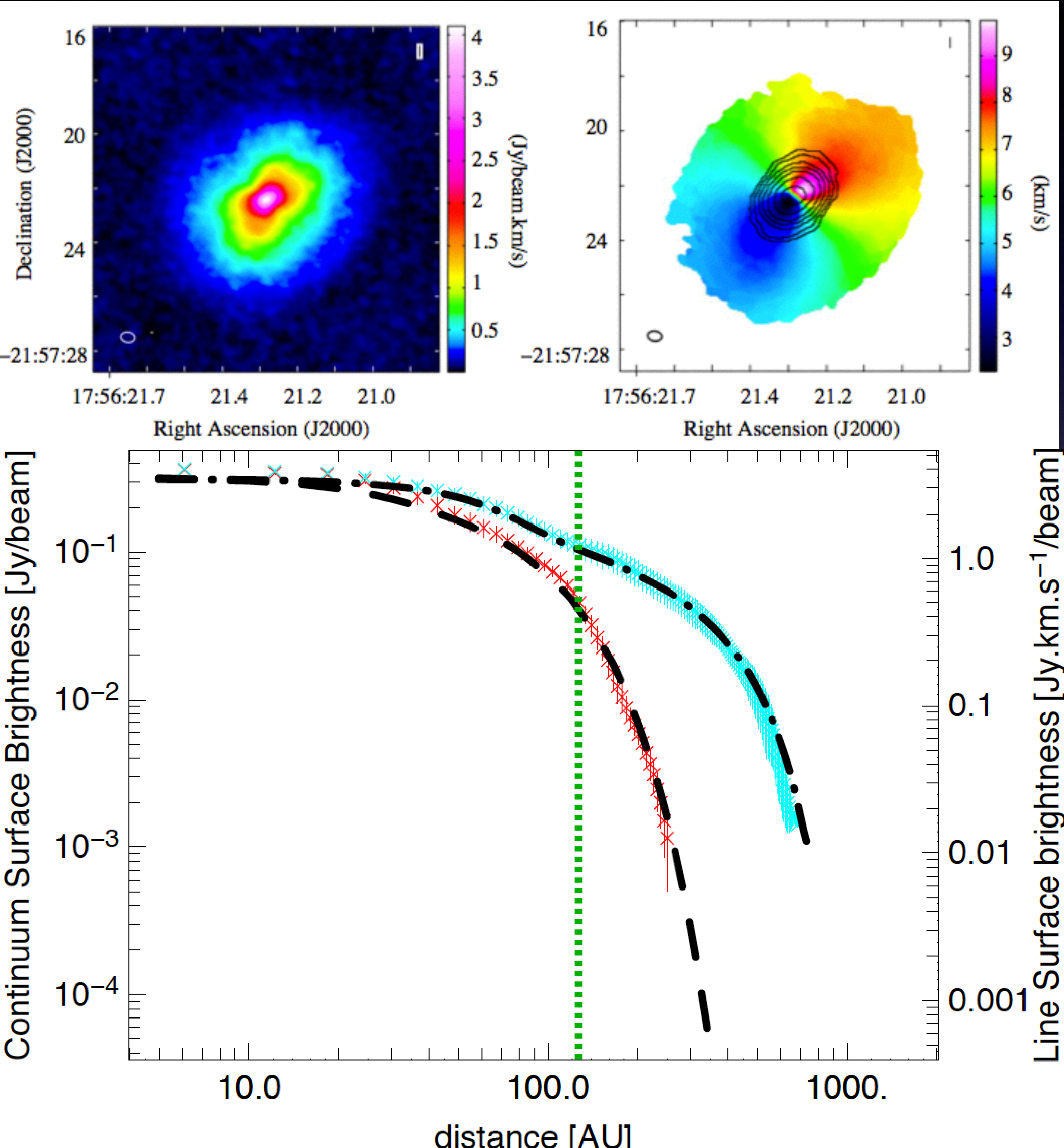


CO isotopes depletion factors:

$^{13}CO \Rightarrow \sim 10$ $([^{13}CO]/[H_2] \sim 10^{-7})$

$C^{18}O \Rightarrow >60$

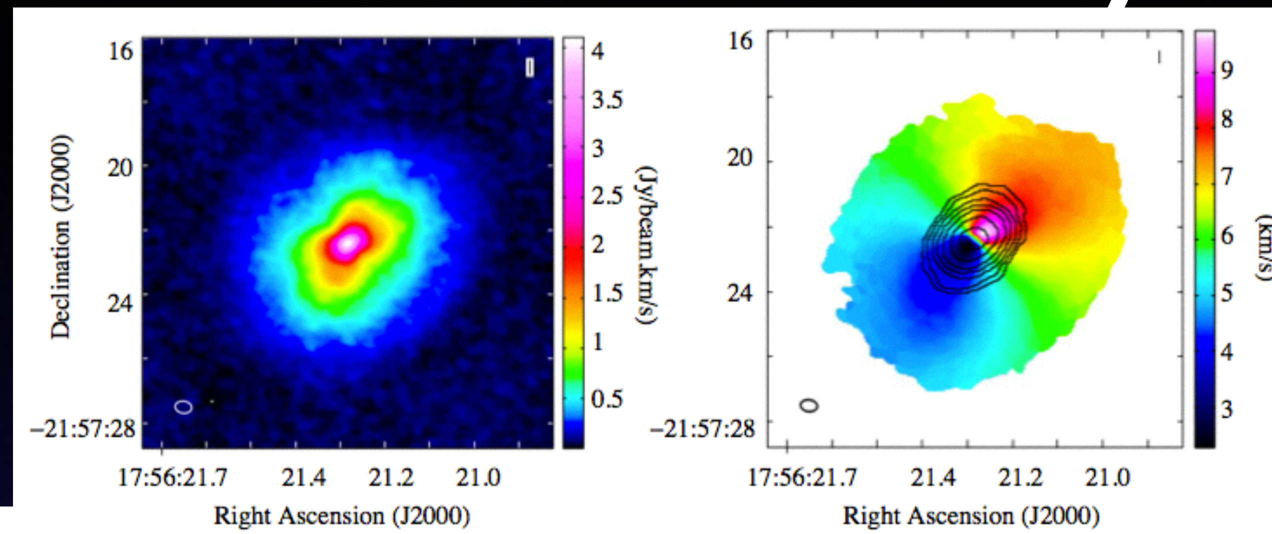
HD163296 as seen by ALMA

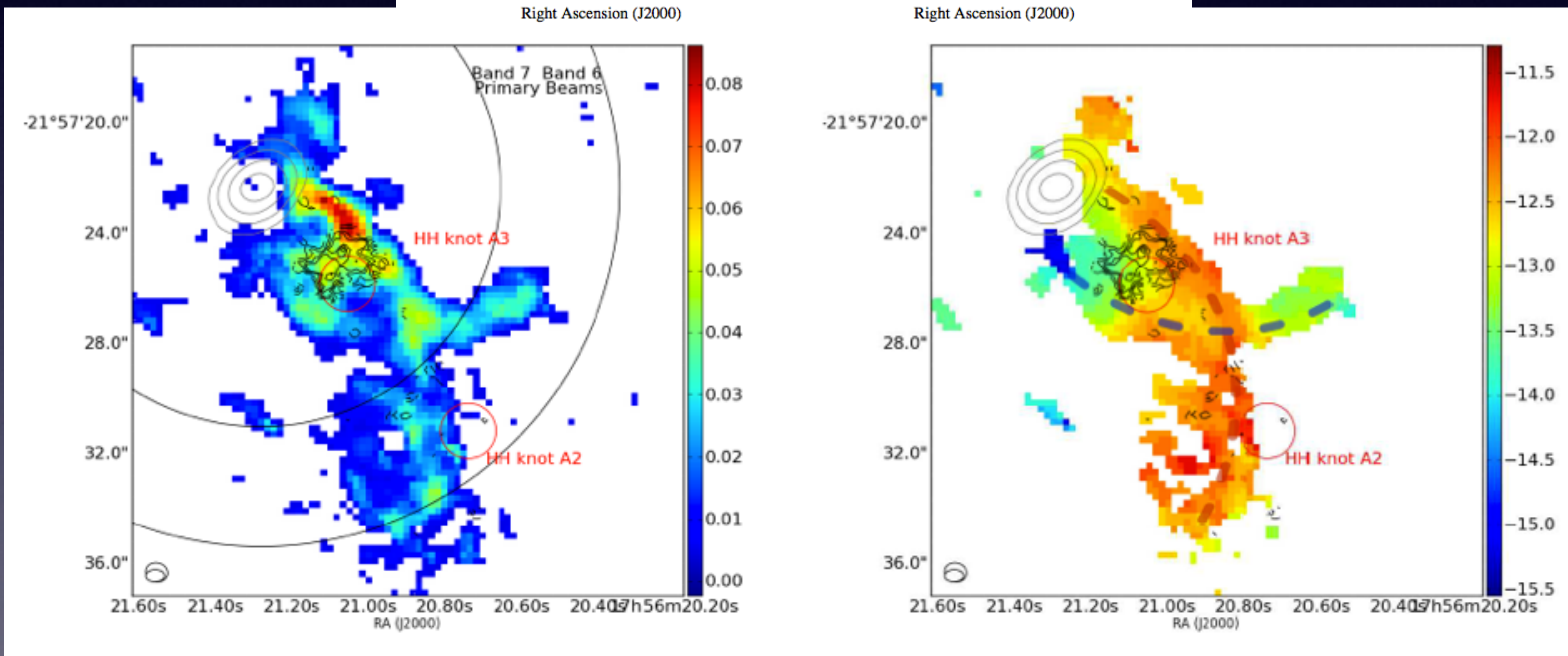


- Extent of the CO disk is much larger than that of the mm-grains disk
- Consistent with expectations from viscous spreading and migration of the larger grains

(deGregorio-Monsalvo+2013)

HD163296 as seen by ALMA

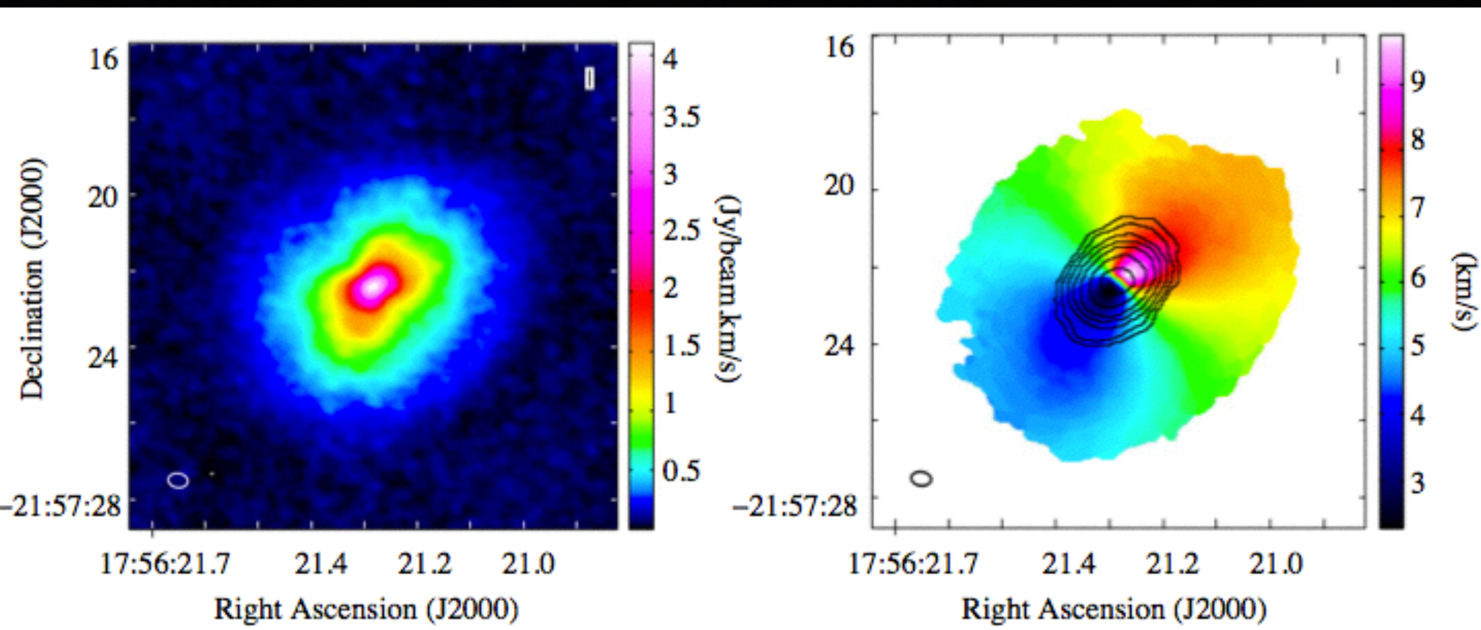




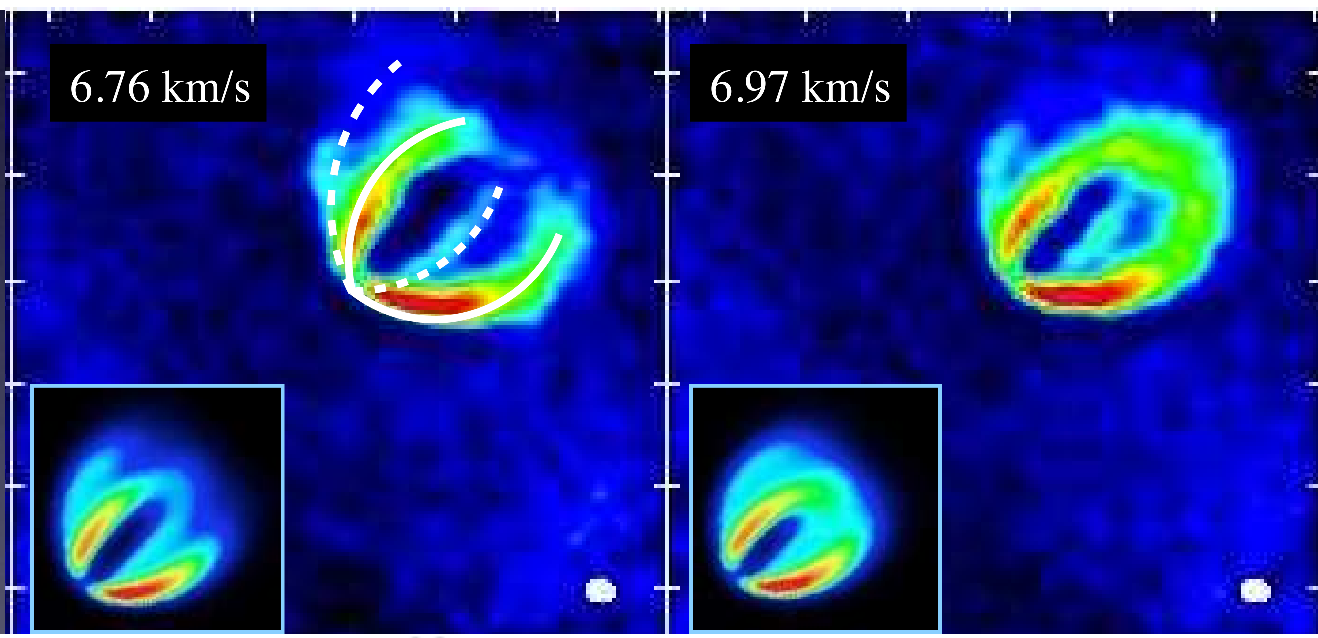
(Klaassen et al. 2013)

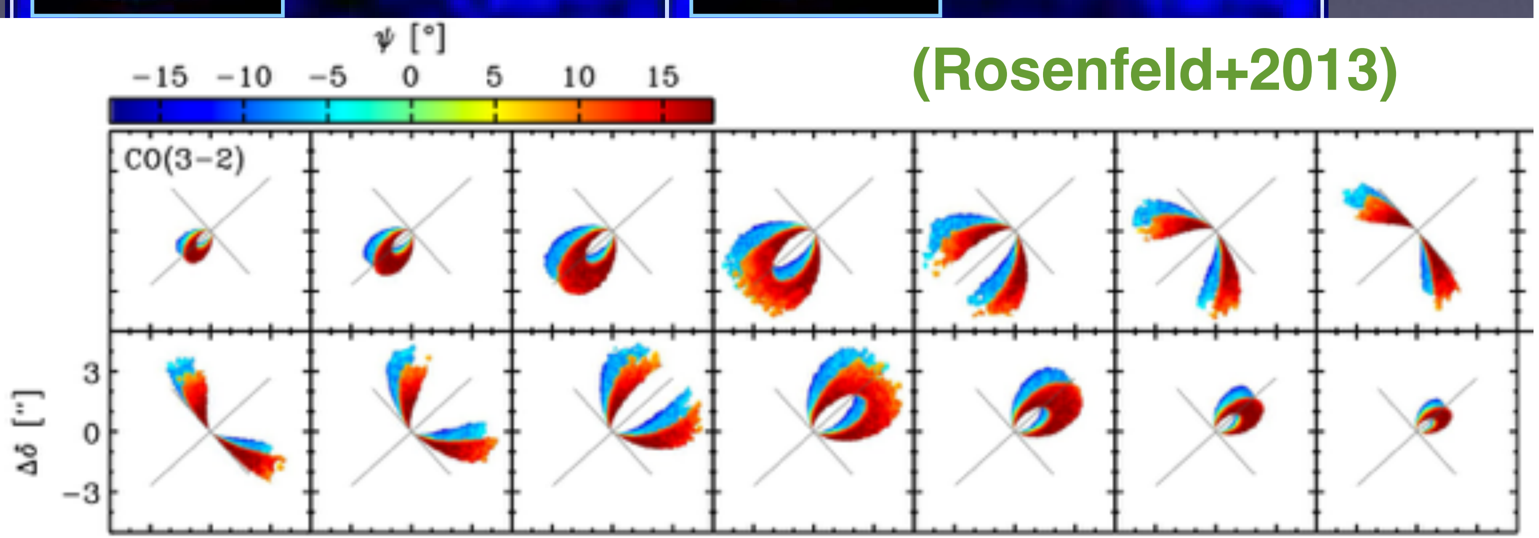
- Evidence for a CO disk wind

HD163296 as seen by ALMA



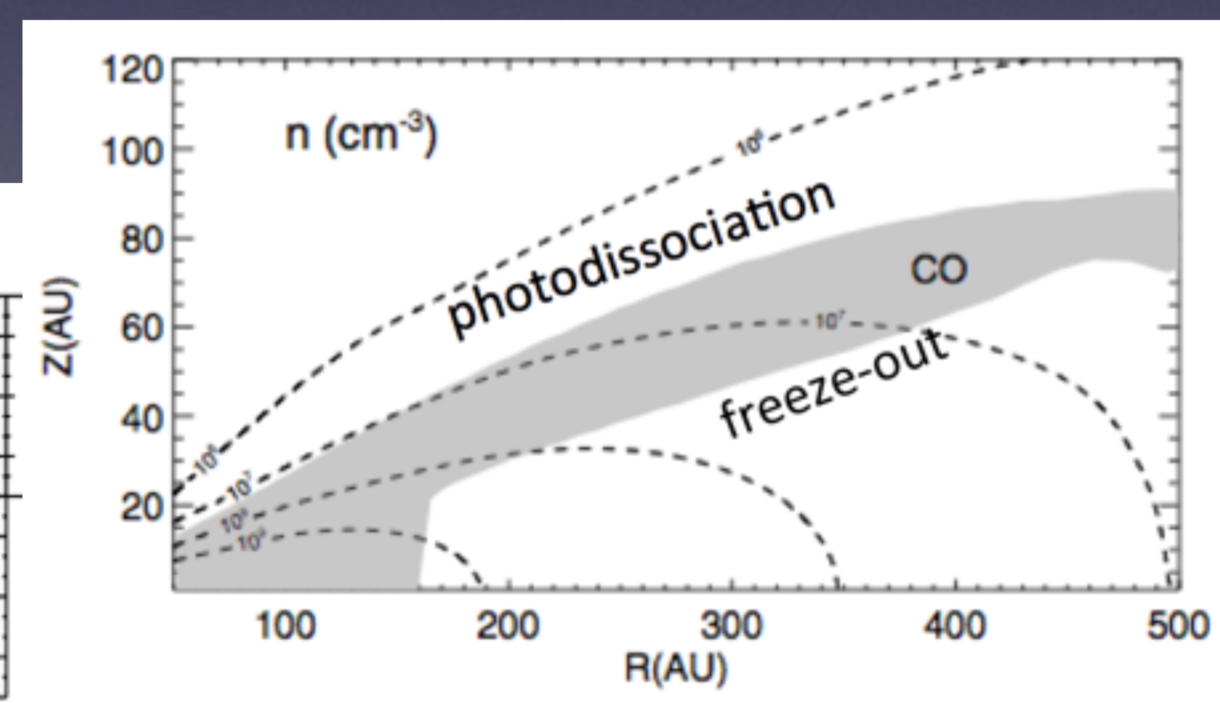
(deGregorio-Monsalvo+2013)





(Rosenfeld+2013)

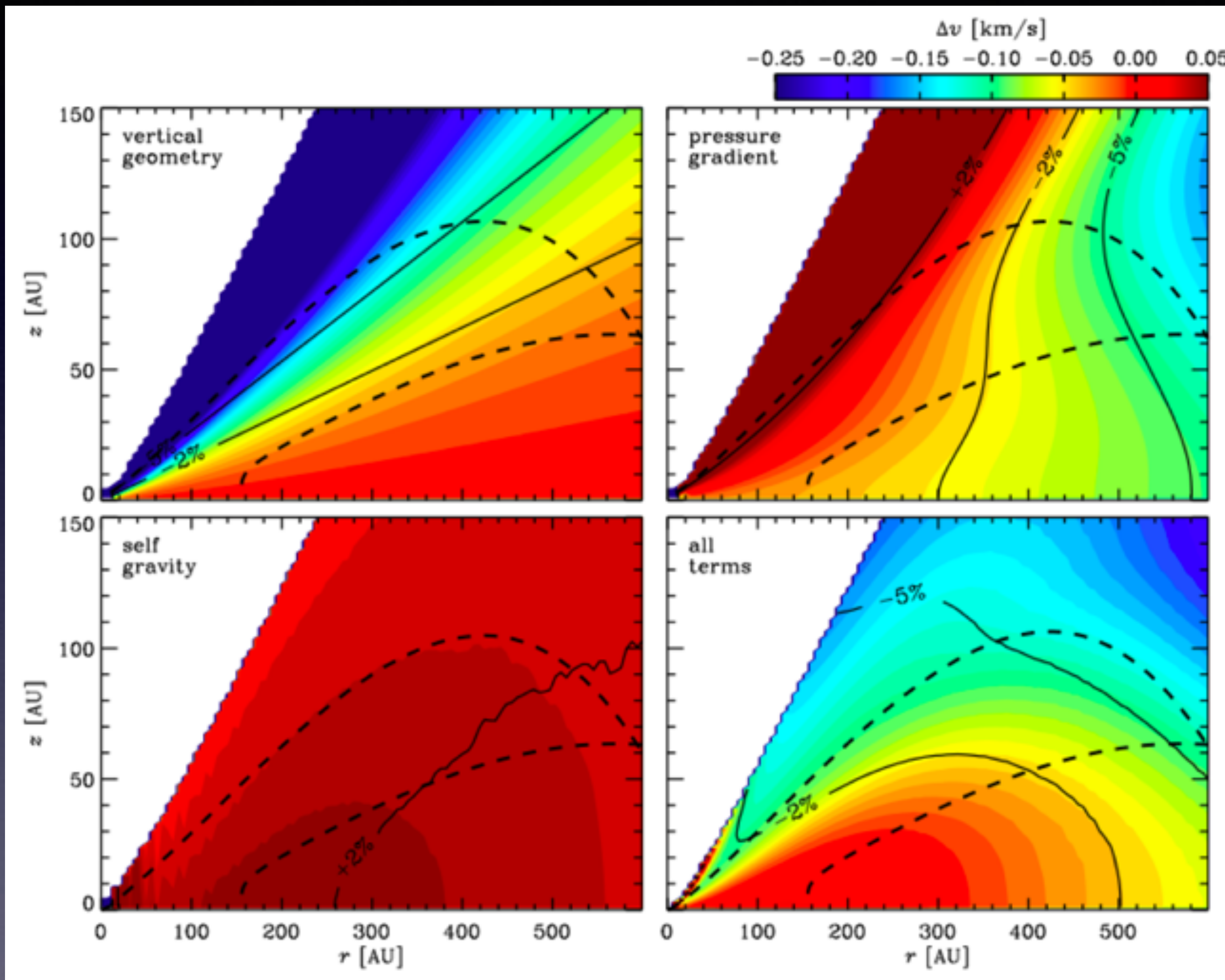
- Direct measurement of disk flaring and CO depletion on the mid plane



5 min pause

- Why CO is our prime probe of gas?
- With $[CO]/[H_2]\sim10^{-4}$, why should it be a better trace of mass than dust ($[d]/[H_2]\sim0.01$)?
- What are the difficulties in using gas as tracer?

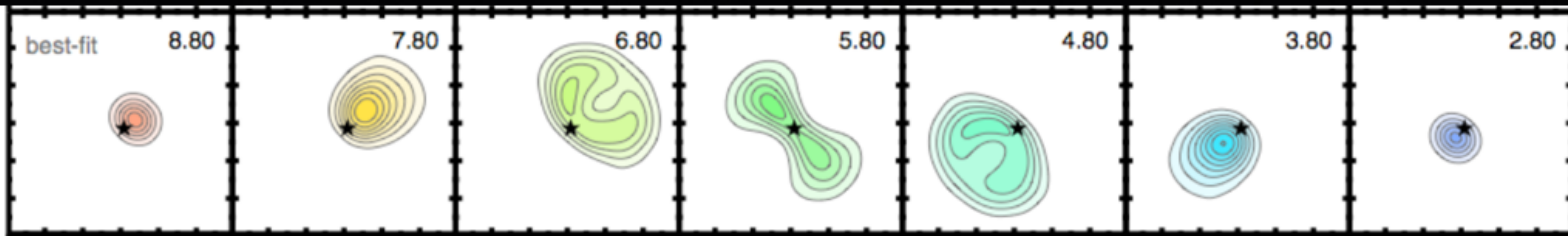
Gas kinematics

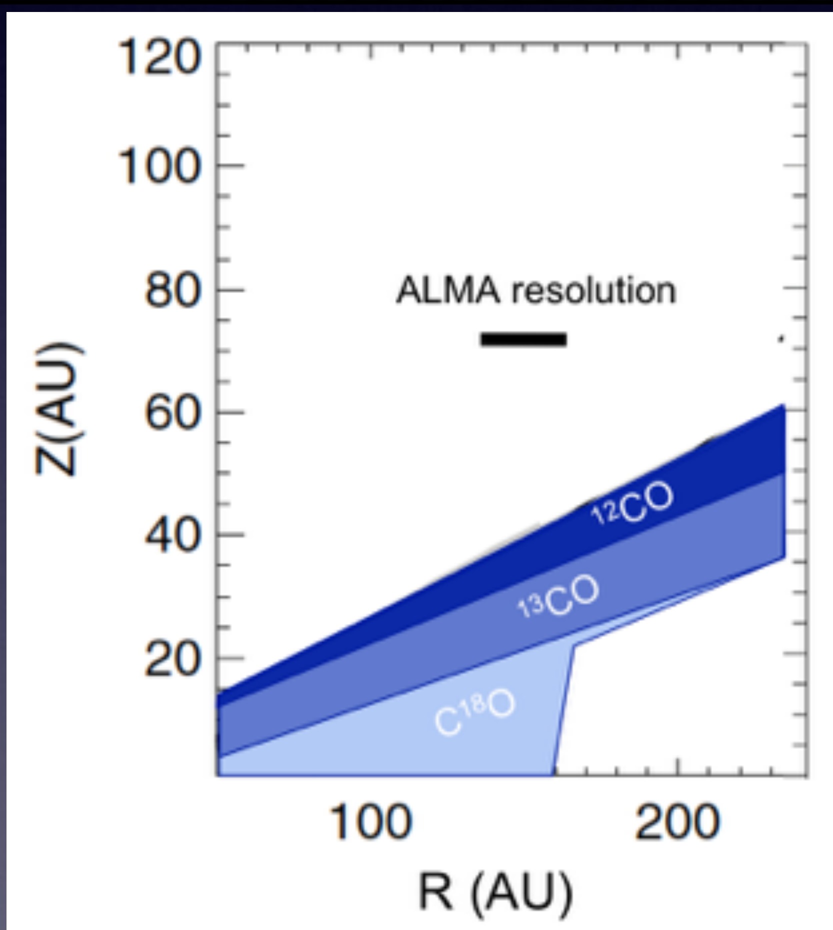


(Rosenfeld et al. 2013)

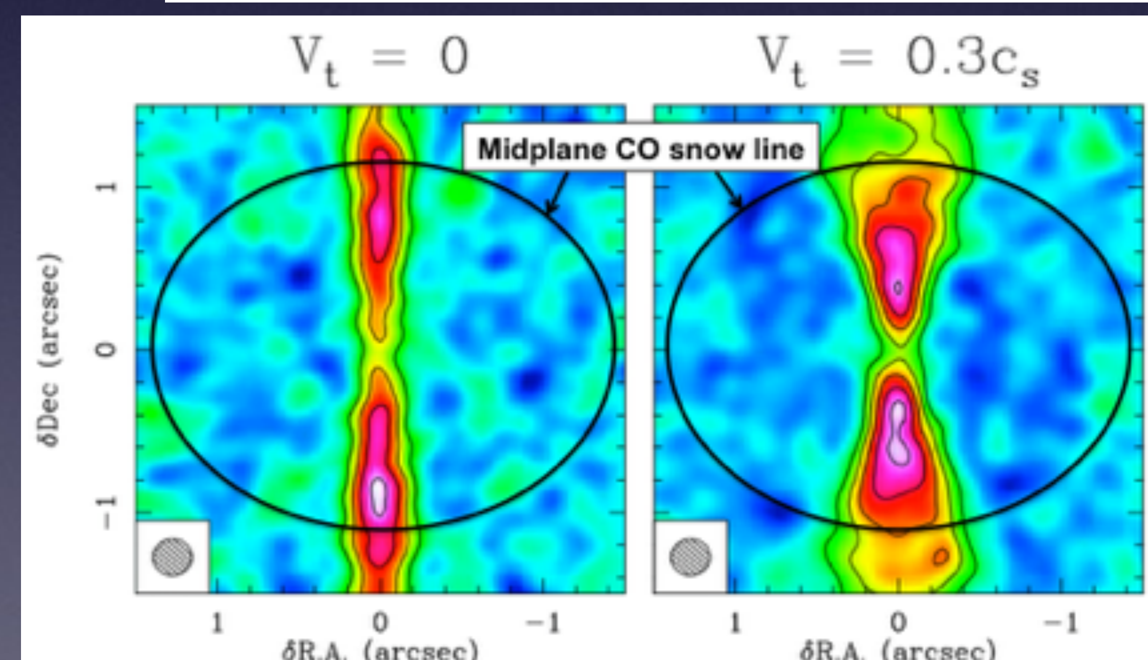
- Potentially a direct measurement of the disk self-gravity
- Not exactly Keplerian
- Largest effect is the pressure term 5%, self gravity 0.1-0.5%

Turbulence



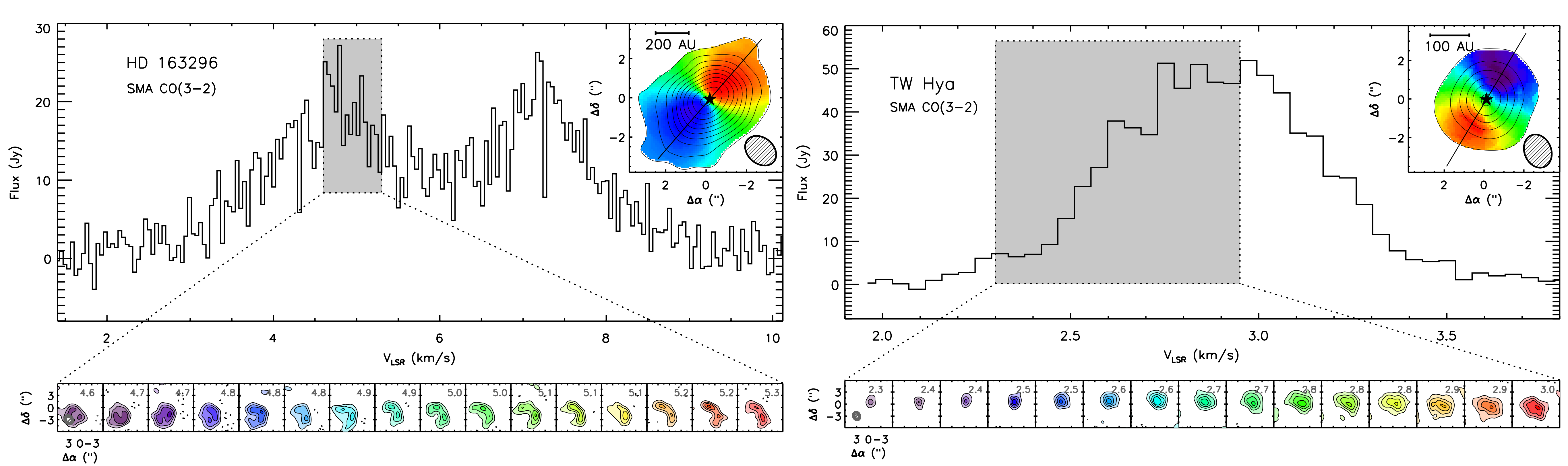


$$\Delta V(r) = \sqrt{\frac{2kT(r)}{\mu m_{\rm H}} + \delta V_{\rm tu}(r)^2}$$



- Turbulence provide an additional line broadening term
- Measureable with ALMA: high S/N and resolution

Turbulence - pre-ALMA

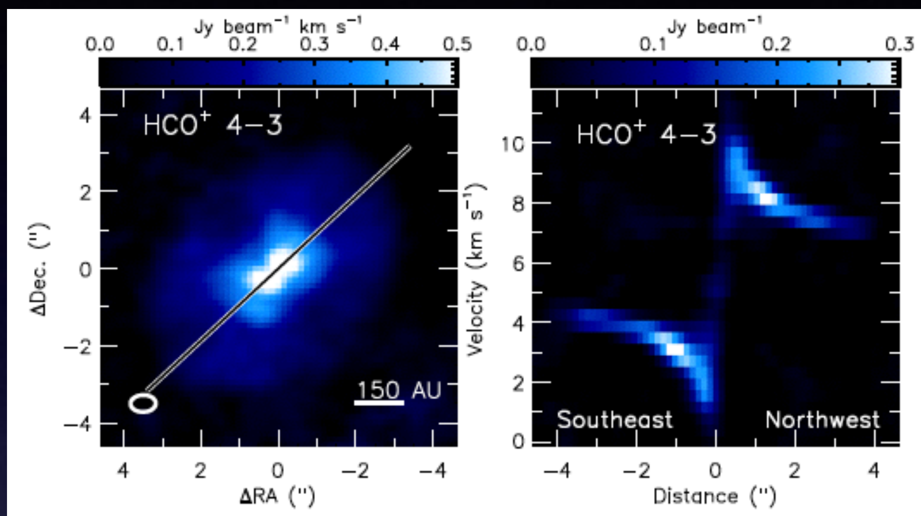


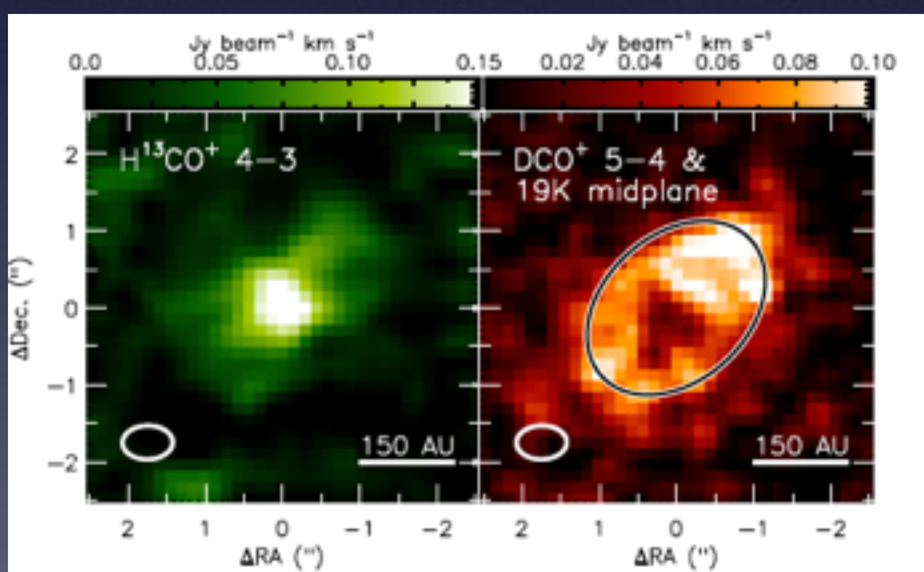
Hughes et al. (2011)

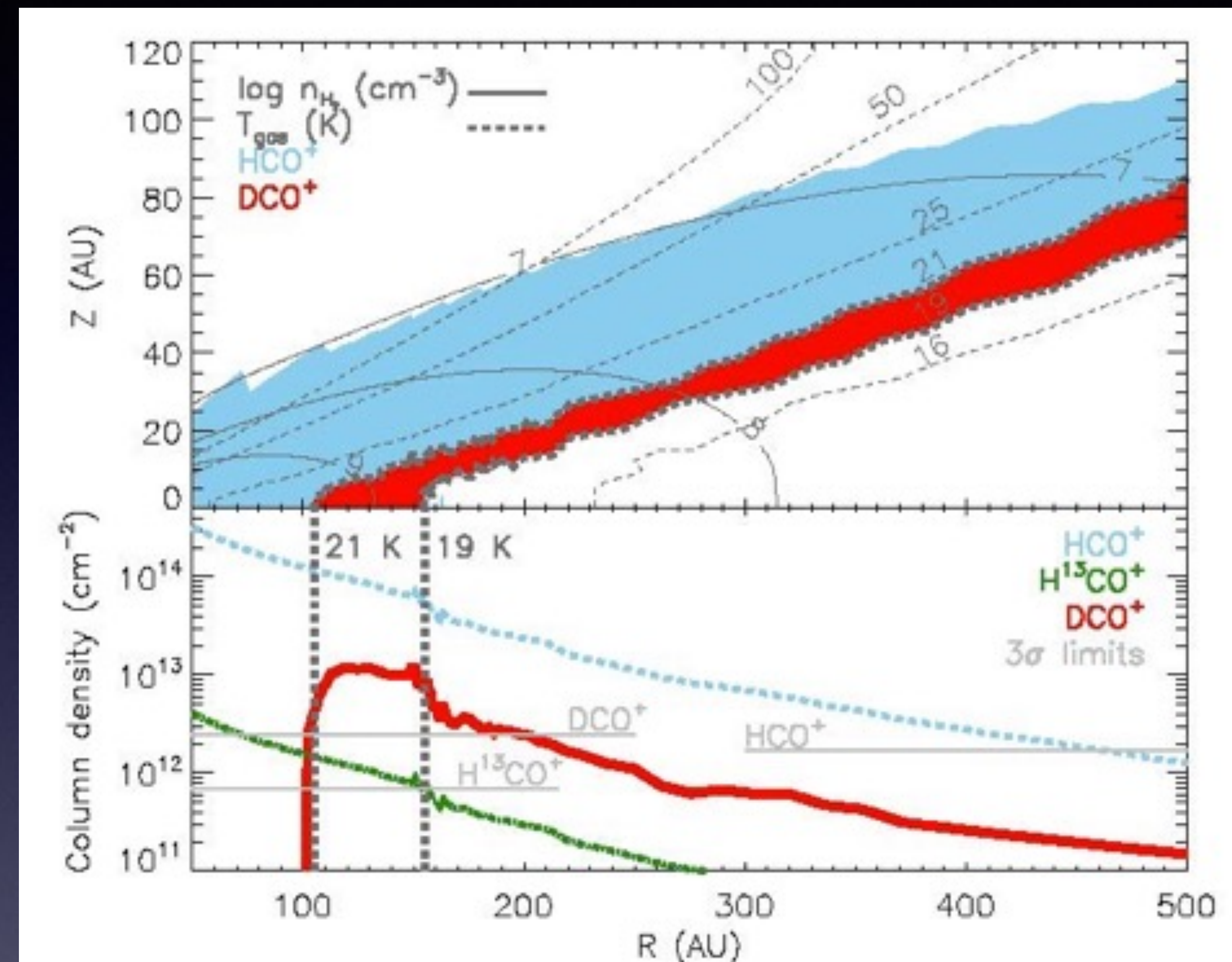
- High S/N spectra limit turbulence to
  - < 40 m/s for TW Hya
  - ~300 m/s for upper layers of HD163296 disk (0.4 Mach)
- DM Tau: 0.4-0.5 Mach at intermediate layers (Guilloteau et al. 2012)
- Important for planet-formation models; mixing of material

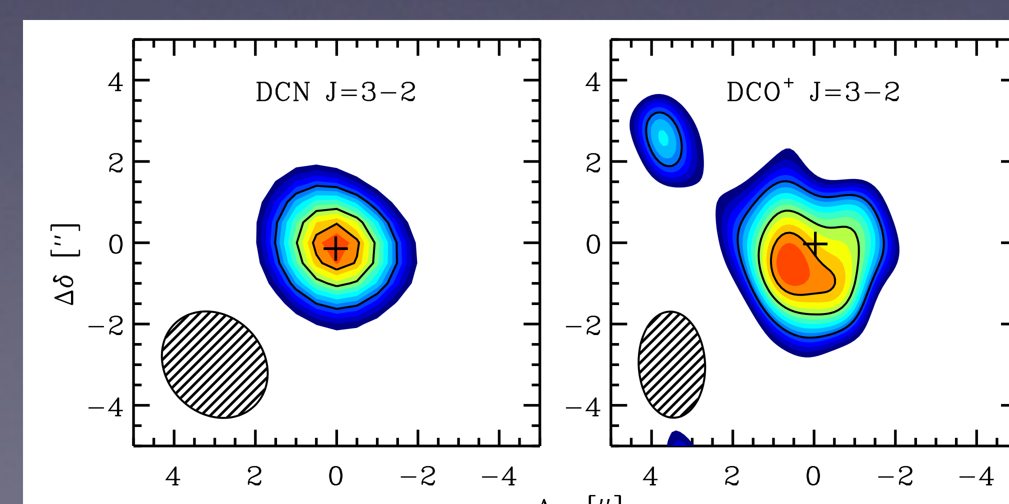
HD163296 as seen by ALMA

(Mathews et al. 2013)







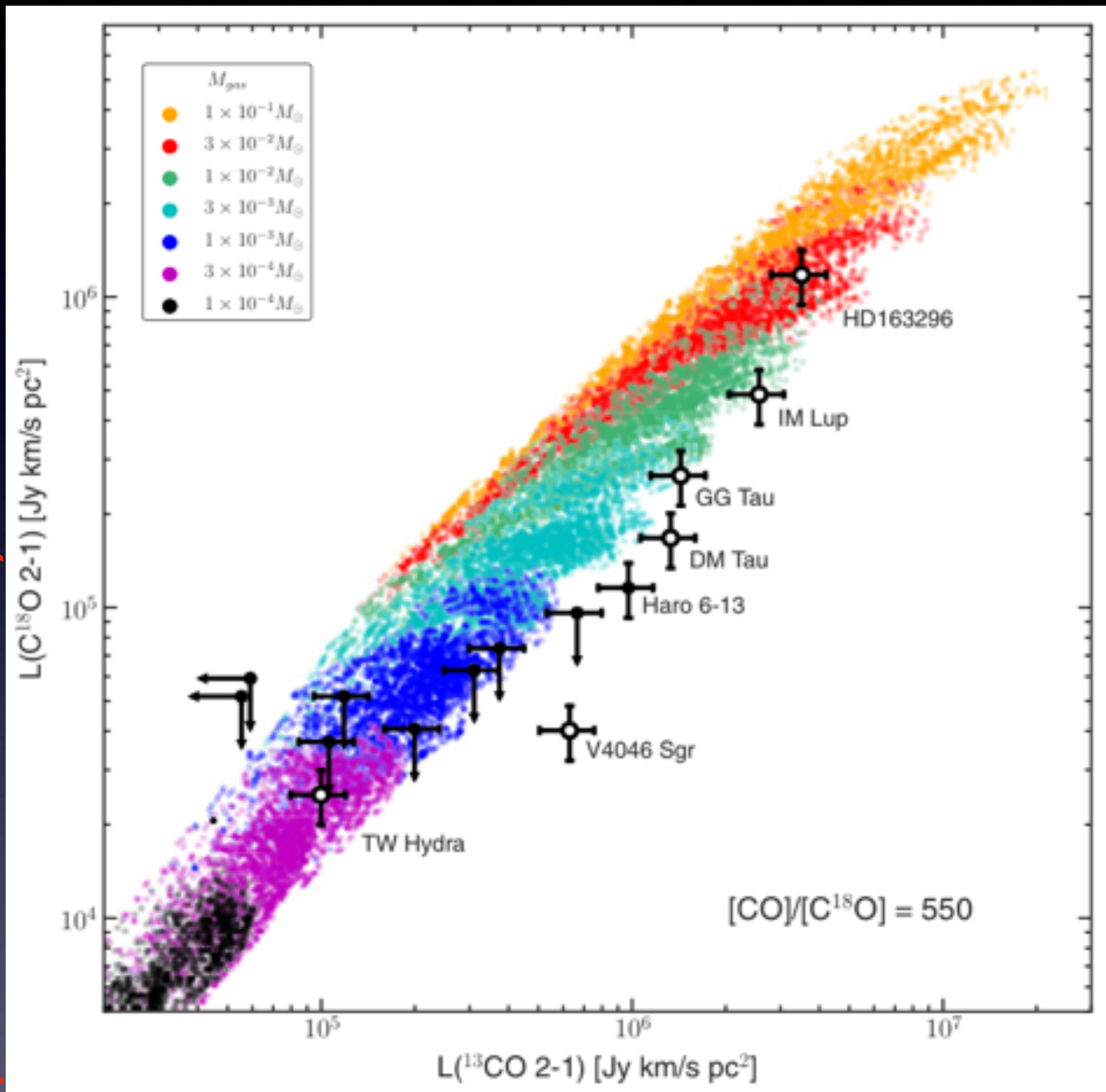


(Oeberg et al. 2012)

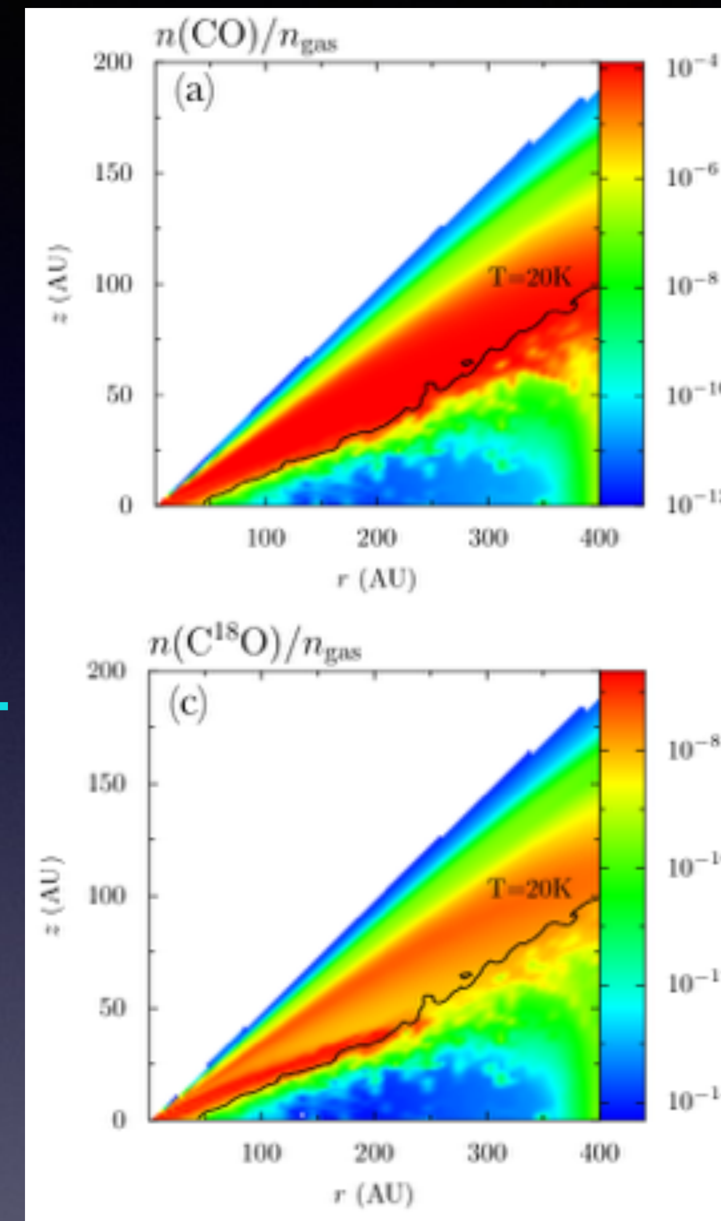
- Chemical measure of CO snowline

Masses from CO and isotopomers

(Williams & Best 2013)



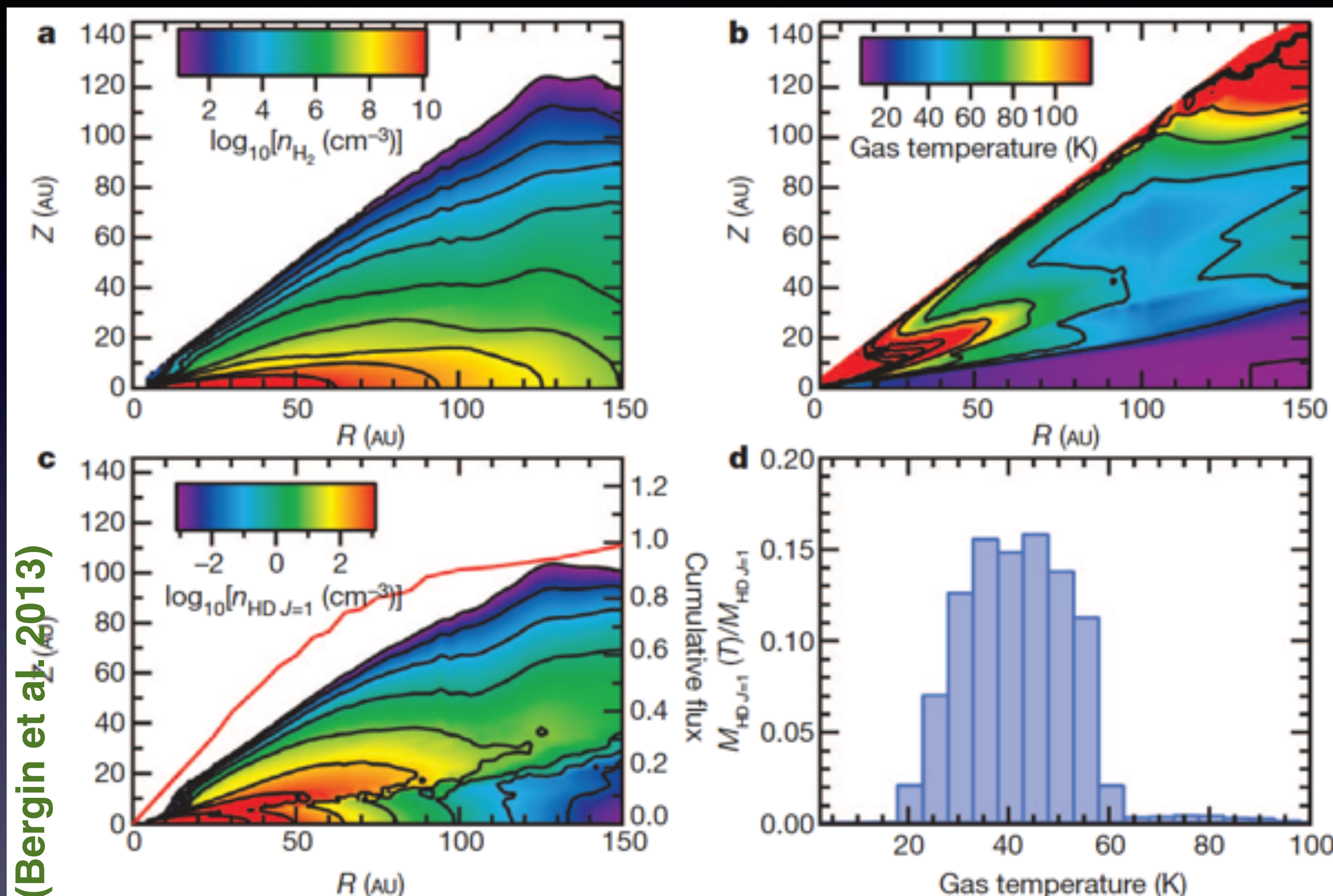
Effect of selective photodissociation

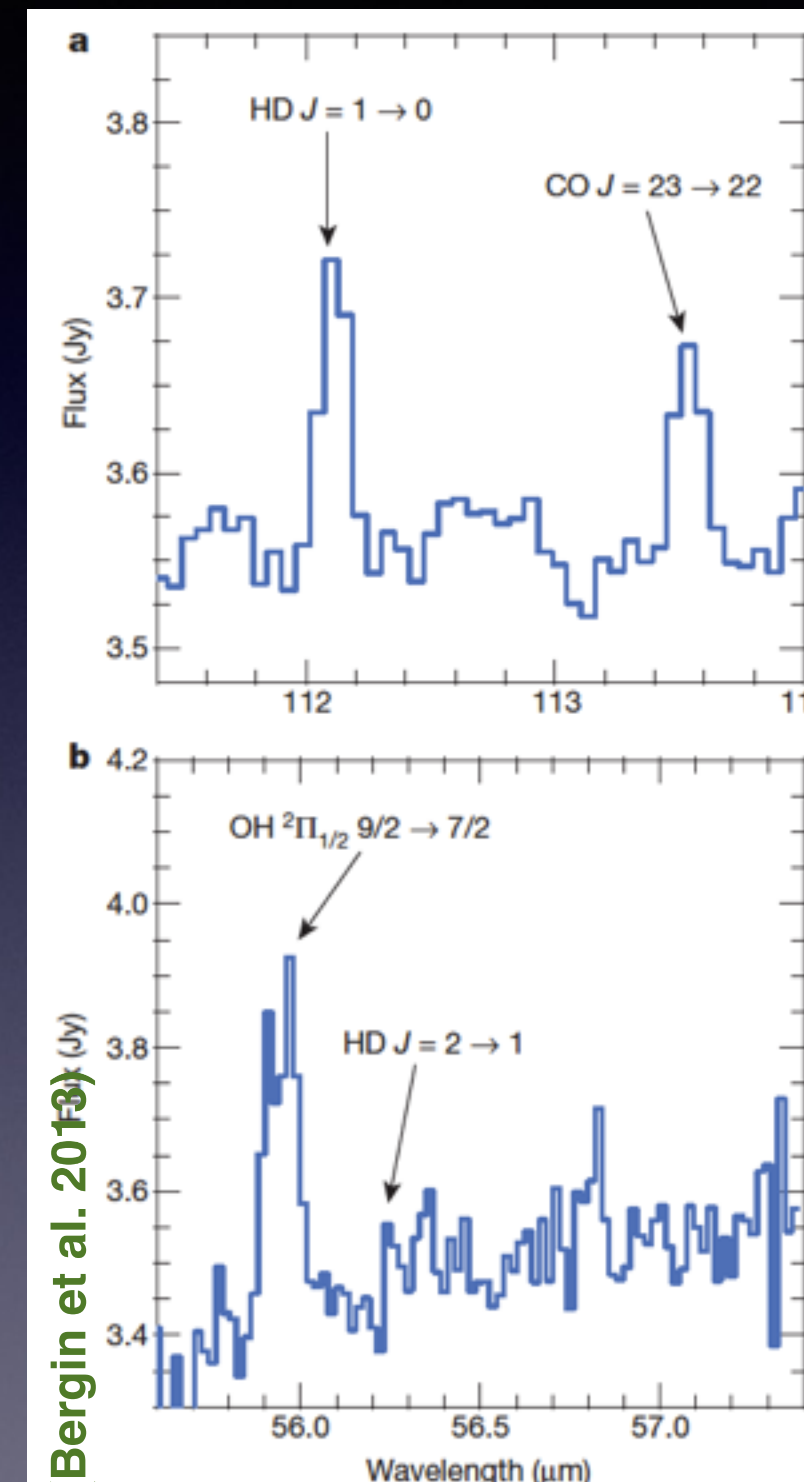


(Miotello+2014)

- CO isotopomers may be good tracers of the gas mass, if treated very carefully
- Taking into account: freeze-out and (selective) photodissociation

Direct measurement from HD





- HD has been detected with Herschel in the nearest disk. This may be a good constraint on the gas mass in disks

Take home points

- Molecular spectroscopy is potentially a very powerful tool to study disk kinematics, physics and chemistry
  - Complex modelling
  - Missing/uncertain key data: collision rates, reaction rates
- ALMA will be the prime tool to study
  - kinematics and chemistry of disks