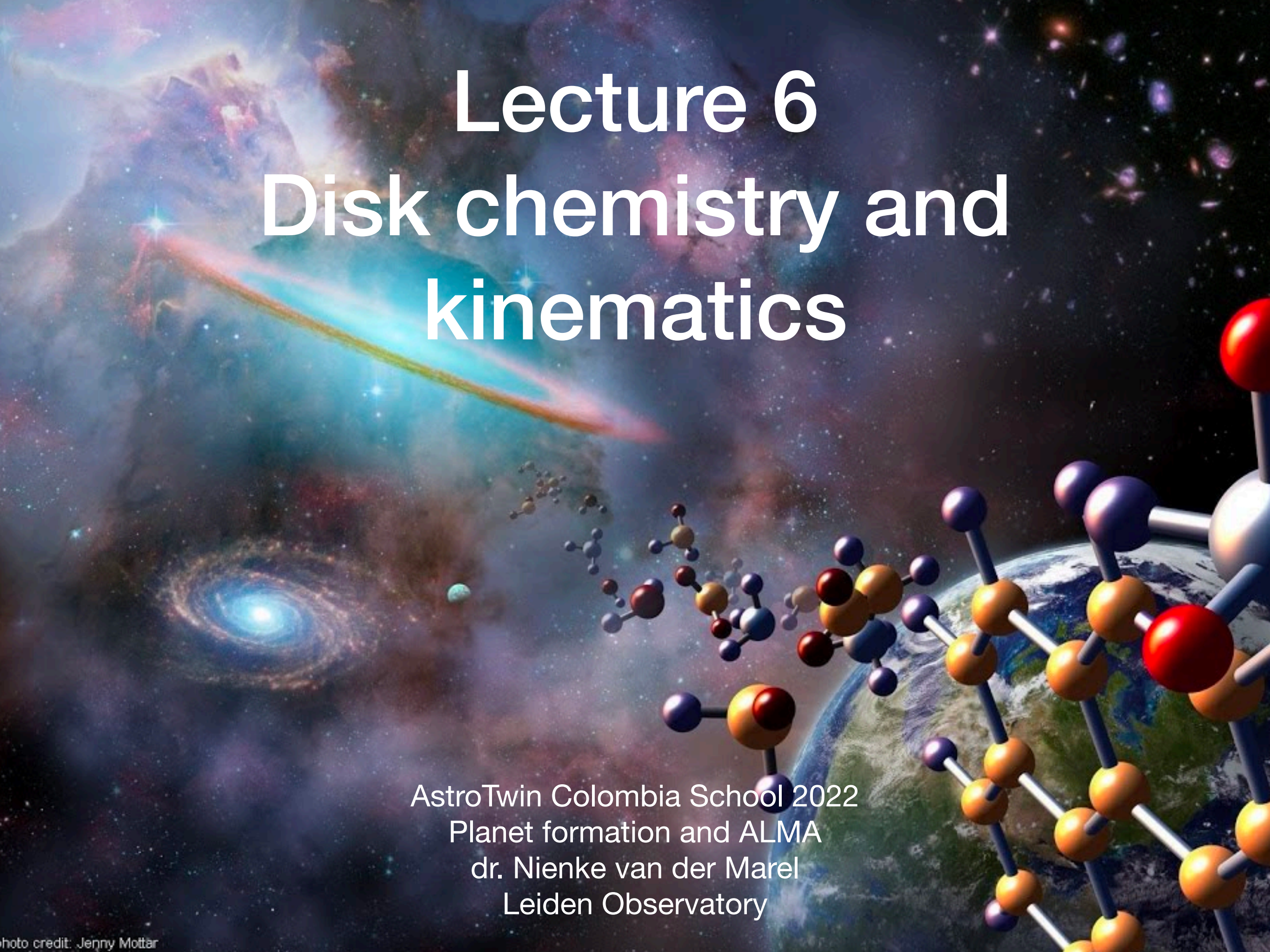


Lecture 6

Disk chemistry and kinematics

The background is a vibrant space scene. On the left, a bright blue jet of gas and dust extends from a central point. In the lower-left, a spiral galaxy with a bright blue core is visible. The right side of the image is dominated by a large, detailed ball-and-stick molecular model of a complex organic molecule, likely a hydrocarbon, with yellow, red, and purple spheres representing different atoms. The overall scene is set against a dark, star-filled background.

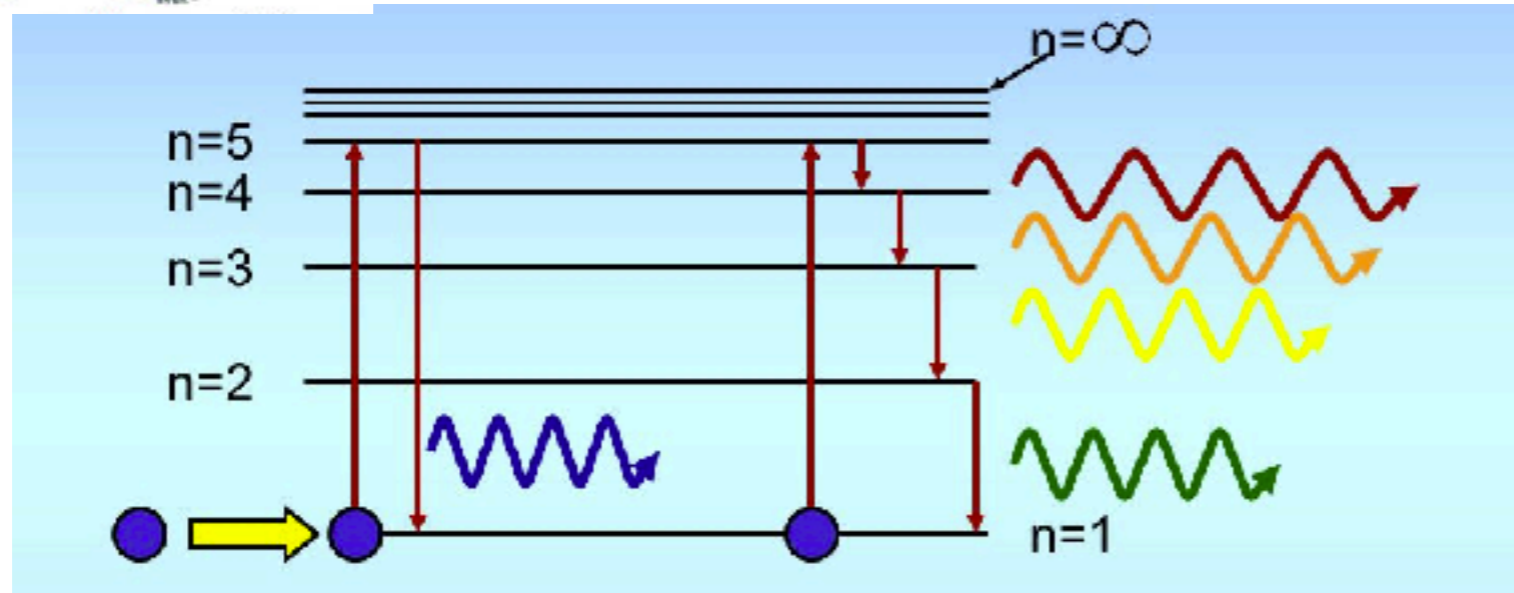
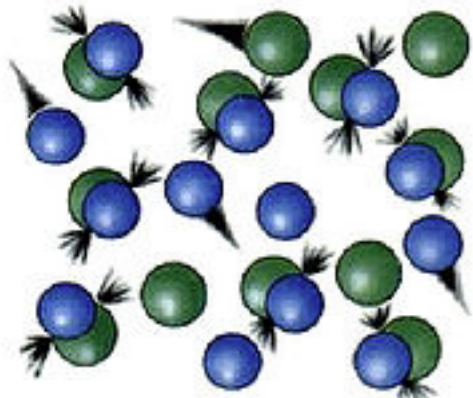
AstroTwin Colombia School 2022
Planet formation and ALMA
dr. Nienke van der Marel
Leiden Observatory

Contents

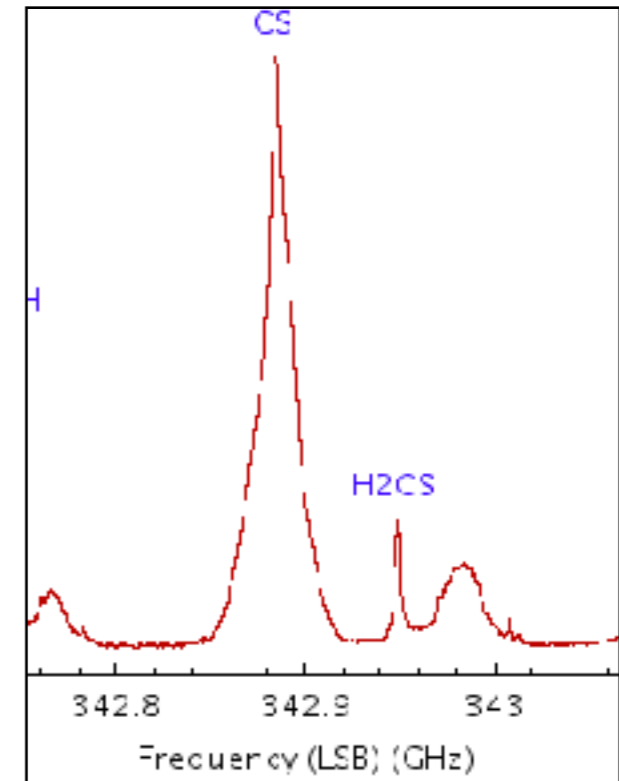
- Chemistry:
 - Astrochemistry overview (incl history)
 - Emission and excitation
 - Ice chemistry
 - Disk chemistry
 - Observational highlights
- Kinematics
 - Channel maps
 - Vertical structure
 - Warps
 - Kinks
 - Turbulence
 - Decomposing the velocity
 - Circumplanetary disks

Recall: line emission

Molecules move around randomly and occasionally collide (more collisions at higher temperature and/or higher density)

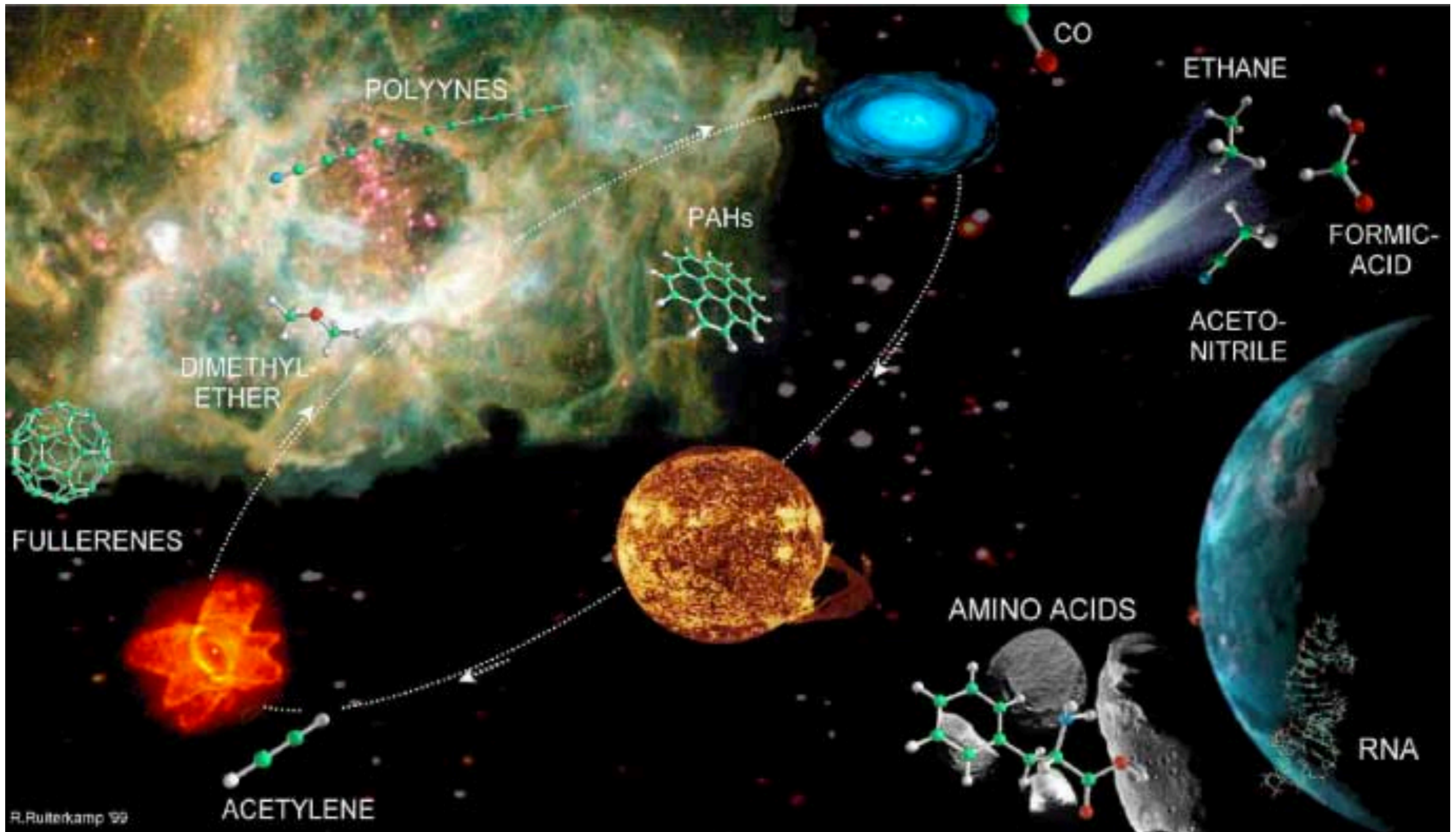


A collision brings a molecule in a higher energetic state



The molecule emits a photon (spontaneous emission) at a specific frequency to get back to lower energy. The frequency is unique for each molecule and each transition ('fingerprint')

Why study chemistry in disks?



Origin of life: what sets the composition of exoplanets?

Astrochemistry

- Molecules as diagnostics of temperature, density, ionisation, velocity, radiation fields, etc.
- Molecules are important coolants of clouds: driving astronomical processes
- Simple molecules form the start of complex organic molecules (COMs) and biomolecules: astrochemical evolution? Origin of life?
- Exotic chemistry: unique chemical laboratory

Astrochemistry

- Time scales:
 - Collision time: ~ 1 month at 10^4 cm^{-3}
 - Chemical time: $\sim 10^5$ yr (dark clouds)
 - Star formation: $\sim 10^6$ yr
 - Lifetime cloud: $\sim 10^7$ yr
- People did not expect to find many molecules since chemical reactions are slow
- Surprise:
interstellar clouds contain a very rich chemistry!

History of astrochemistry

- Simple gas-phase molecules in optical
 - CH: Swings & Rosenfeld 1937
 - CN: McKellar 1940
 - CH⁺: Douglas & Herzberg 1941
- First astrochemical models
 - Kramers & Ter Haar 1946, Bates & Spitzer 1951

History of astrochemistry

- Development of radio astronomy
 - H I 21 cm: Ewen & Purcell 1951
 - OH 18 cm: Weinreb et al. 1963
 - NH₃ 1 cm: Cheung, Townes et al. 1968
 - First polyatomic molecule!
 - H₂O 1 cm (22 GHz): Cheung et al. 1969
- Development of UV astronomy
 - 1970: H₂
- Development of millimeter astronomy
 - 1970: CO
- >1970: flood of new molecules

History of astrochemistry

- OVRO 230 GHz spectral line survey Orion

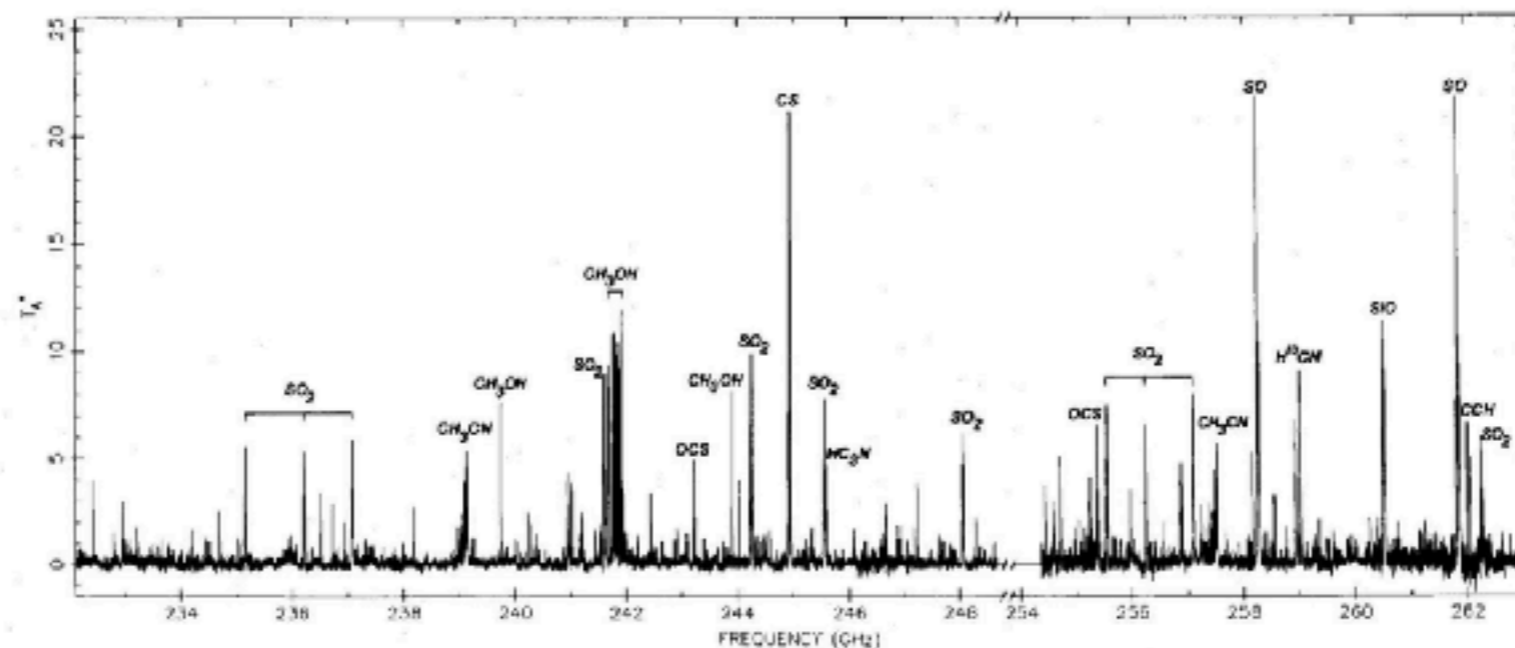
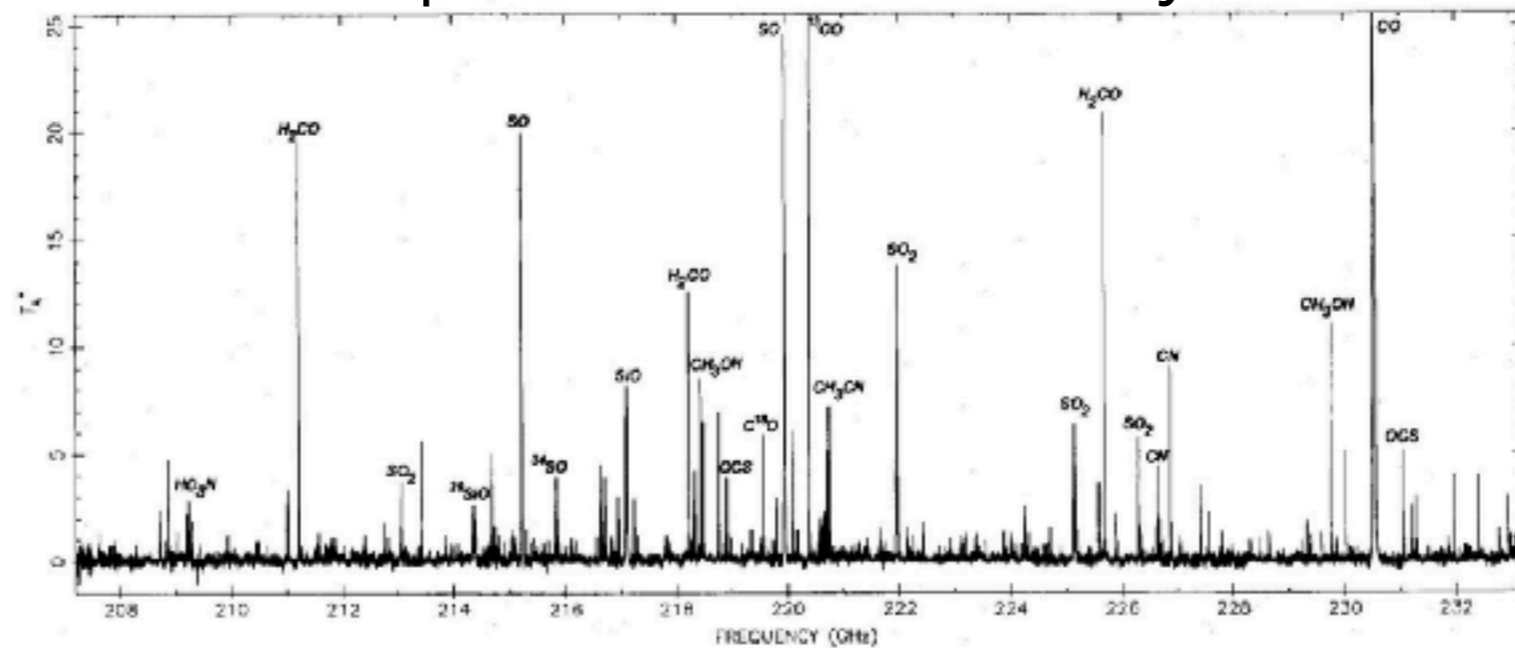


FIG. 1.—Compressed view of the OVRO spectral line survey of OMC-1

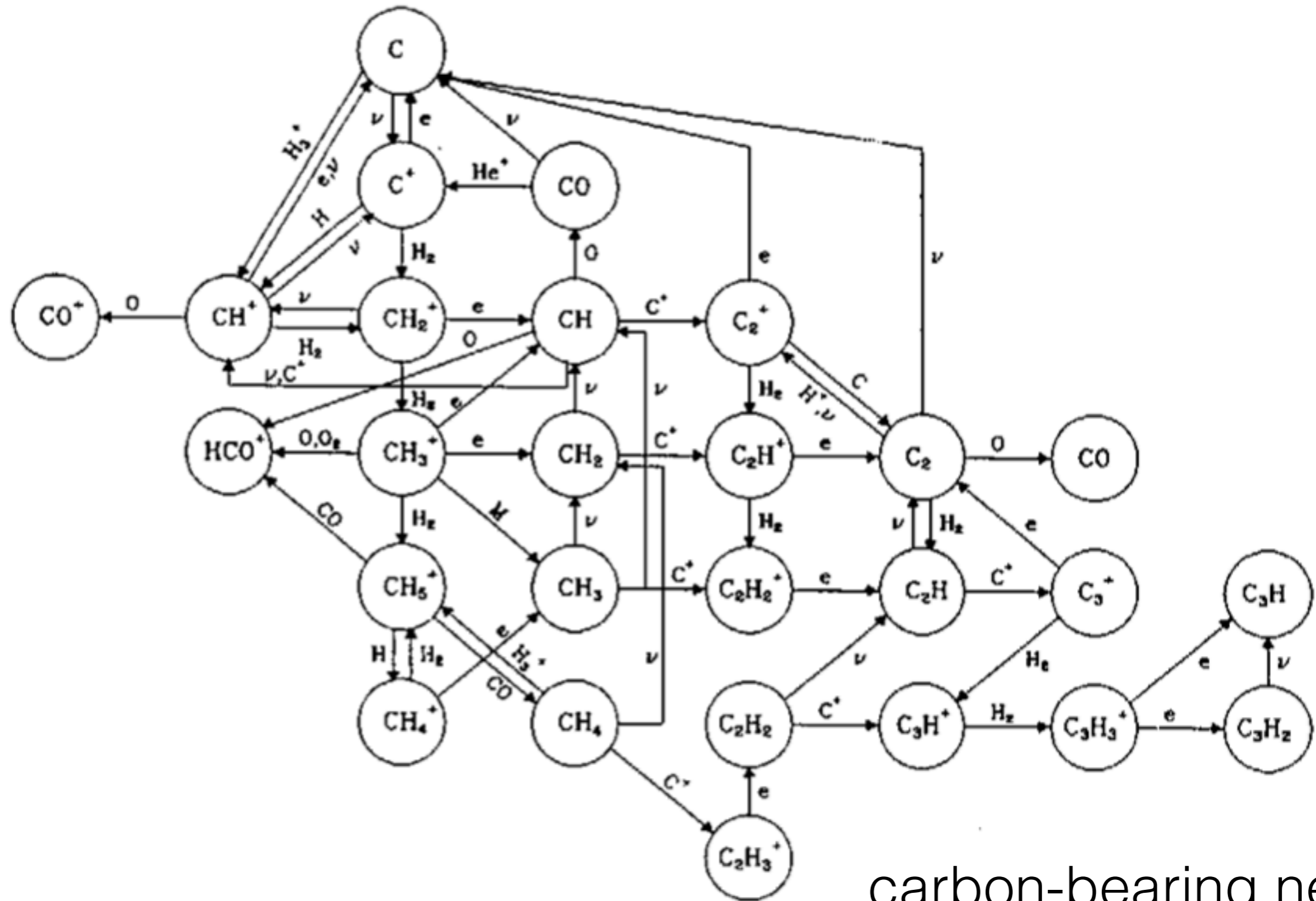
History of astrochemistry

- **Development of IR astronomy**
- 1983: IRAS
 - First full-sky survey at 12, 25, 60 and 100 μm
 - Cirrus clouds and dust properties
- 1995 – 98: Infrared Space Observatory (ISO)
 - First complete 2-200 mm spectra
 - H_2O , OH, [O I] far-IR lines
 - Symmetric molecules: C_6H_6 , CH_3 , C_2H_4 , CO_2 ,...
- 2003-2009: Spitzer Space Telescope
 - Ices and silicates toward low mass protostars and disks
- 2009-2013: Herschel Space Telescope
 - Multi-transition CO
 - Detections of H_2O and HD and various other molecules
- 2022-... : JWST!

Chemical reactions

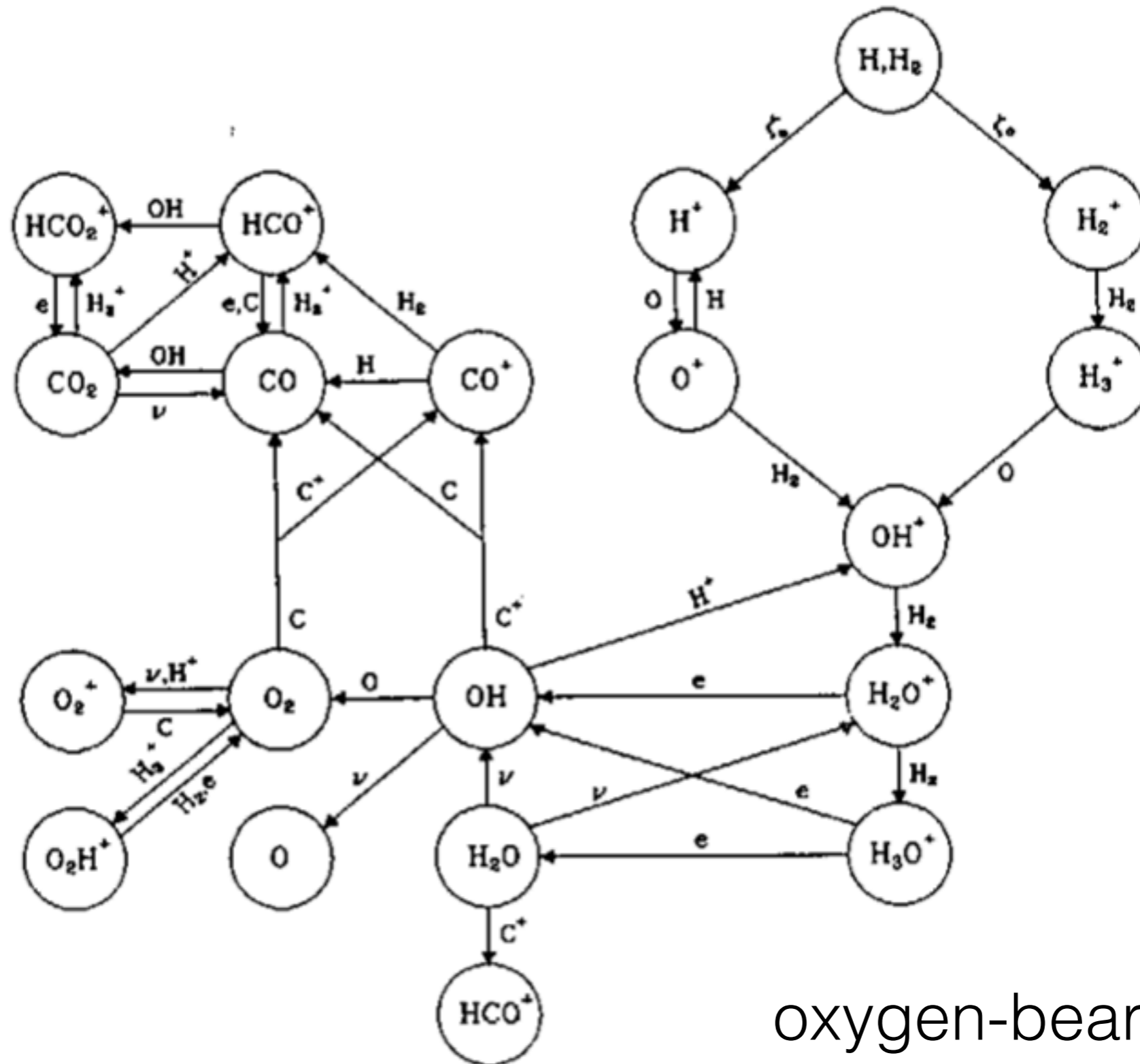
- Because of low densities and temperatures, chemistry is controlled by two-body reactions:
=> abundances depend on physical conditions (temperature, density, radiation field, history)
- Three-body reactions not important until $n \sim 10^{12} \text{ cm}^{-3}$
- Reaction rate (often T-dependent):
 $k n(x) n(y) \text{ cm}^{-3} \text{ s}^{-1}$

Chemical reactions



carbon-bearing network

Chemical reactions

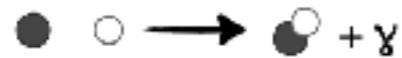


Types of reactions

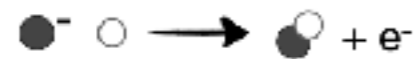
Gas-phase chemistry

Bond formation

Radiative association



Associative detachment



Bond destruction

Photo-dissociation



Dissociative recombination



Bond rearrangement

Ion-molecule, neutral-neutral or charge transfer



- Formation of bonds
 - Radiative association $X^+ + Y \Rightarrow XY + h\nu$
 - Associative detachment $X^- + Y \Rightarrow XY + e$
 - (Grain surface) $X + Y:g \Rightarrow XY + g$
- Destruction of bonds
 - Photodissociation $XY + h\nu \Rightarrow X + Y$
 - Dissociative recombination $XY^+ + e \Rightarrow X + Y$
 - (Collisional dissociation) $XY + M \Rightarrow X + Y + M$
- Rearrangement of bonds
 - Ion-molecule reactions $X^+ + YZ \Rightarrow XY^+ + Z$
 - Charge-transfer reactions $X^+ + YZ \Rightarrow X + YZ^+$
 - Neutral-neutral reactions $X + YZ \Rightarrow XY + Z$

Line excitation

Local Thermodynamic Equilibrium (LTE): collisions lead to excitation and spontaneous emission photon: Boltzmann distribution

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp(-h\nu / kT_{ex})$$

$$= \frac{g_u}{g_l} \exp(-(E_u - E_l) / kT_{ex})$$

g = degeneracy of energy level

Example ^{12}CO :

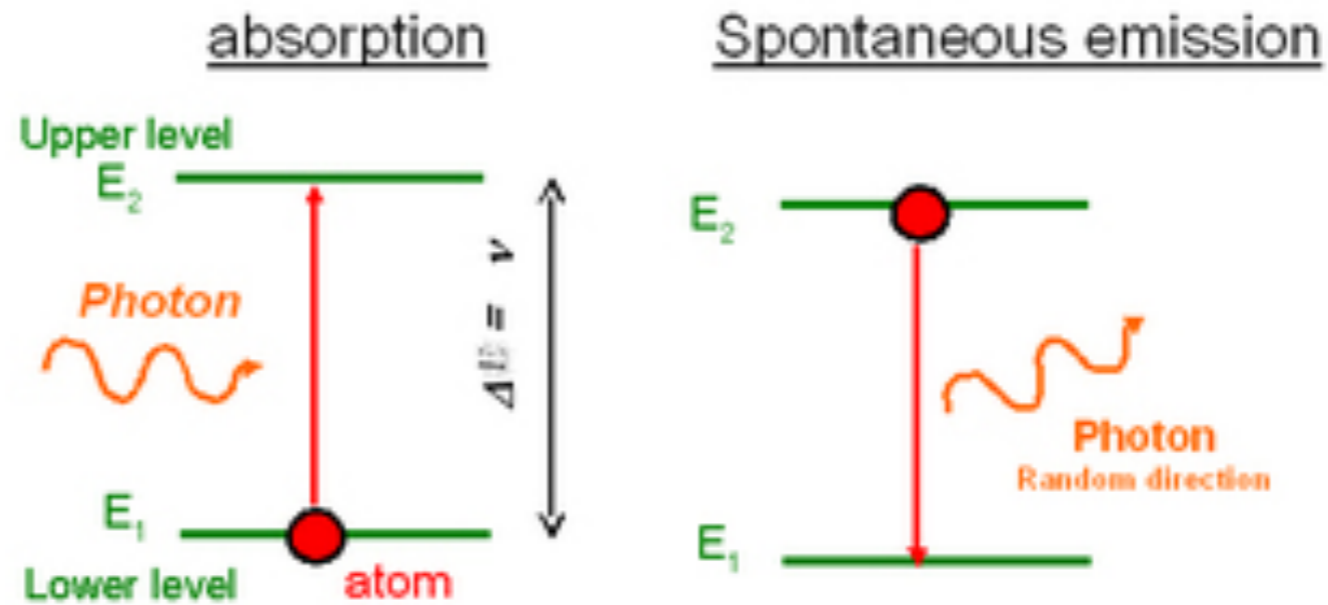
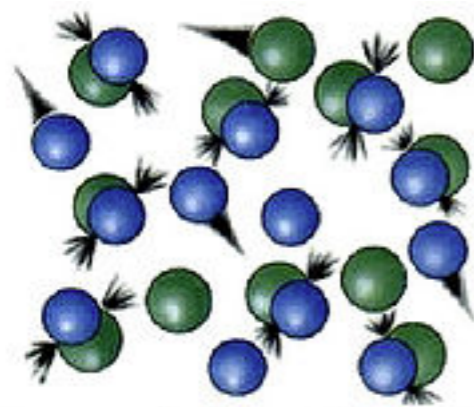
J=1-0: 115.271 GHz, $E_u=5.5$ K

J=2-1: 230.538 GHz, $E_u=17$ K

J=3-2: 345.596 GHz, $E_u=33$ K

..

J=6-5: 691.473 GHz, $E_u=116$ K



Find transitions + frequencies:
<http://www.splatalogue.net>

Line excitation

Local Thermodynamic Equilibrium (LTE): collisions lead to excitation and spontaneous emission photon: Boltzmann distribution

1. Calculate N_u , the column density of the upper energy population level of a molecular transition, using the integrated line flux

$$N_u^{\text{thin}} = \frac{4\pi S_\nu \Delta\nu}{A_{ul} \Omega hc}$$

Flux linewidth
Emitting area

The rate of spontaneous emission is set by the Einstein coefficient A_{ul} (property of transition)

2. Calculate N_T , the total column density of a molecule using the energy level E_u , the partition function $Q(T)$ (summing over all N_u/N_l combinations) and an assumed temperature T_{rot}

$$\frac{N_u}{g_u} = \frac{N_T}{Q(T_{\text{rot}})} e^{-E_u/kT_{\text{rot}}}$$

$Q(T)$ is a property of the molecule

Find E_u , A_{ul} , $Q(T_{\text{rot}})$ for each molecular transition on <http://www.splatalogue.net>

Line excitation

If you have multiple transitions of a slab of material, you can calculate a combination of N_T and T_{rot} using a linear fitting procedure, assuming LTE, opt. thin emission and all emission coming from the same region and temperature: a rotational diagram

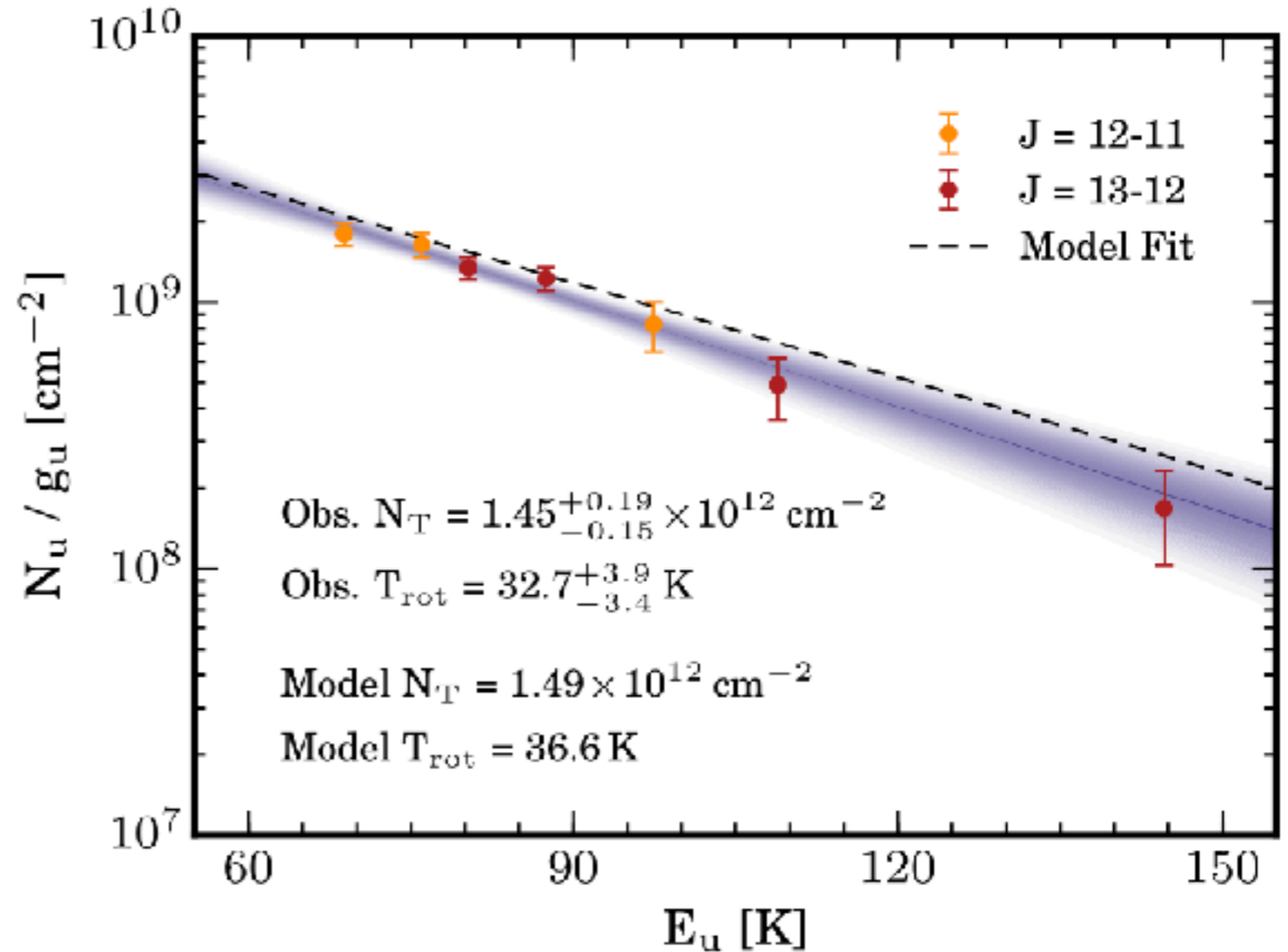
$$\frac{N_u}{g_u} = \frac{N_T}{Q(T_{\text{rot}})} e^{-E_u/kT_{\text{rot}}}$$

Take logarithm:

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N}{Q(T)}\right) - \frac{E_u}{kT} = -\frac{1}{T} \frac{E_u[\text{erg}]}{k} + \ln\left(\frac{N}{Q(T)}\right)$$

From obs. line flux

$$\underbrace{\ln\left(\frac{N_u}{g_u}\right)}_y = \underbrace{-\frac{1}{T}}_a \underbrace{E_u[\text{K}]}_x + \underbrace{\ln\left(\frac{N}{Q(T)}\right)}_b$$



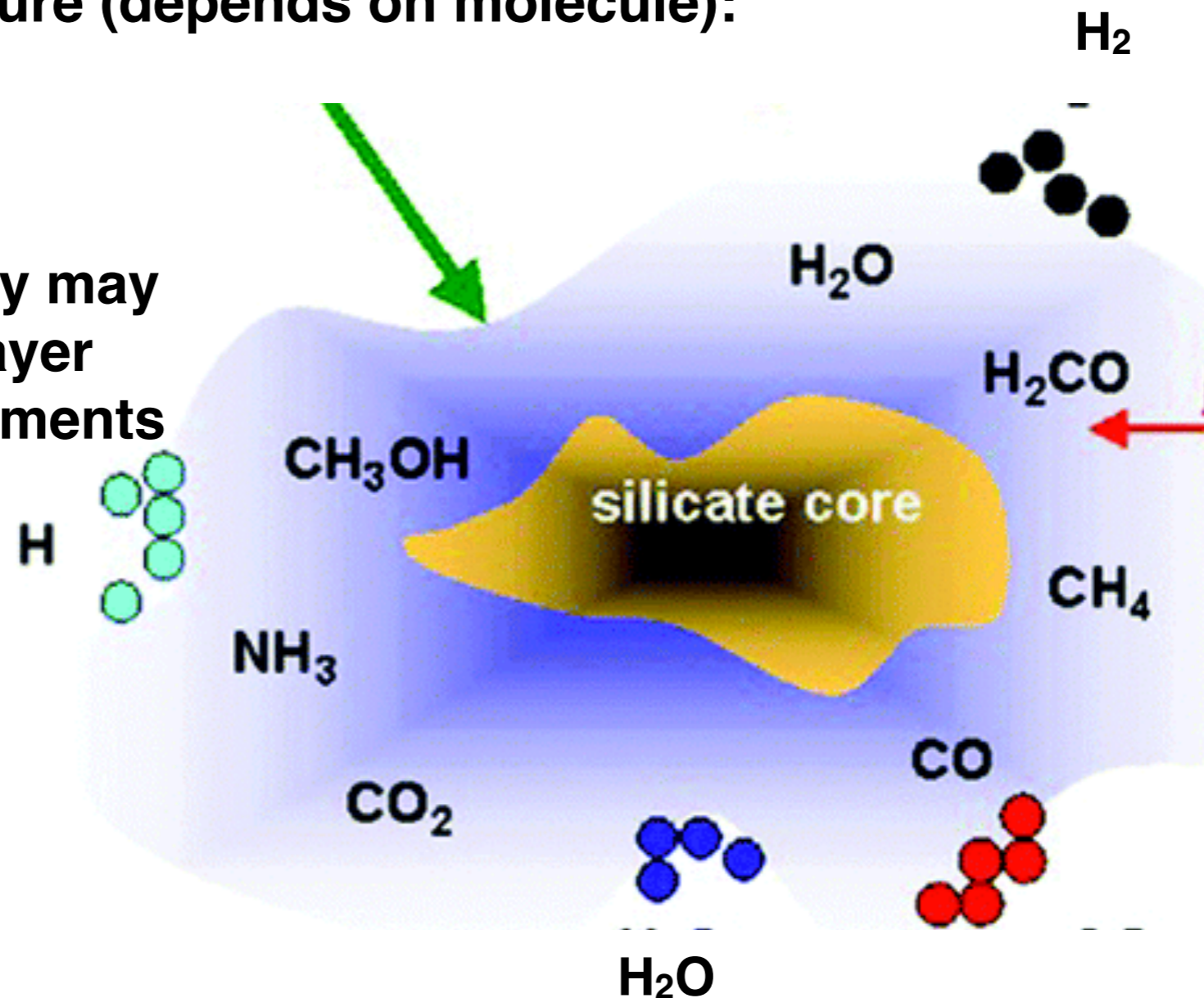
So in the end you just do a linear fit and a and b give you column density N and temperature T

Ice chemistry

Molecules can freeze out onto dust grains when temperature is below freeze-out temperature (depends on molecule):

=> ice layer

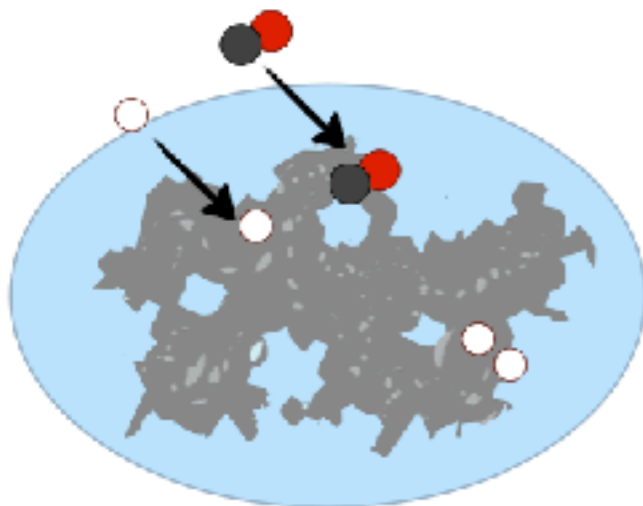
Additional chemistry may happen inside ice layer through H bombardments and radiation fields



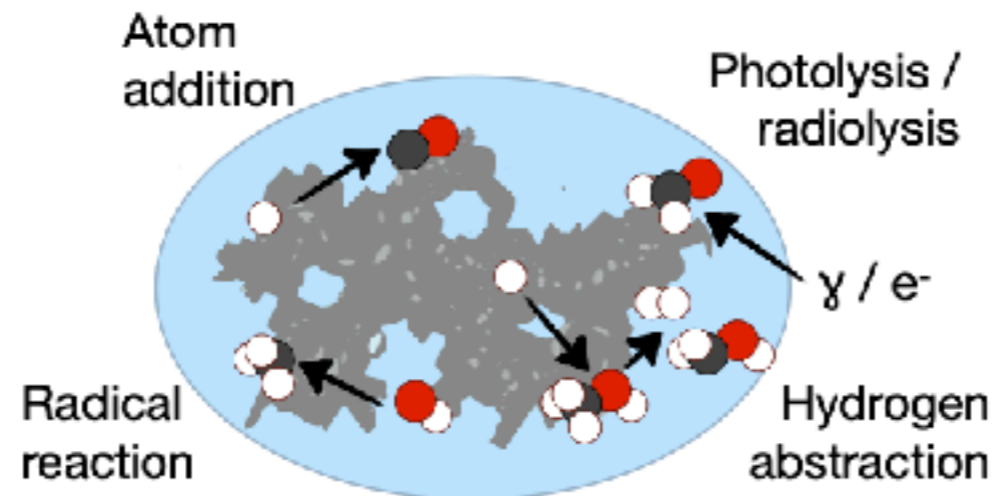
Ice chemistry

Grain-surface and ice processes

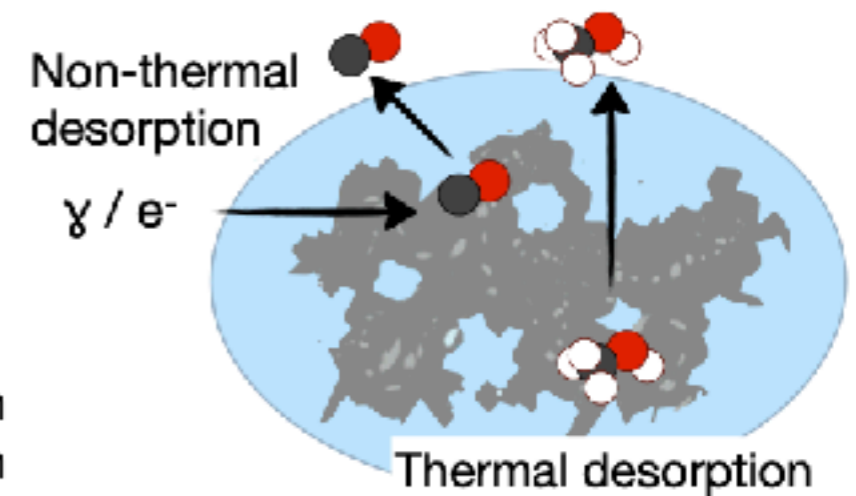
Freeze-out / adsorption



Grain surface and ice chemistry



Ice sublimation / desorption



Many possible chemical reactions, followed by ice sublimation

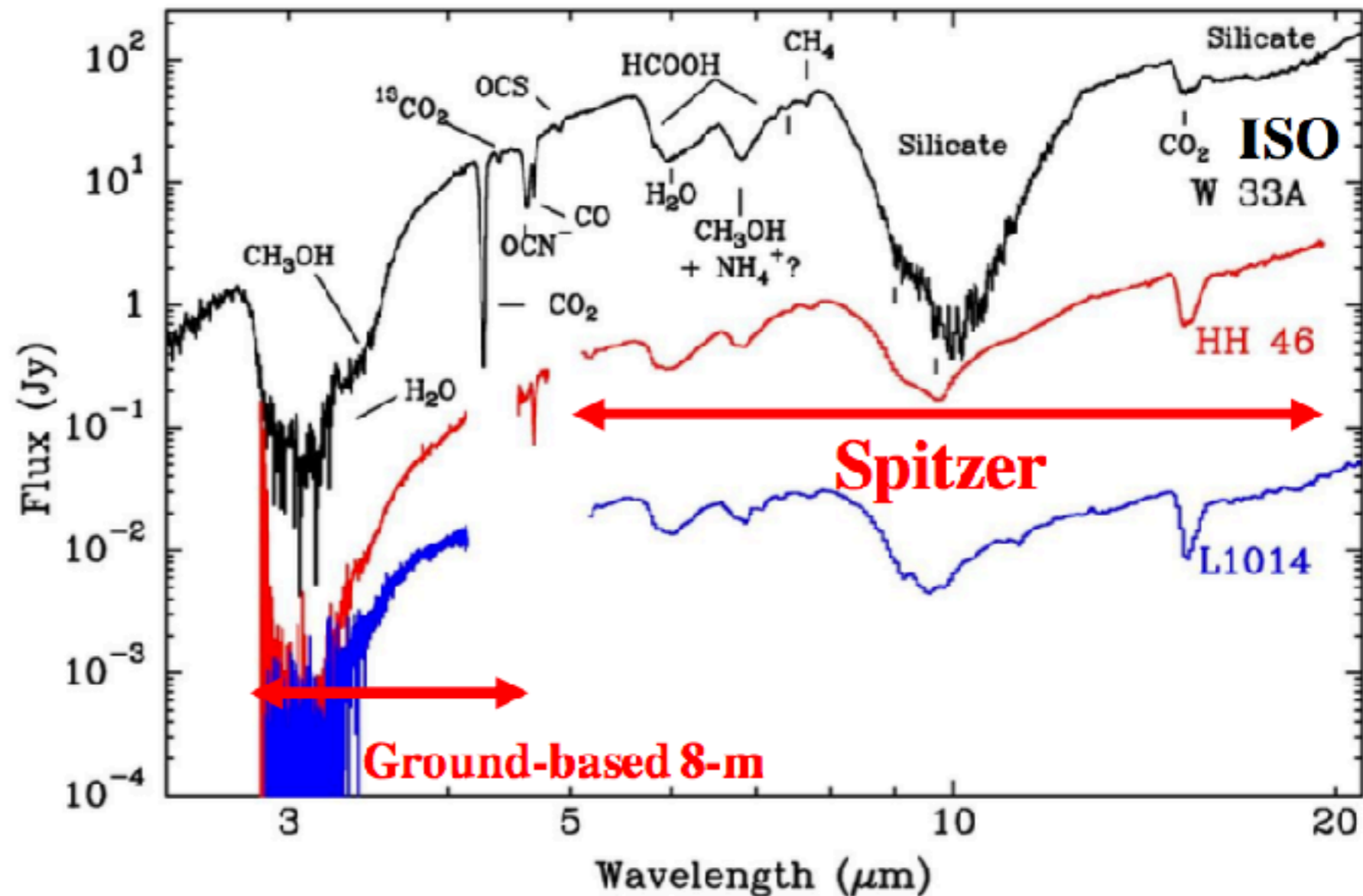
=> more chemical complexity!

Evidence for ice chemistry

Infrared: ice absorption spectra!

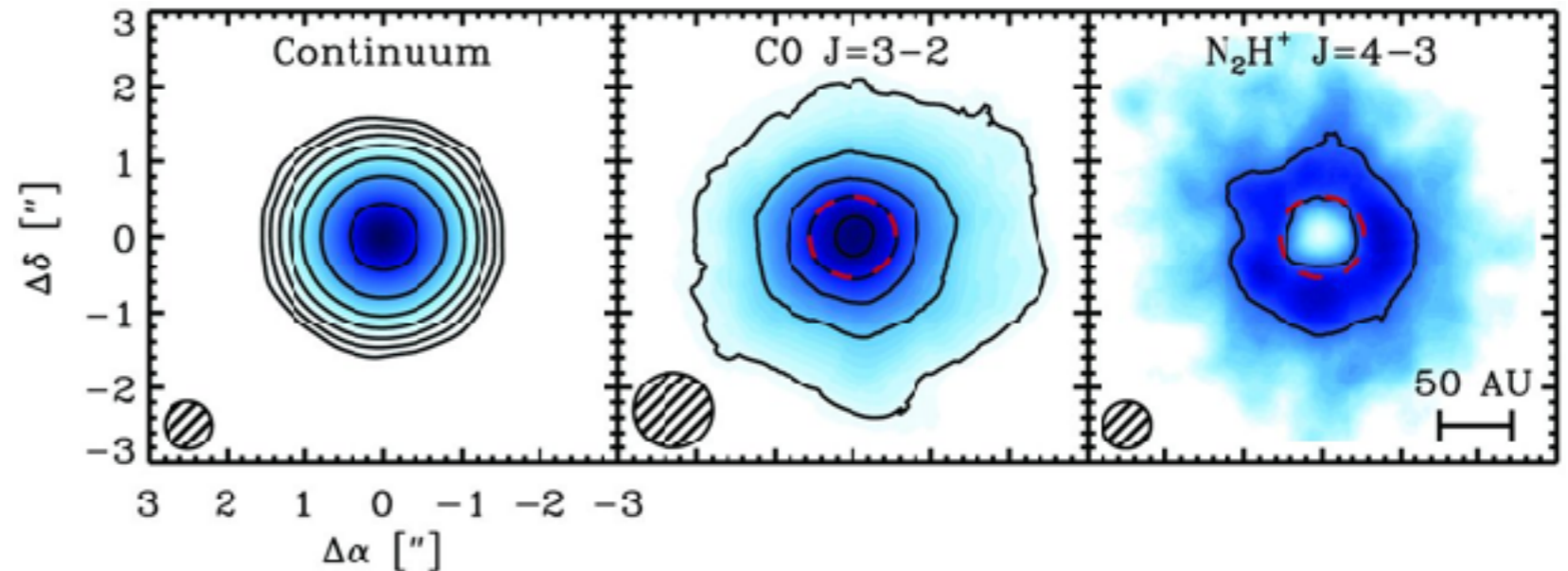
Taking these spectra require a bright background source and can only be done from space:

Spitzer and ISO did some of the brightest disks, but JWST will take many more ice spectra



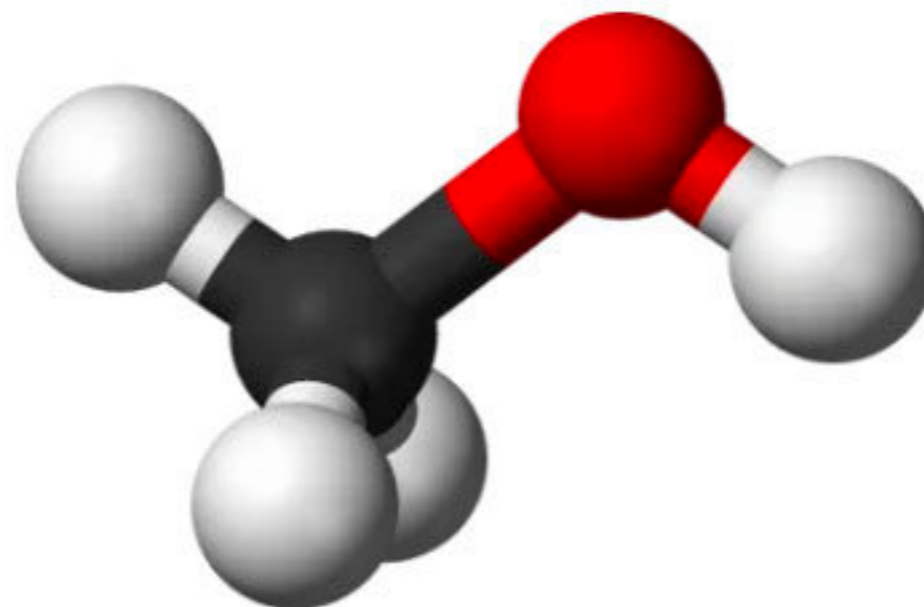
Evidence for ice chemistry

Anti-correlation between N_2H^+ and CO: evidence CO snowline



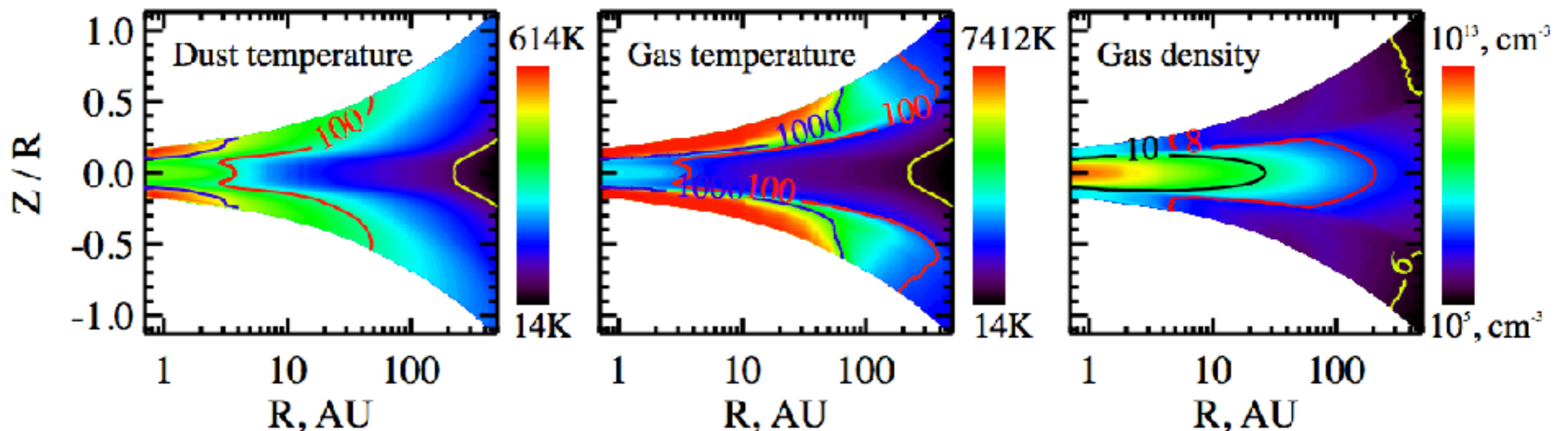
High abundances of complex organic molecules, like methanol:

=> can only form efficiently in the ice (followed by sublimation), no efficient formation in the gas-phase



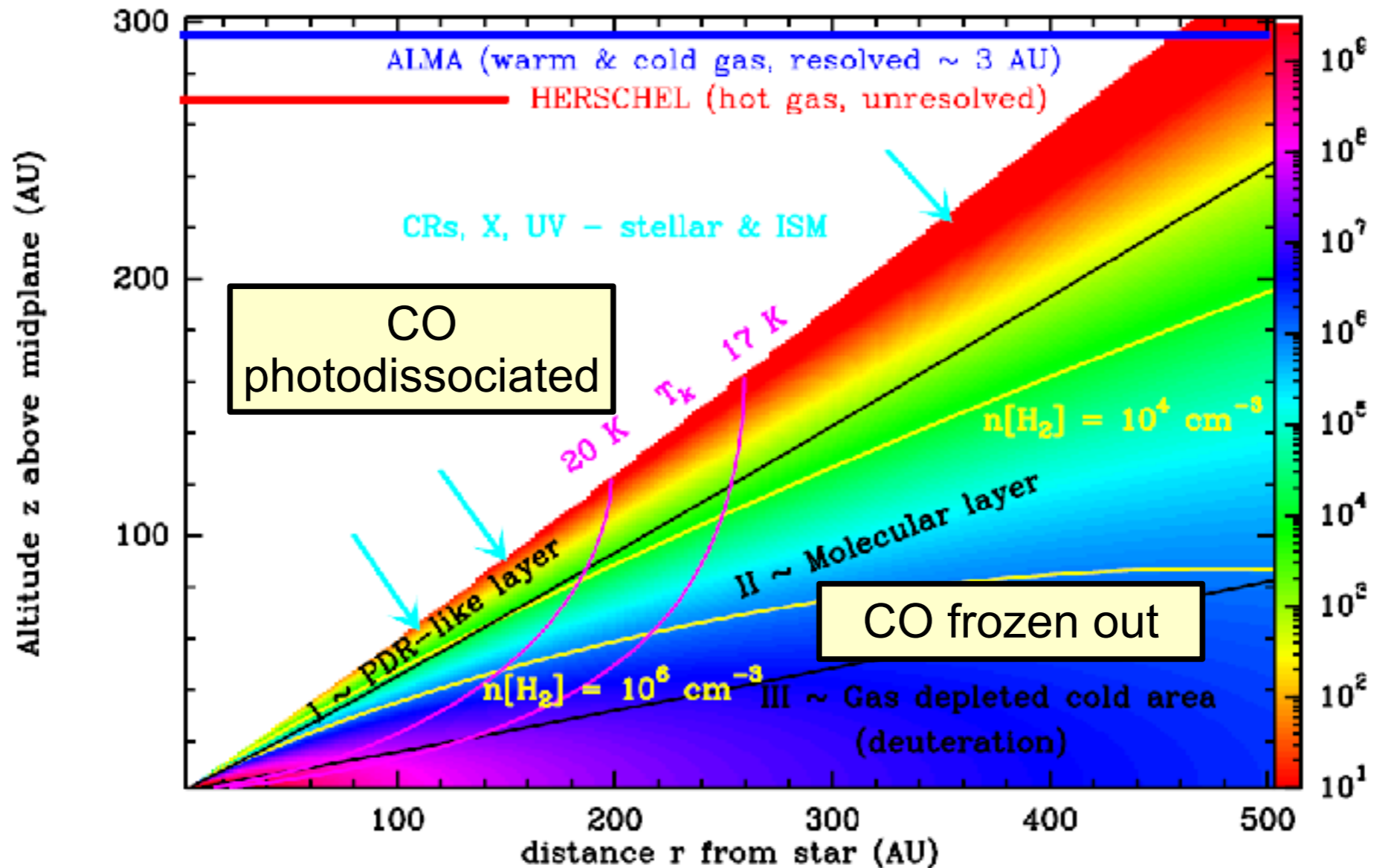
Disk chemistry

- Chemistry in the disk
 - large gradients in temperature, density and UV radiation field which all influence the local chemistry
 - chemical networks include thousands of reactions even for simple molecules
 - line emission relatively weak

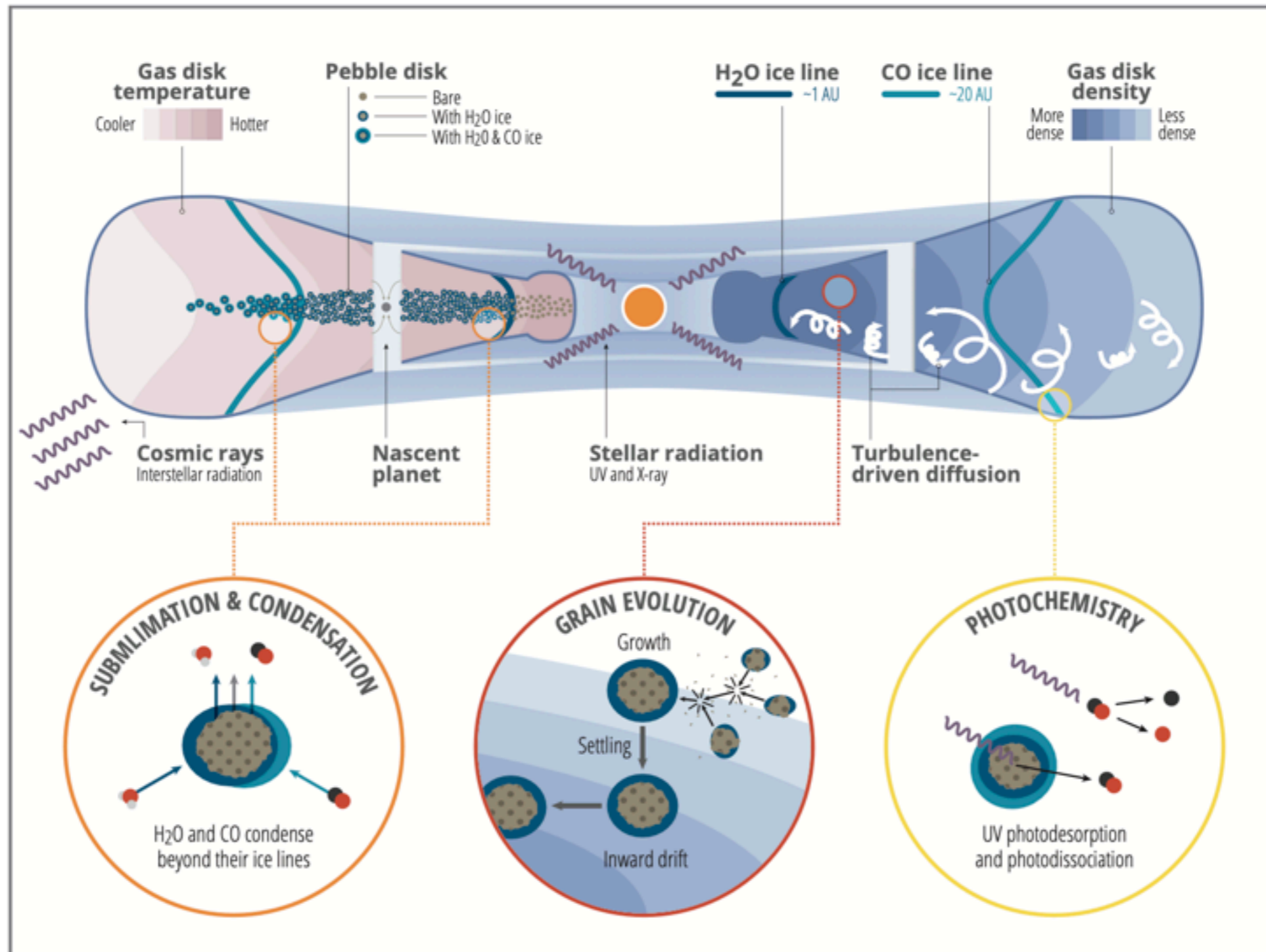


Disk chemistry

Example: CO molecular abundance



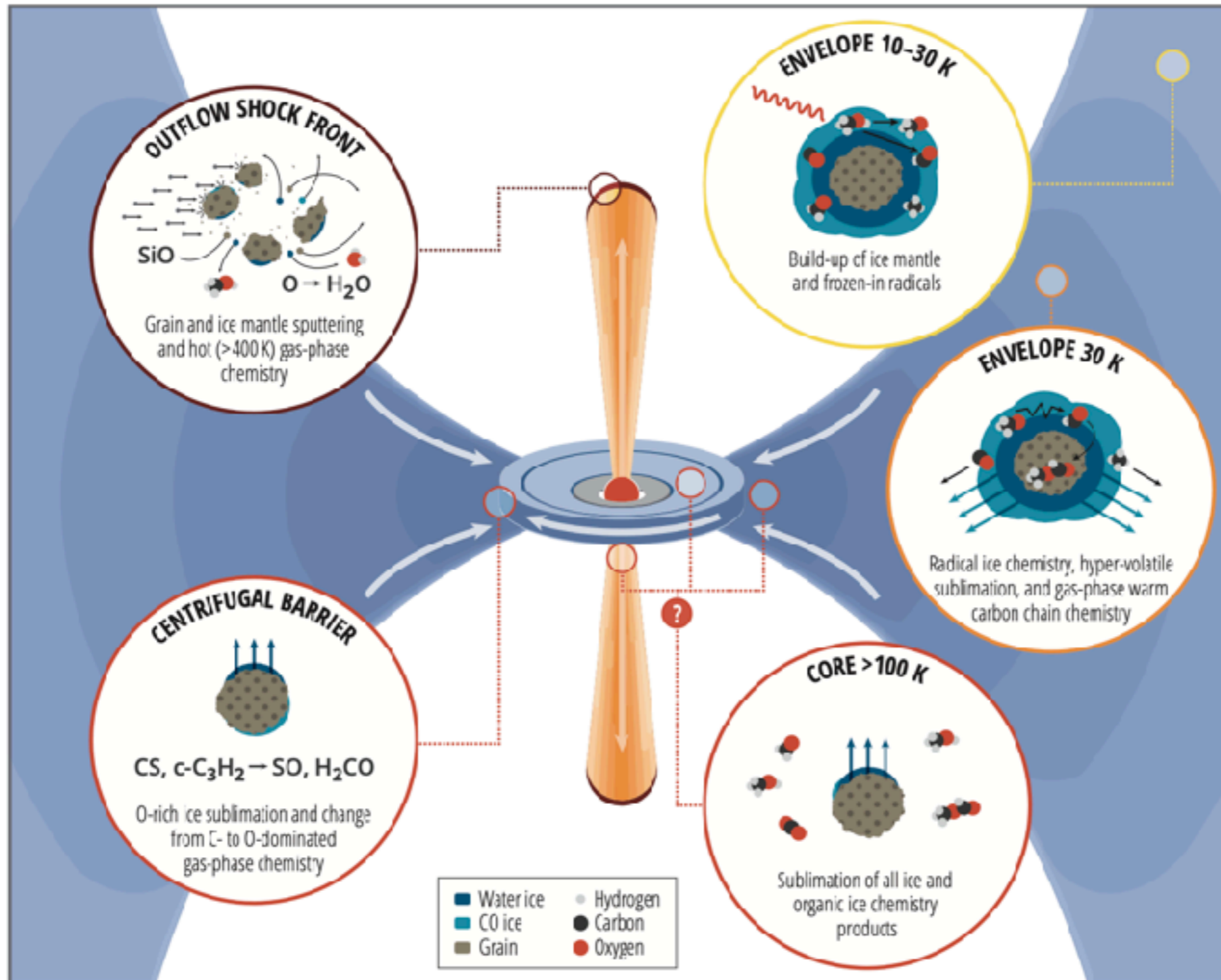
Disk chemistry



Studying chemistry in disks is a complex problem due to the number of physical processes and conditions in the disk

Disk chemistry

Does the cloud chemical composition reflect the disk composition? Or is there a 'reset'?



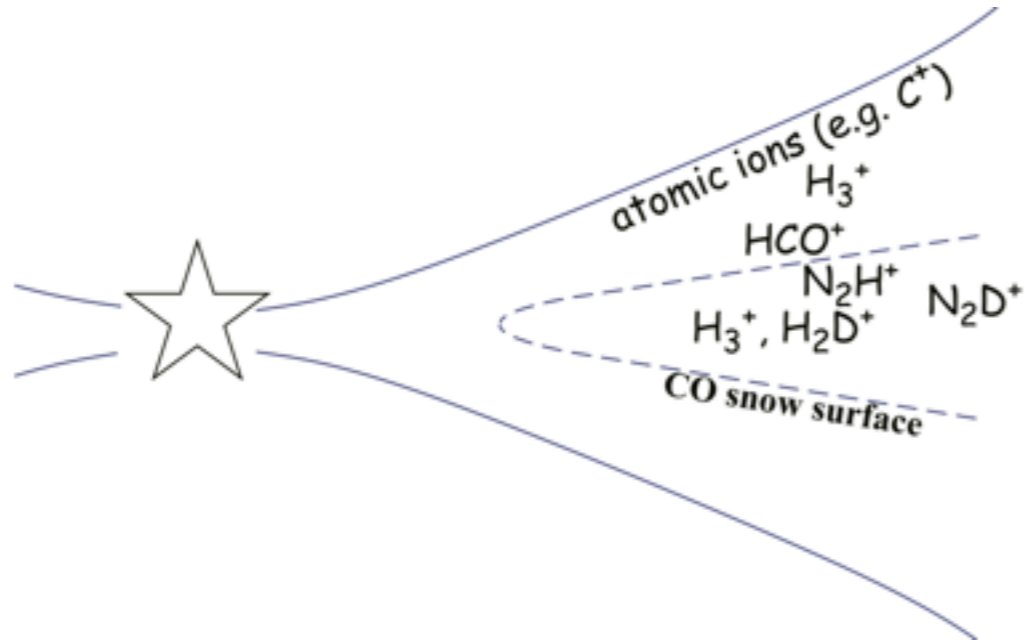
Disk chemistry: detected molecules to date

Table 6

List of Molecules, Including Rare Isotopic Species, Detected in Protoplanetary Disks, with References to Representative Detections

2 Atoms		3 Atoms		4 Atoms		5 Atoms		6 Atoms	
Species	Ref.	Species	Ref.	Species	Ref.	Species	Ref.	Species	Ref.
CN	1, 2	H ₂ O	3, 4, 5	NH ₃	6	HC ₃ N	7	CH ₃ OH	8
C ¹⁵ N	9	HCO ⁺	1, 2	H ₂ CO	2	HCOOH	10	CH ₃ CN	11
CH ⁺	12	DCO ⁺	13	H ₂ CS	14, 15	c-C ₃ H ₂	16		
OH	17, 5	H ¹³ CO ⁺	18, 13	C ₂ H ₂	19	CH ₄	20		
CO	21	HCN	1, 2						
¹³ CO	22	DCN	23						
C ¹⁸ O	24	H ¹³ CN	25						
C ¹⁷ O	26, 27	H ¹⁵ CN	25						
¹³ C ¹⁸ O	39								
¹³ C ¹⁷ O	40								
H ₂	28	HNC	2						
HD	29	DNC	14						
CS	30, 31, 32	H ₂ S	33						
C ³⁴ S	14, 15	N ₂ H ⁺	34, 35						
¹³ CS	14, 15	N ₂ D ⁺	36						
SO	37	C ₂ H	2						
		C ₂ D	14						
		CO ₂	38						

Disk ionisation: HCO⁺

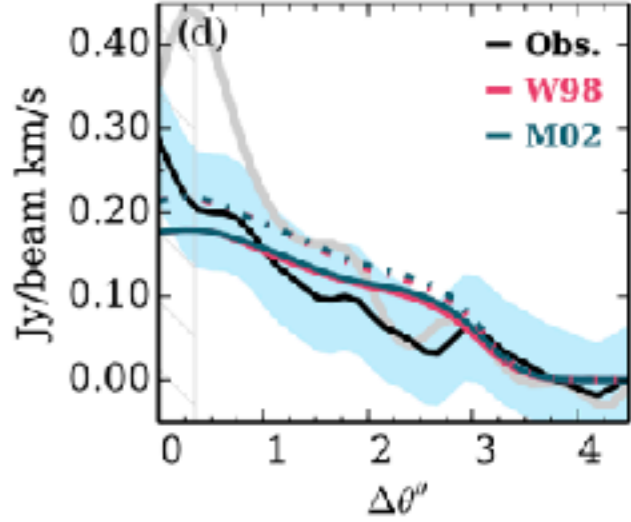
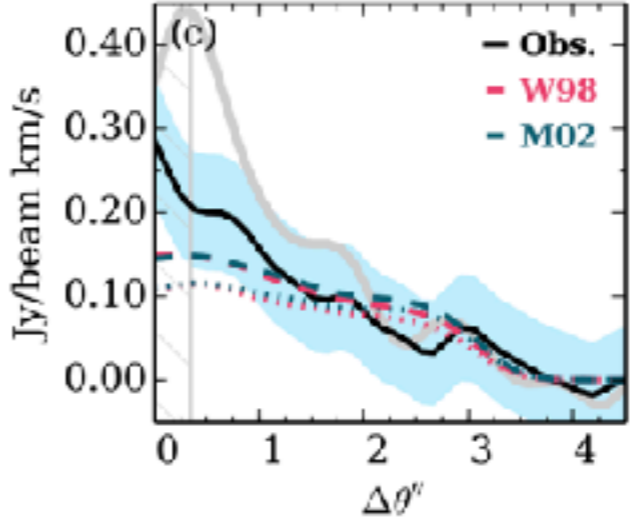
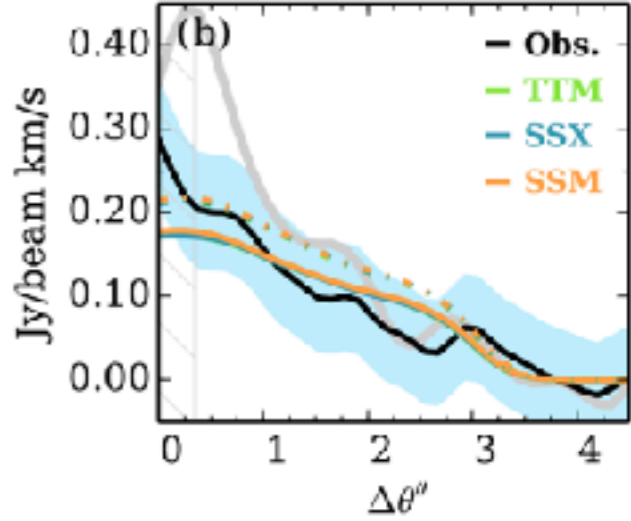
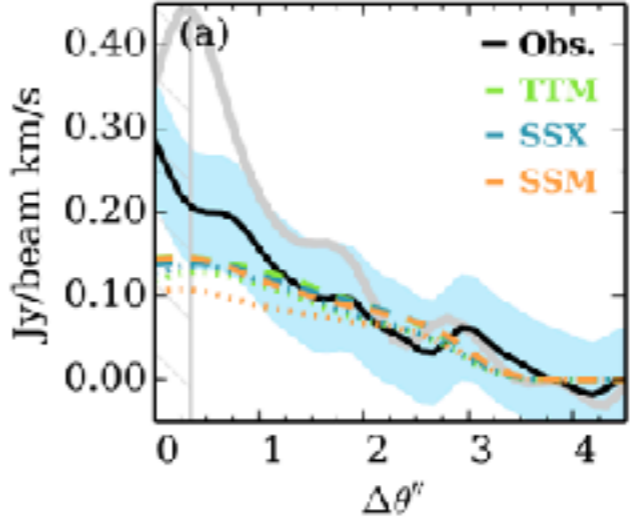


Low Cosmic Rays

High Cosmic Rays

Low X-rays

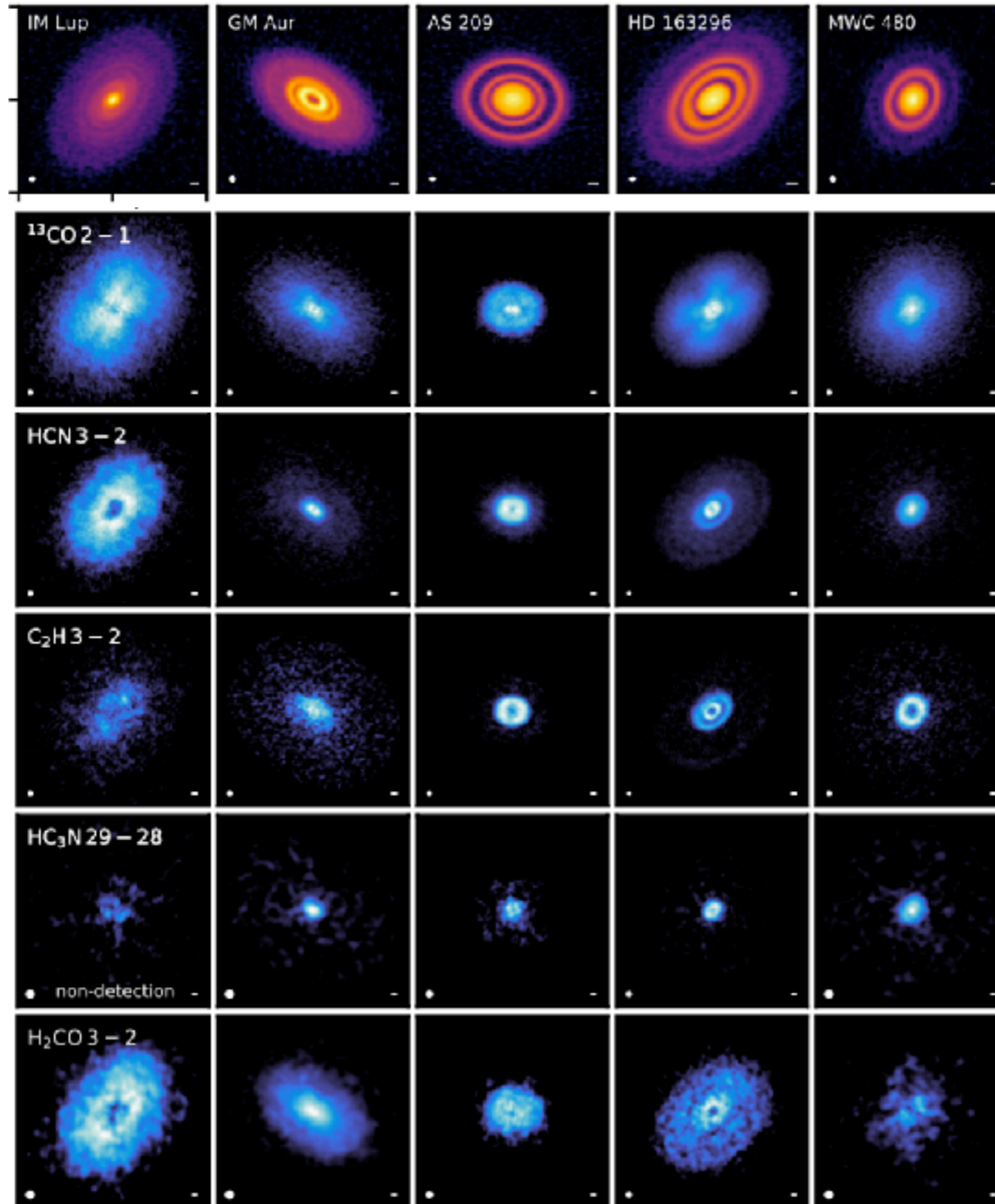
High X-rays



HCO⁺ is a good tracer of ionisation of the disk, and is sensitive to both cosmic rays and X-rays from the star, which are usually not constrained:

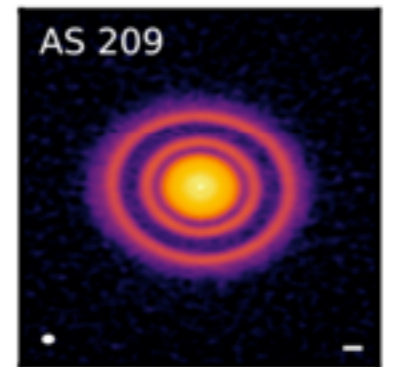
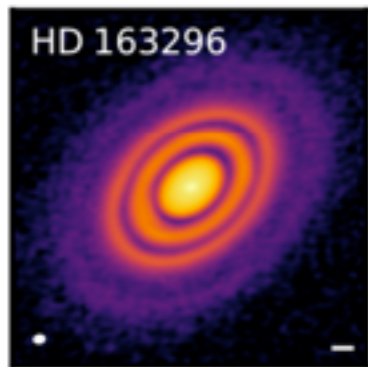
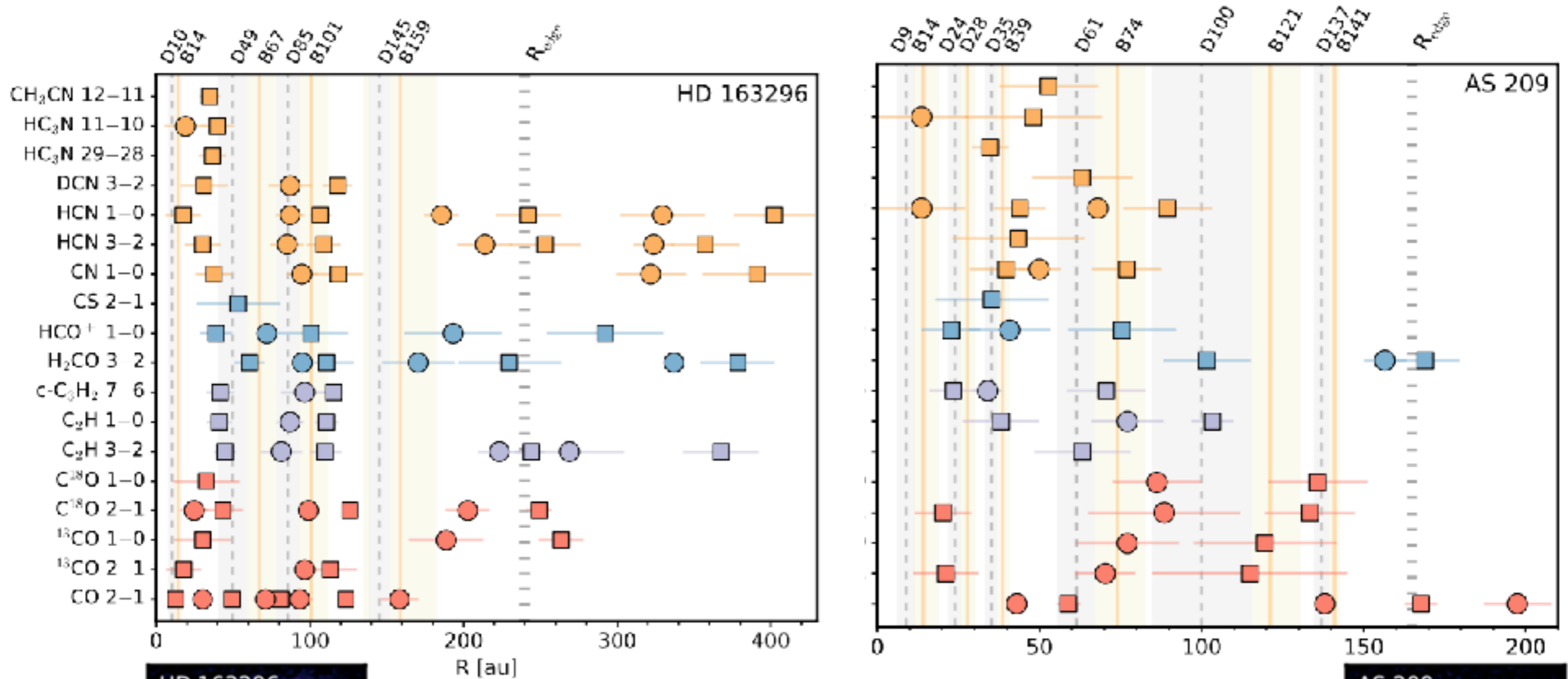
Use the strength of HCO⁺ emission to determine cosmic ray and X-ray rates

Disk chemistry survey: MAPS



**Large diversity in
gaps in various
molecules**

MAPS: molecular gaps?

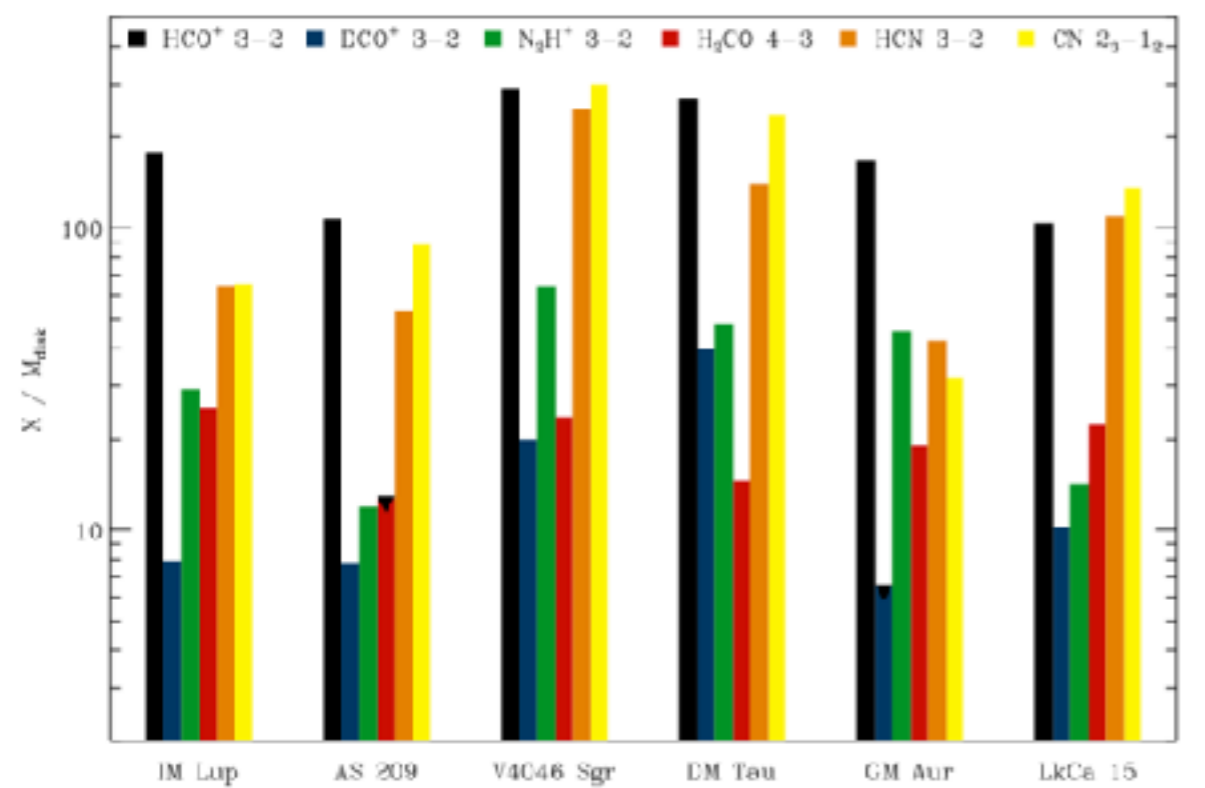


Some gaps in molecules overlap with dust, others do not, there are no clear trends: no link and multiple mechanisms must be responsible for emission

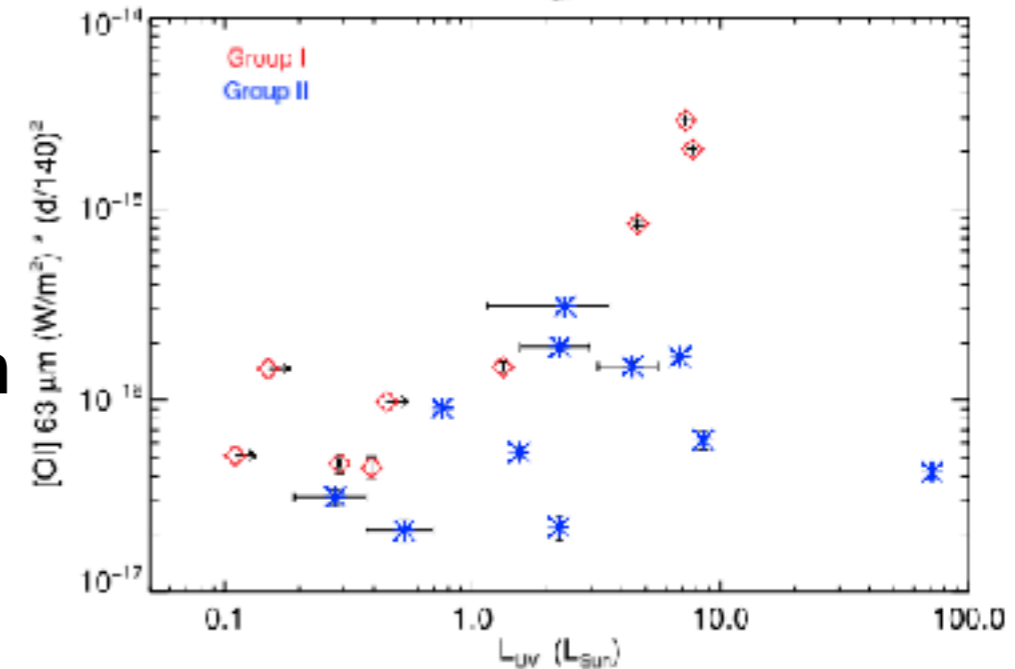
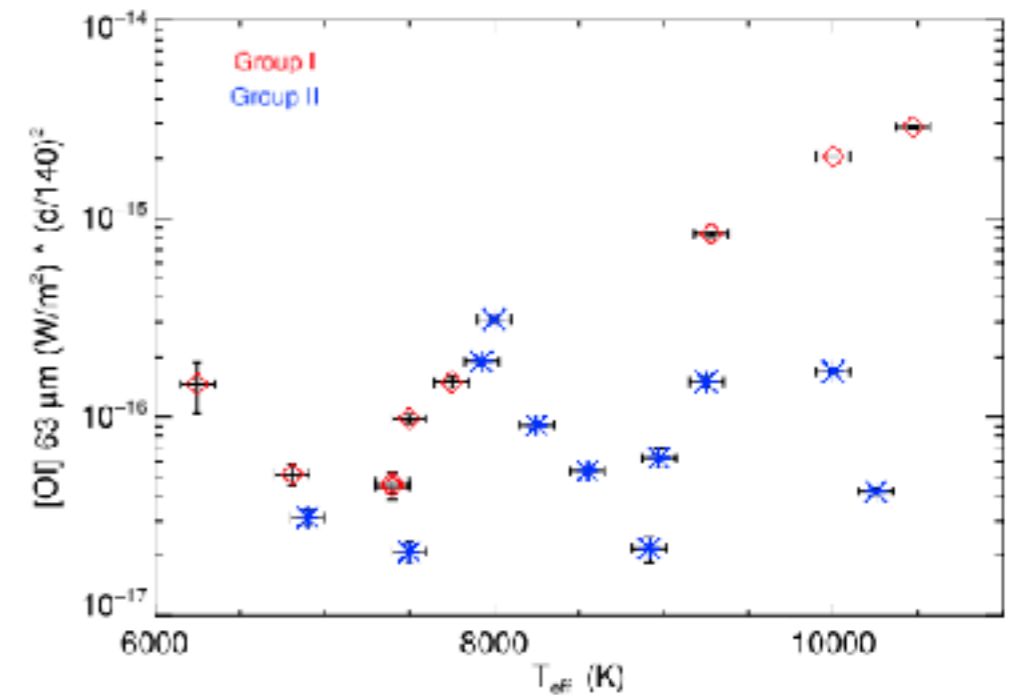
Often no clear origin for molecular emission

Solution: look for trends (or lack thereof) of larger samples

Disk integrated fluxes (pre-ALMA...)



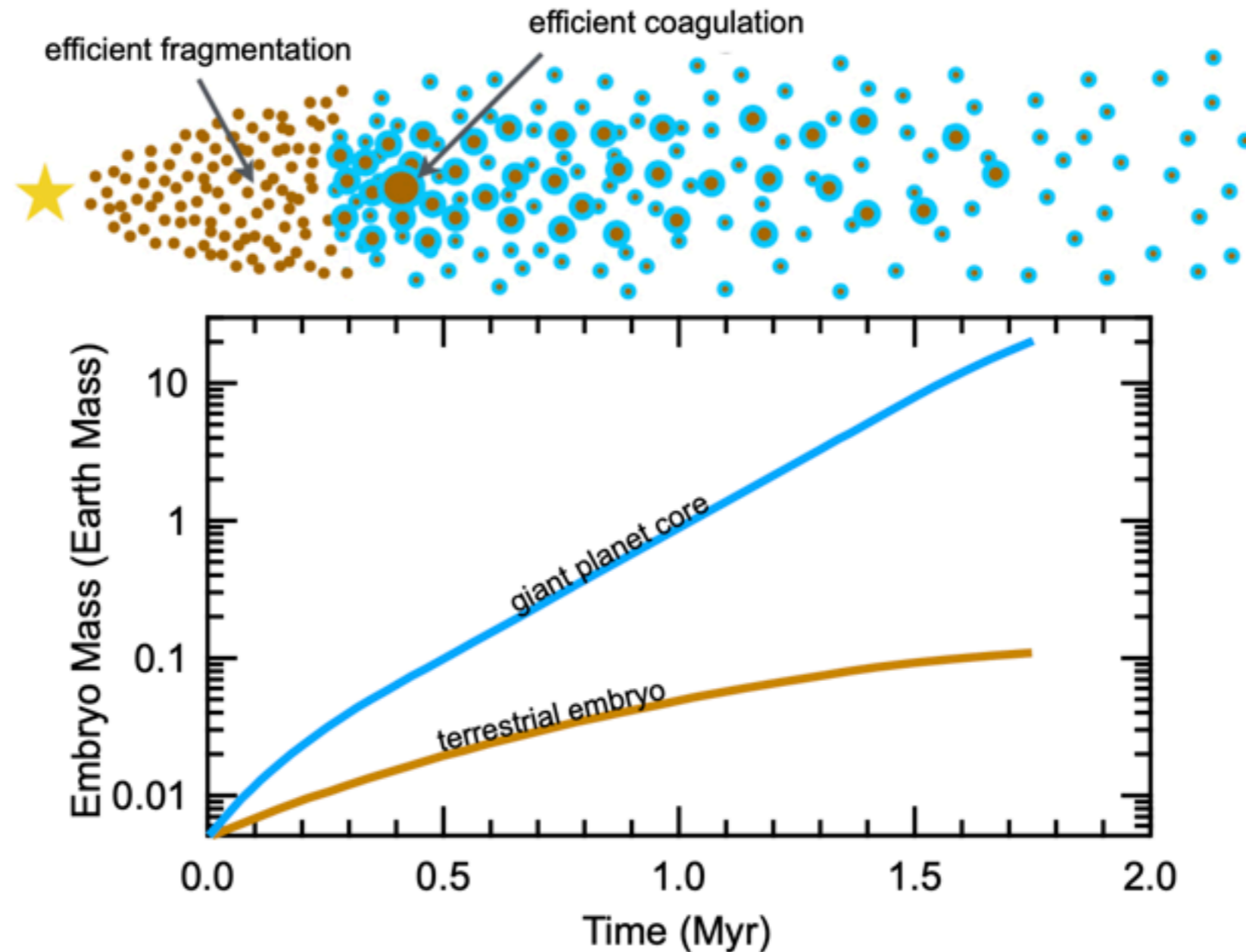
Look for correlations with disk/stellar properties



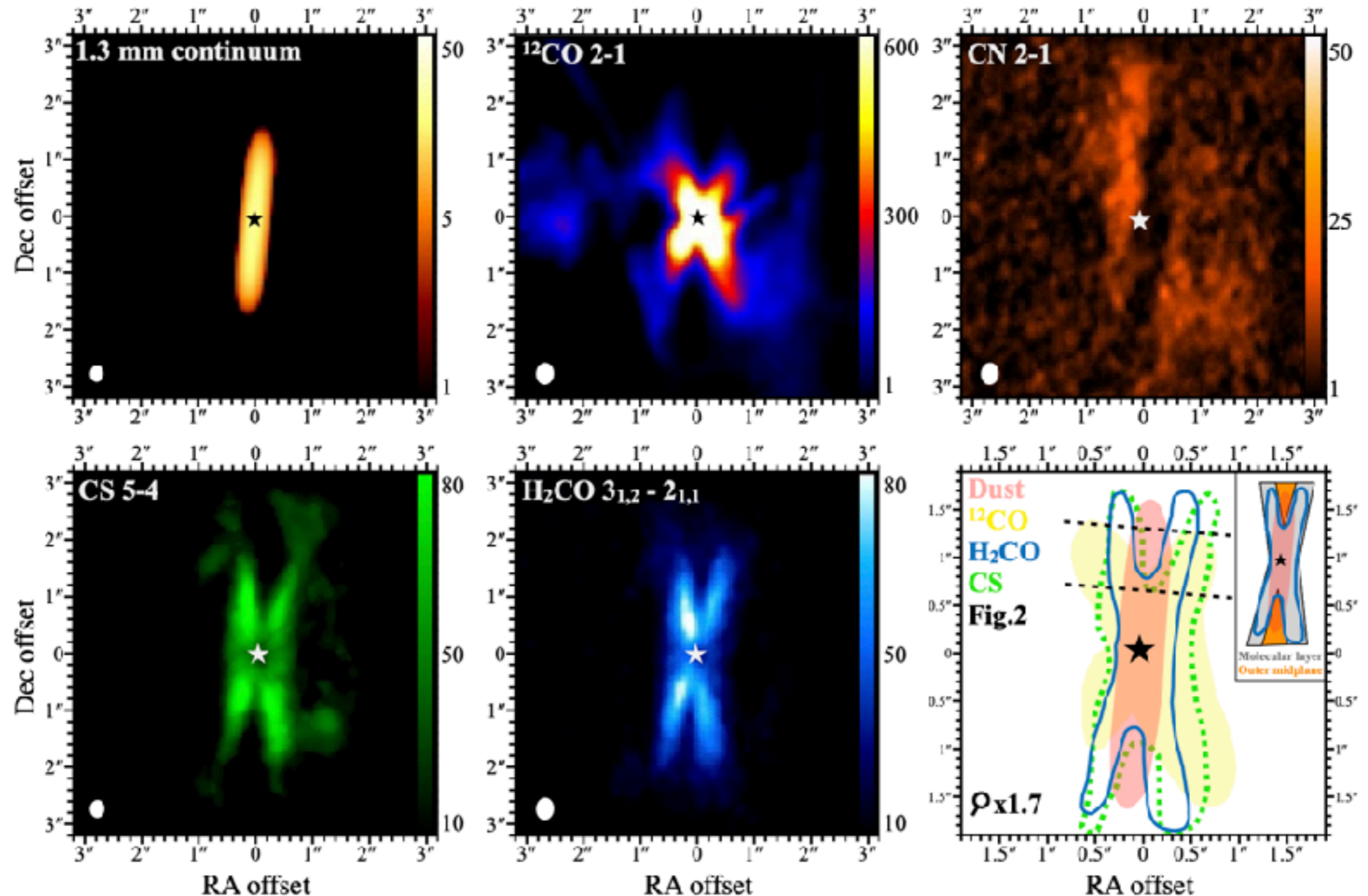
Oberg et al. 2011
 Carr & Najita 2011
 Salyk et al. 2011
 Meeus et al. 2012

Disk chemistry: ices

Snowlines in a disk have been proposed to be key locations for planet formation due to the stickiness of dust grains

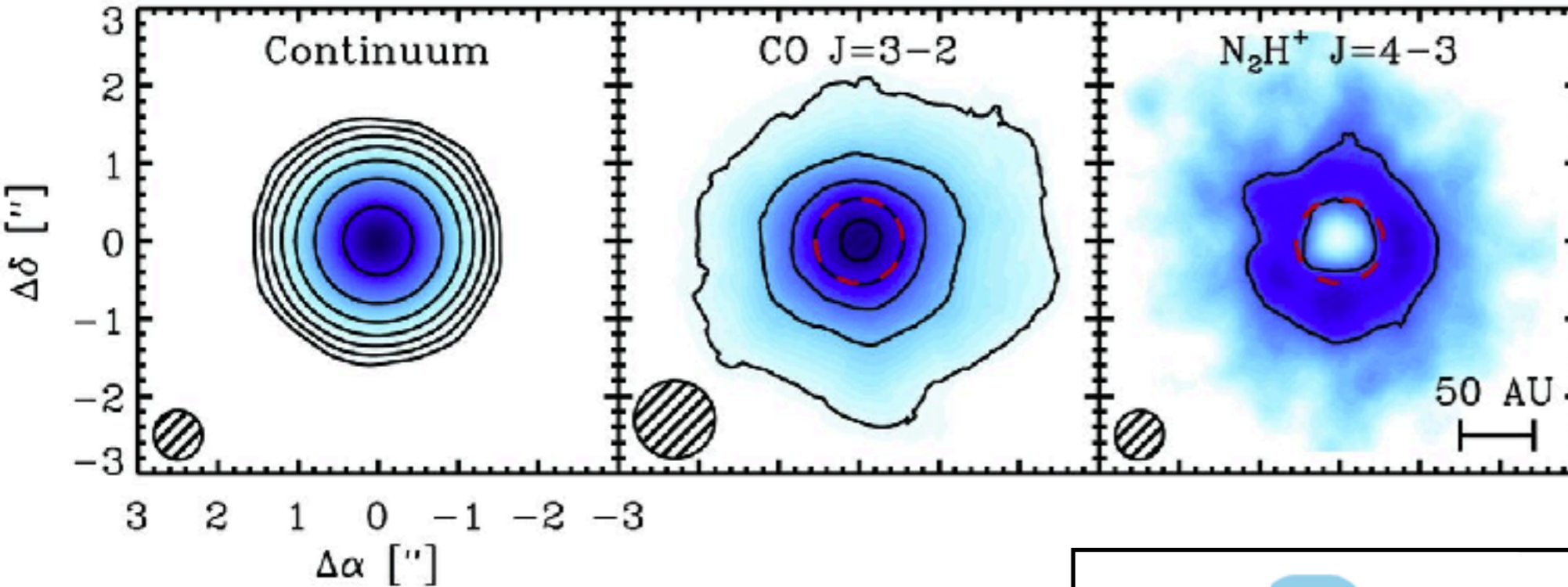


Disk chemistry: vertical structure

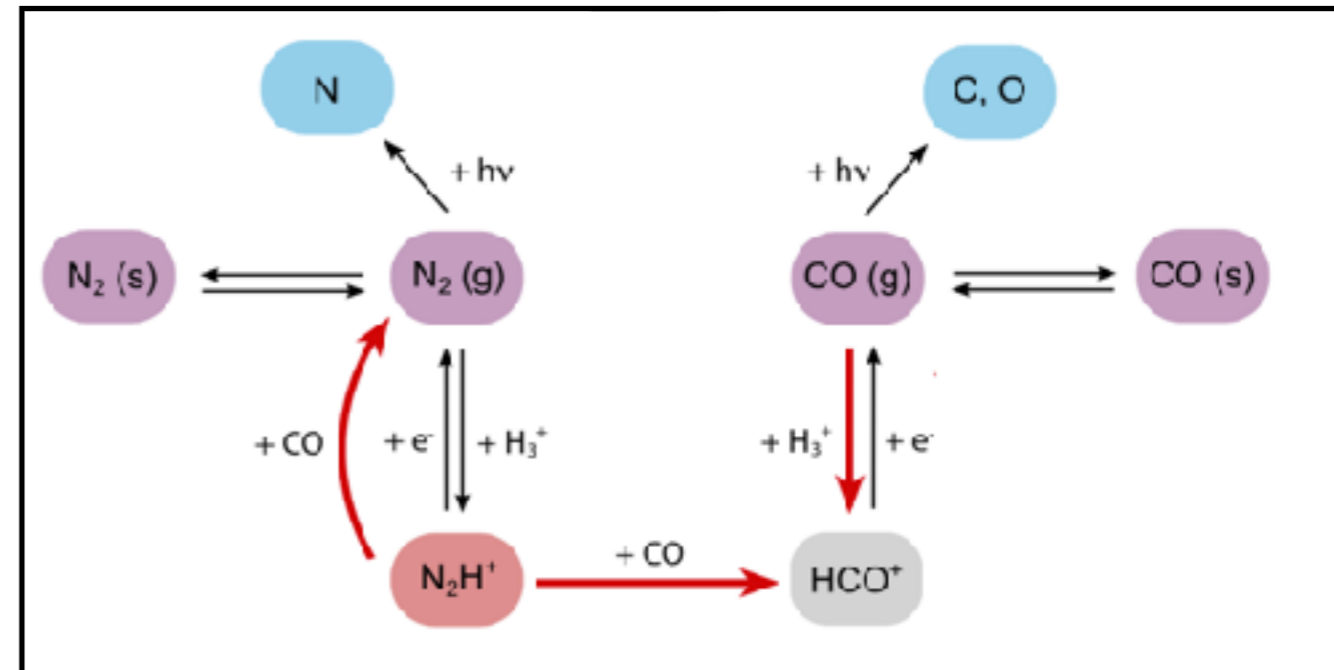


In edge-on disks it is possible to resolve the vertical structure of the molecules: temperature structure

Snowlines

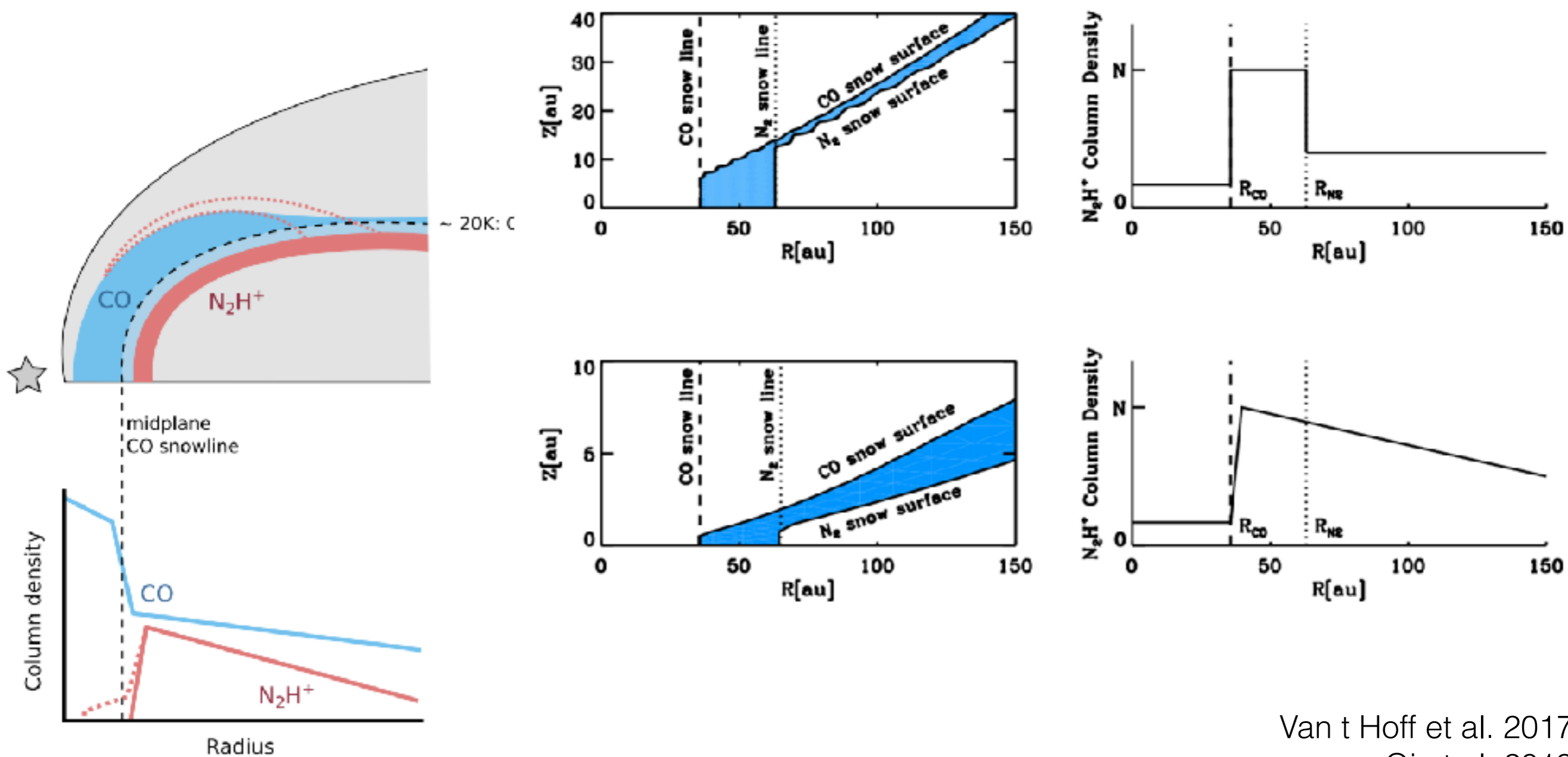


**Disk with an N_2H^+ ring:
CO snowline ($T_{\text{subl}} \sim 22$ K)?
 $\Rightarrow N_2H^+$ can only form
when CO is frozen out**



Snowlines

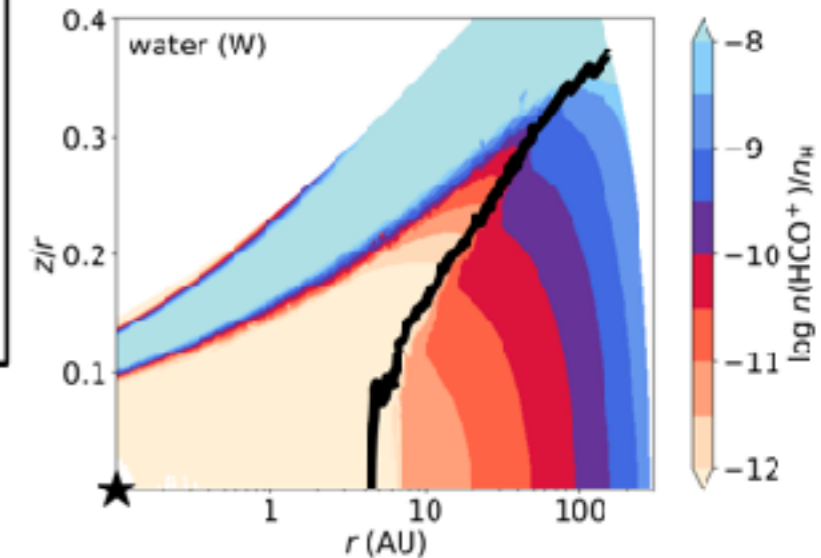
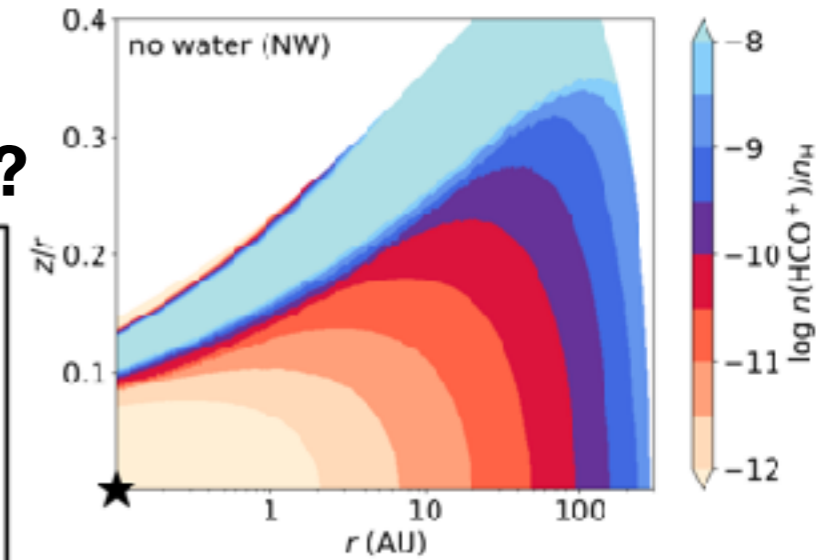
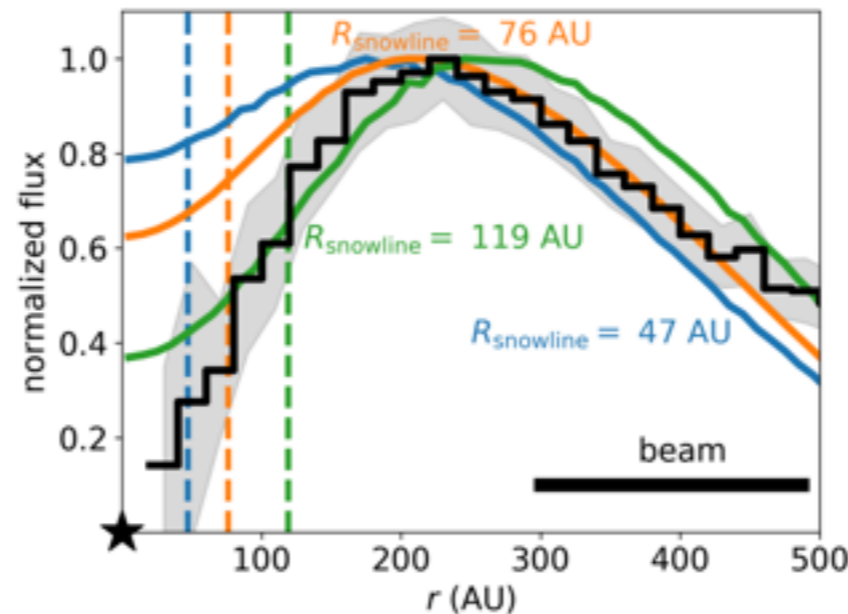
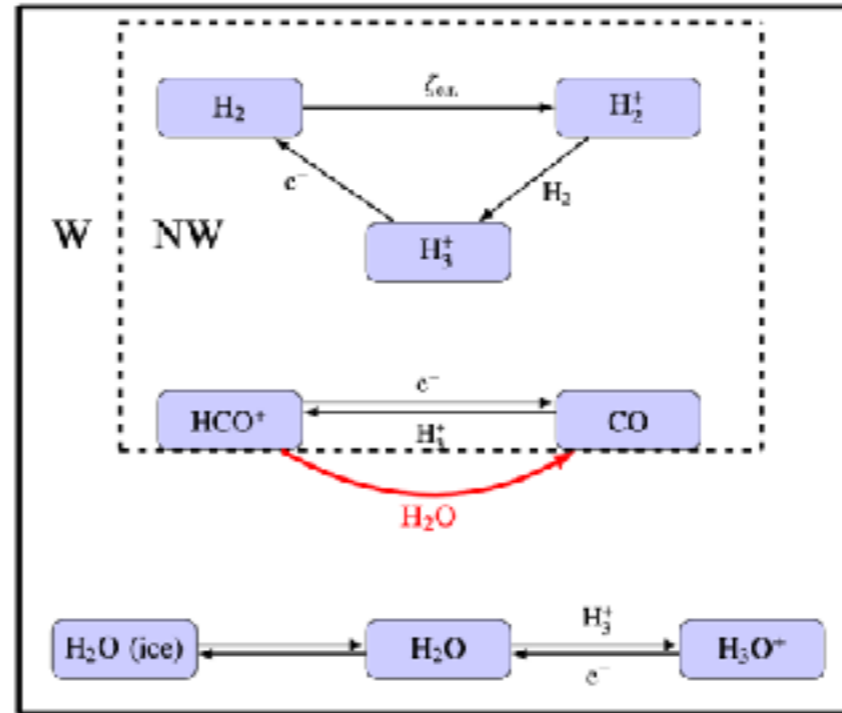
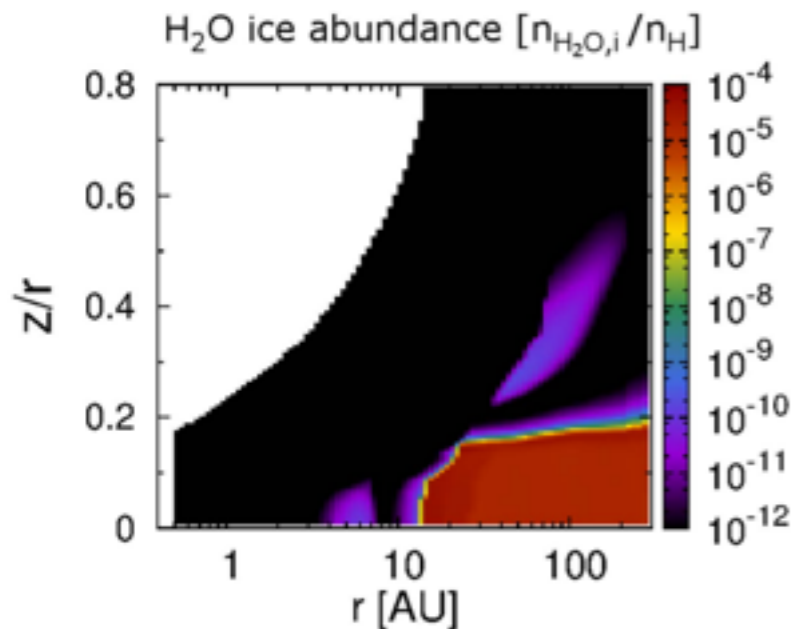
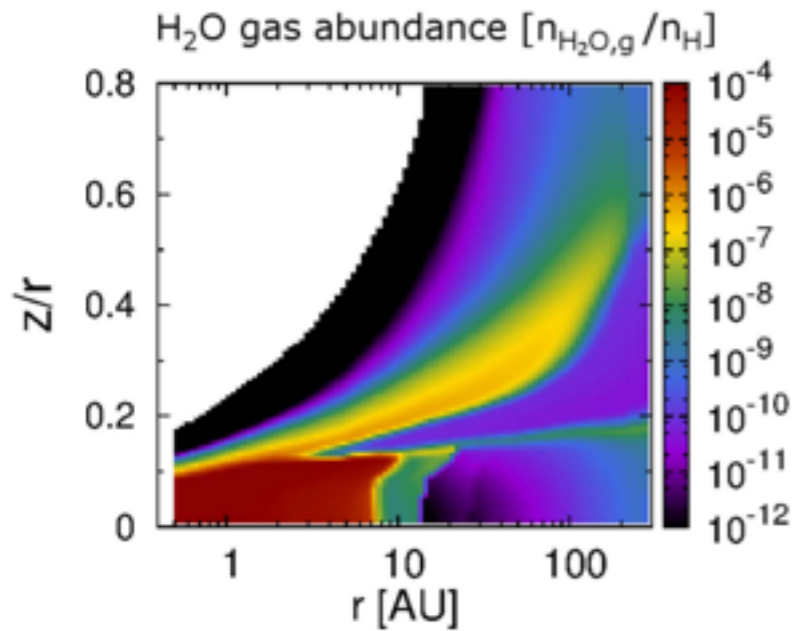
Modeling: CO snowline is actually CO snow surface



H₂O snowline

H₂O snowline ($T_{\text{subl}} \sim 120$ K) tricky:
close to host star and
inaccessible from ground

HCO⁺ as tracer?

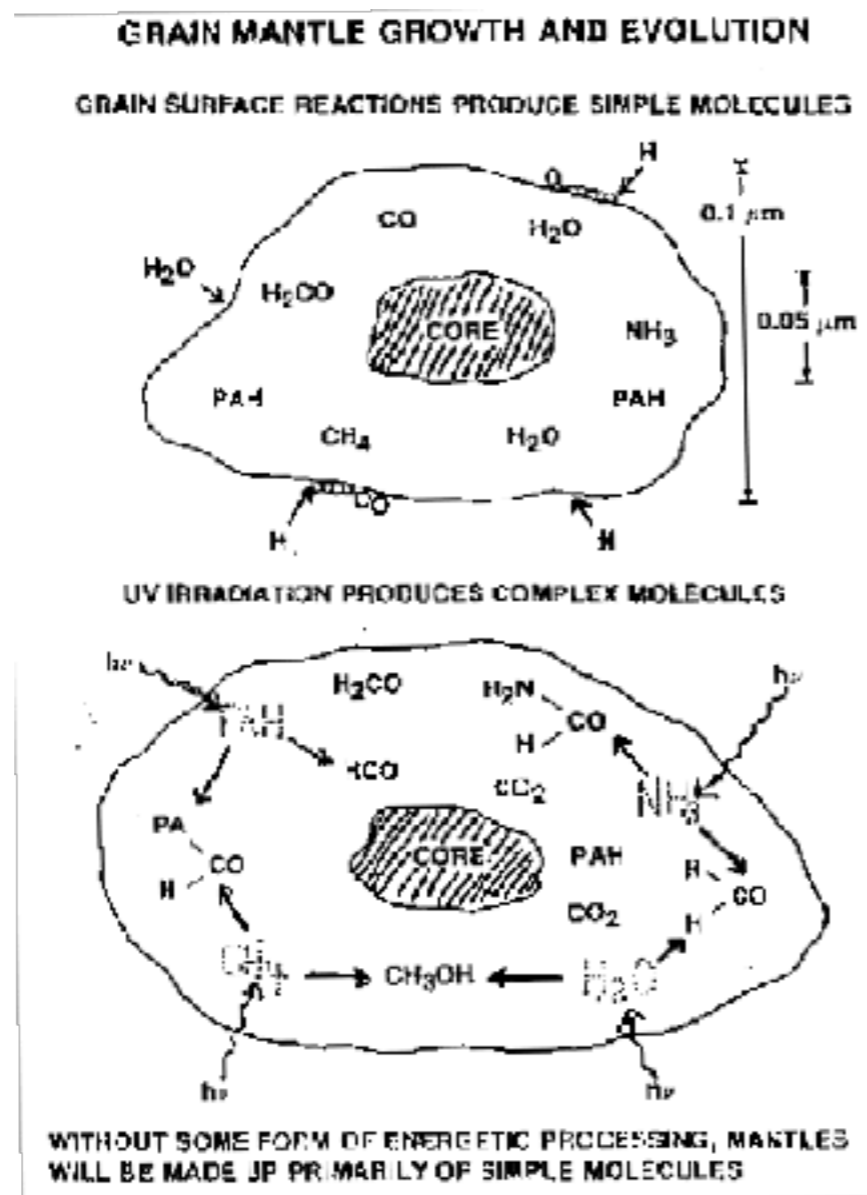
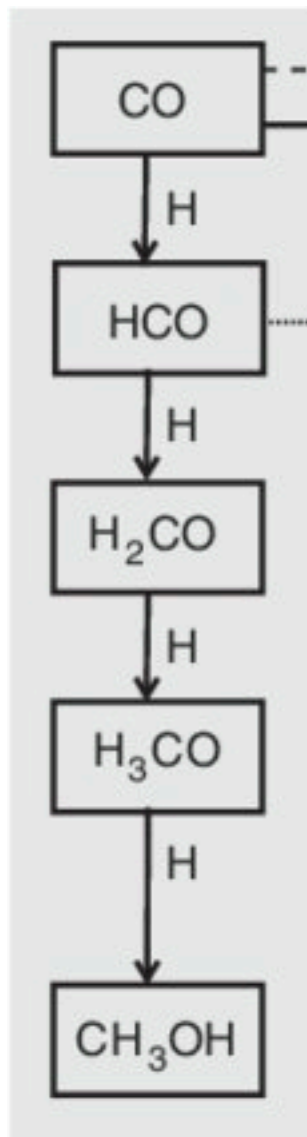


**V883 Ori: outburst
(100* brighter):
Snowline further out!**

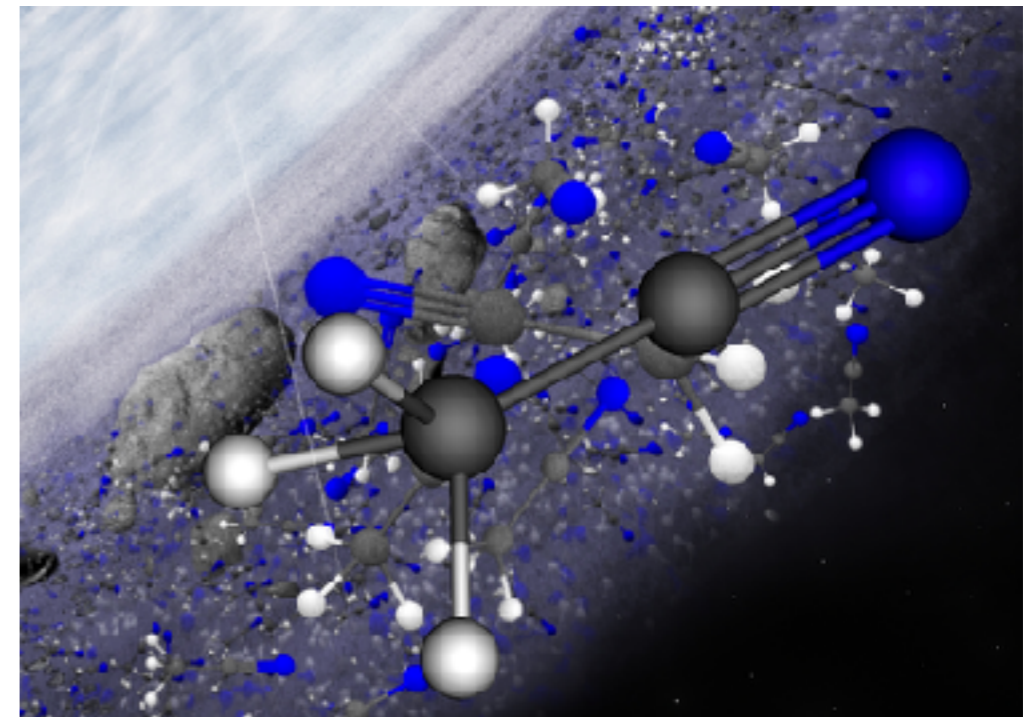
Notsu et al. 2017
Van t Hoff et al. 2018
Leemker et al. 2021

Complex organic molecules

Hydrogenation of CO-ice:
(e.g. Watanabe & Kouchi 2002)



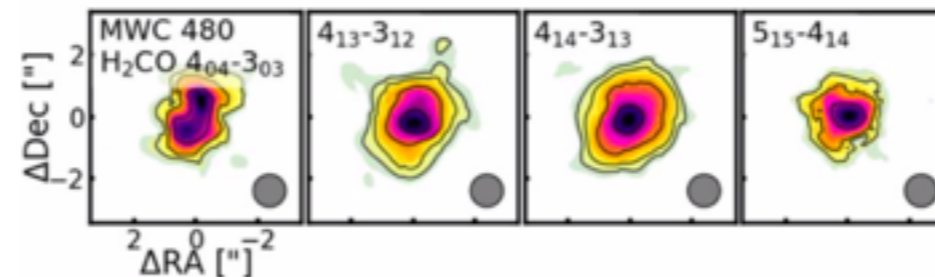
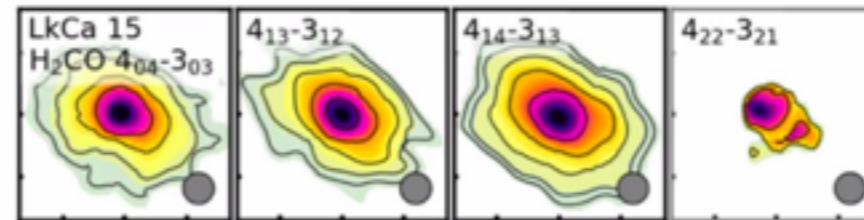
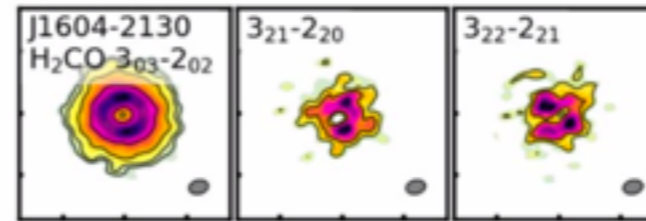
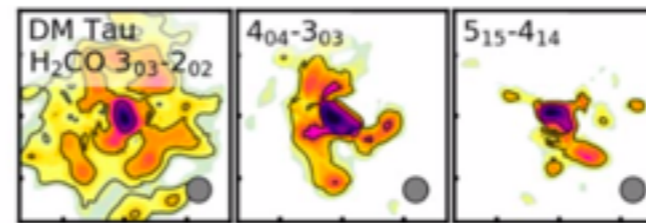
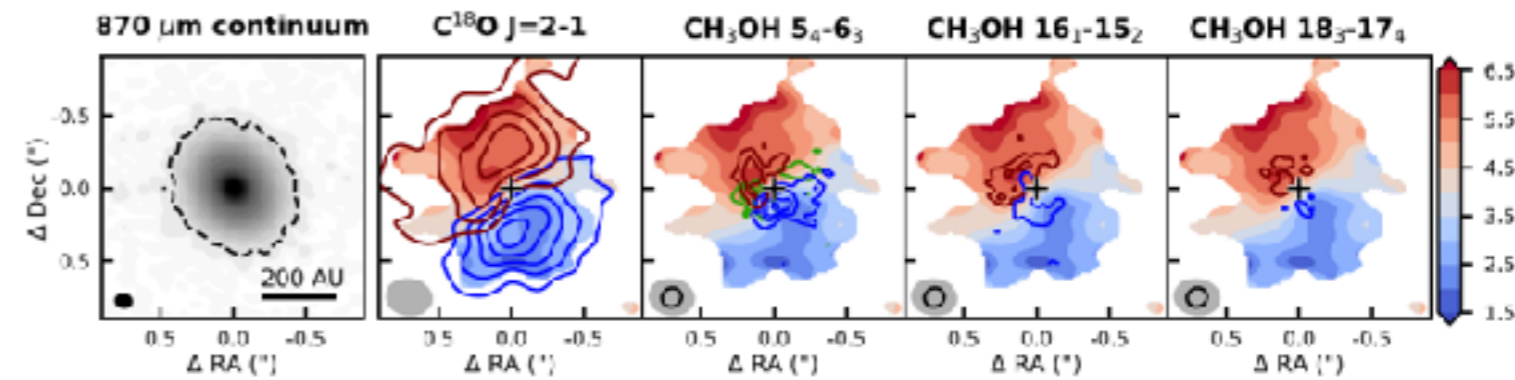
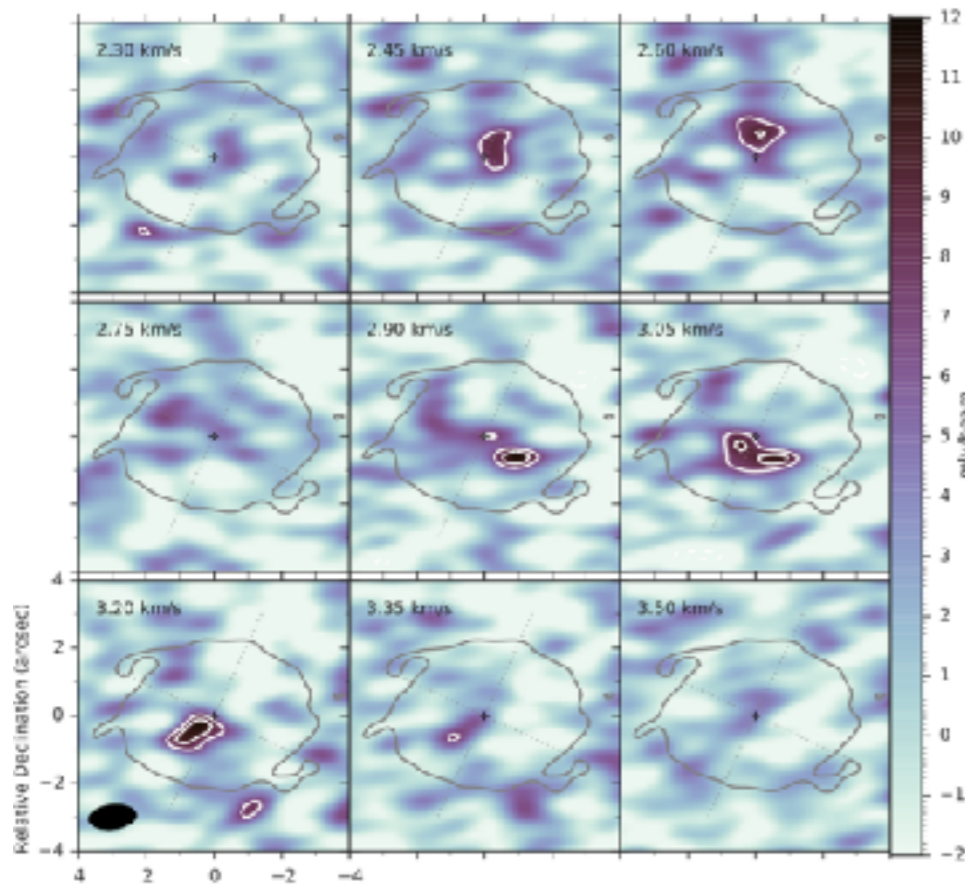
=> start of complex organic molecule (COM) chemistry: biomolecules?



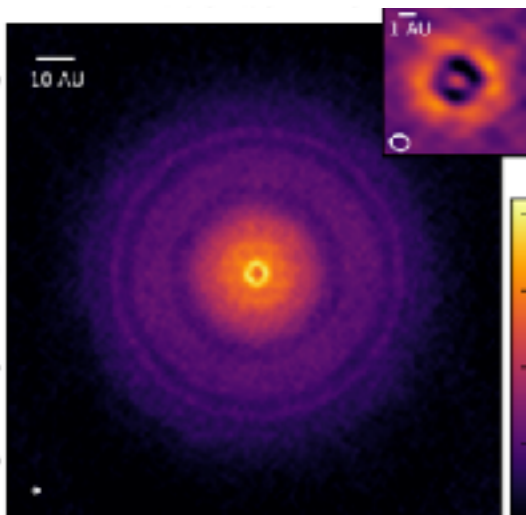
CH₃OH and H₂CO

V883 Ori: CH₃OH

TW Hya: CH₃OH (nearest disk)

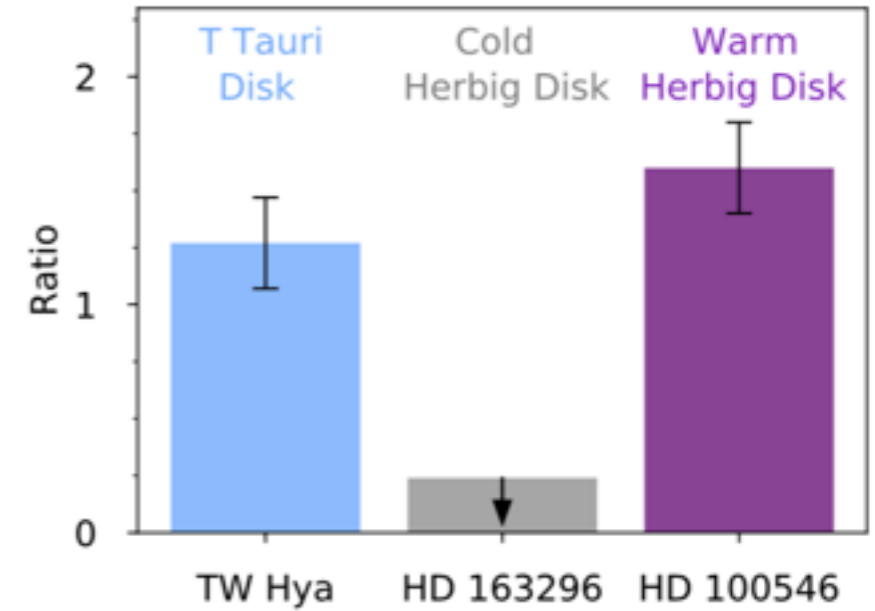
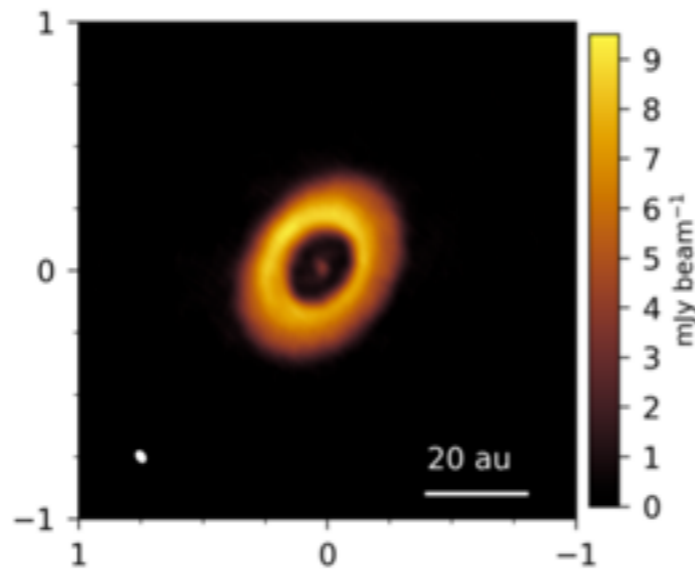
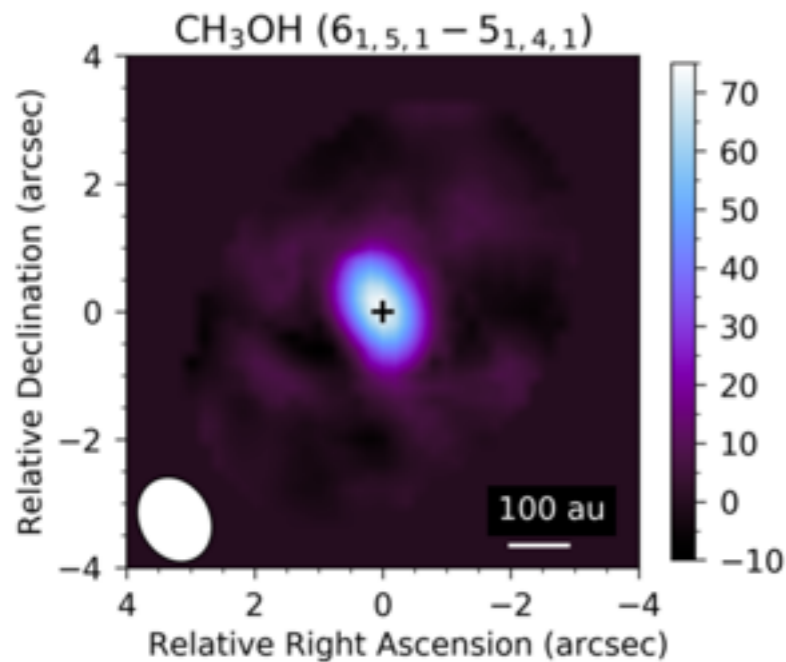


Many disks:
H₂CO (also gas-phase
formation)

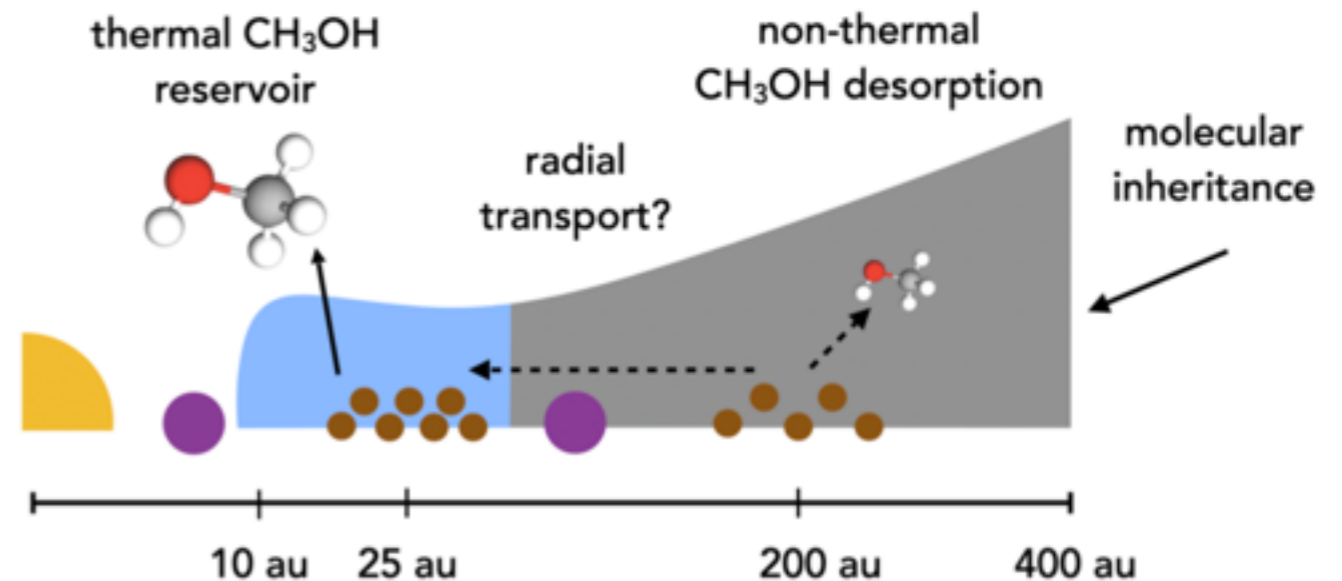


CH₃OH in warm disk?

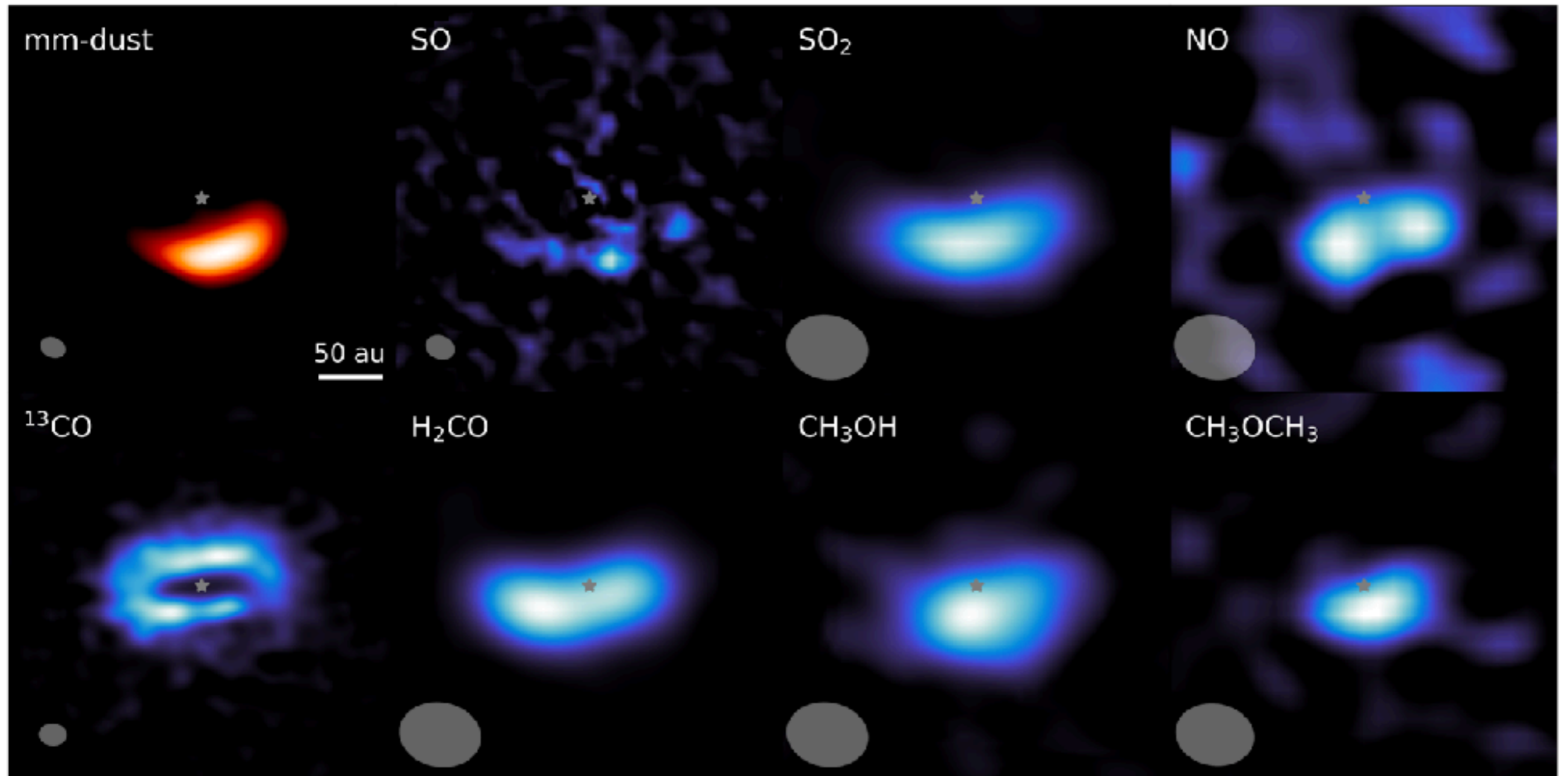
HD100546: warm disk (hot star) => no CO ice reservoir?



CH₃OH ice must be formed in early cloud phase and inherited



CH₃OH in ice trap in warm disk?

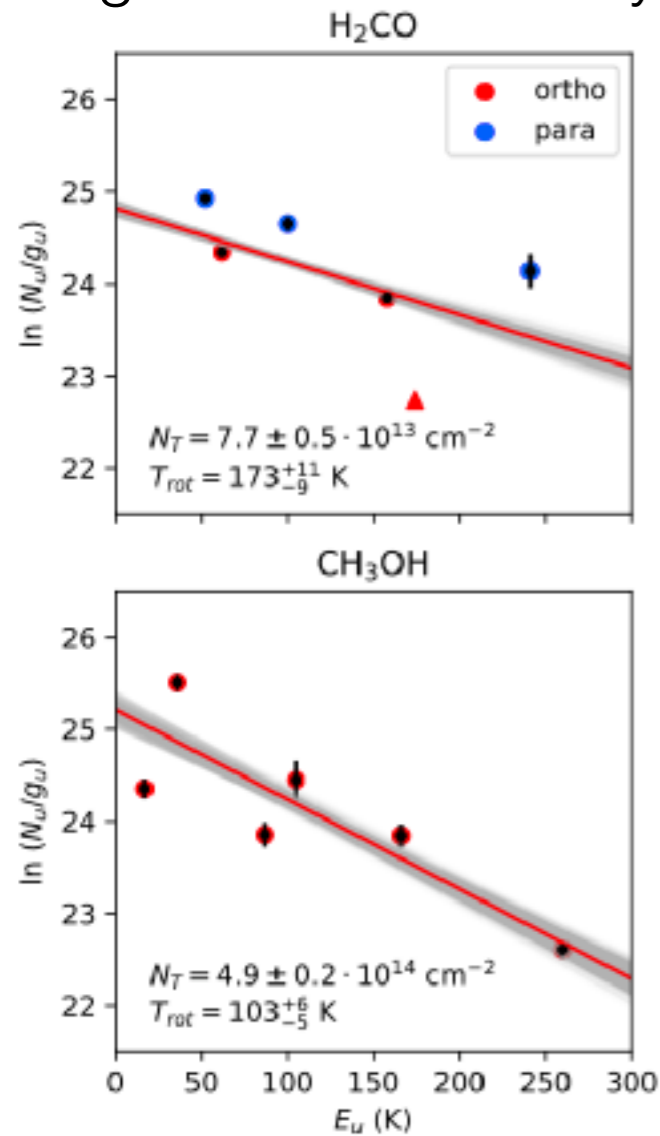


**Various complex organic molecules cospatial
with dust trap: must originate from icy pebbles**

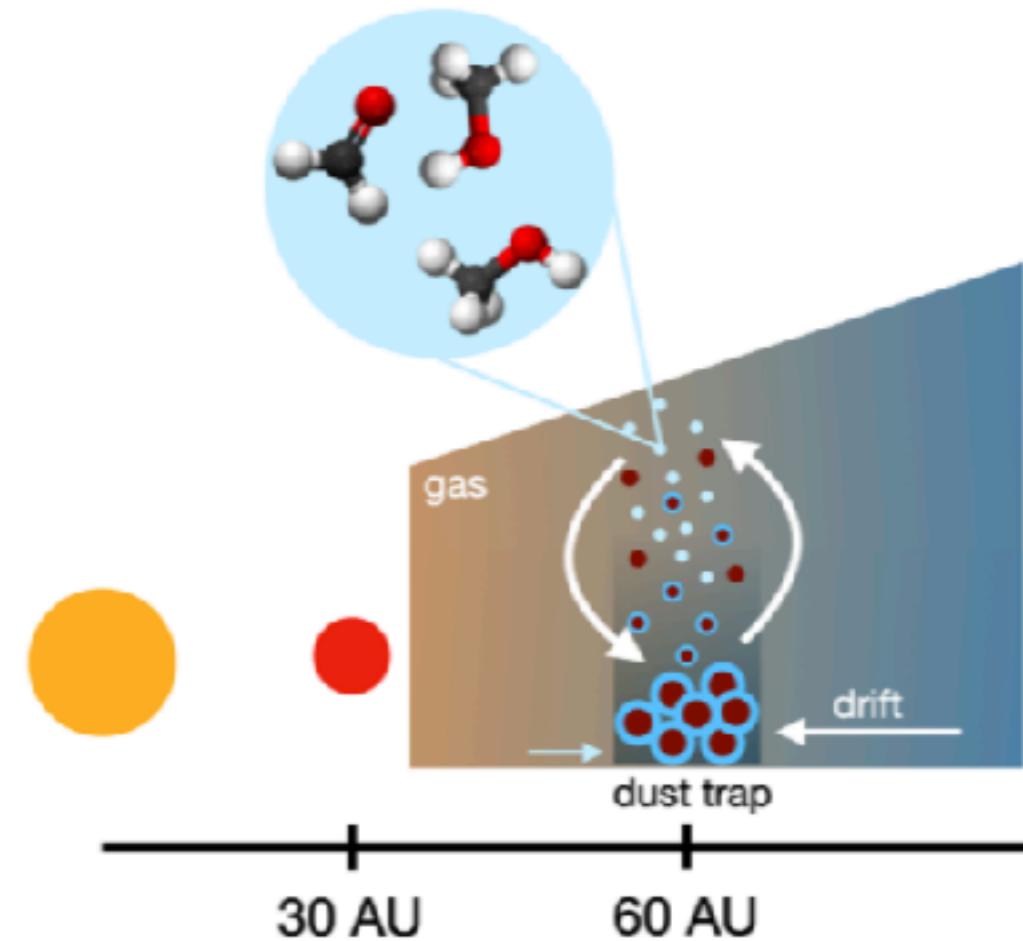
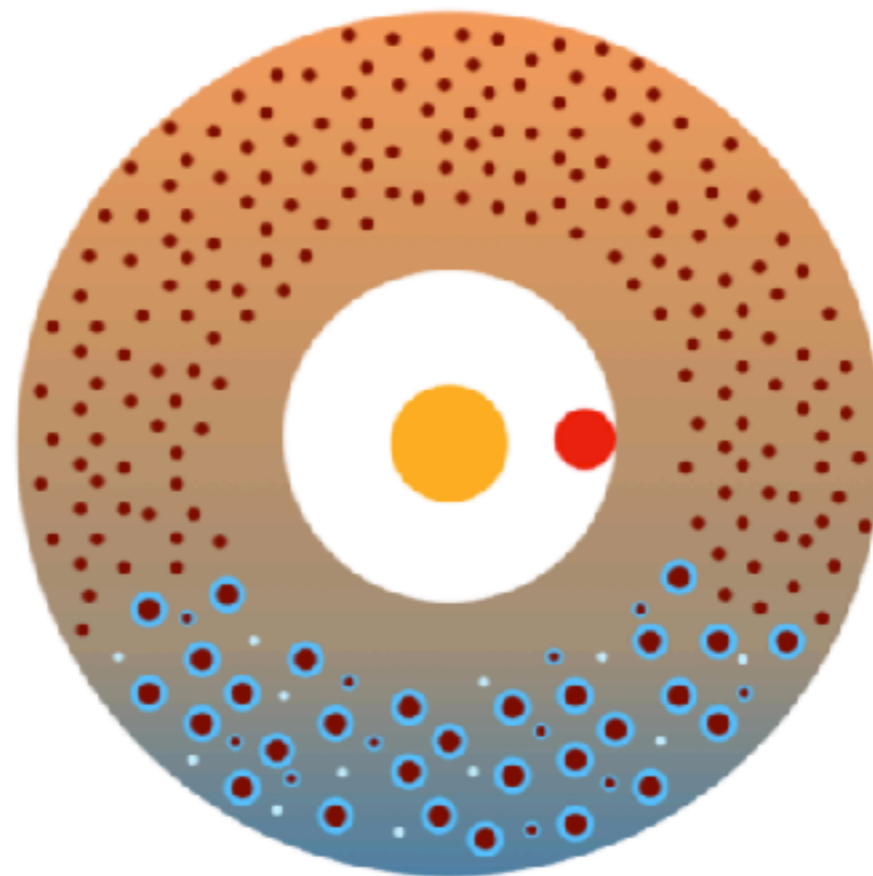
Van der Marel et al. 2021b
Booth et al. 2021
Brunken et al. 2022

CH₃OH in ice trap

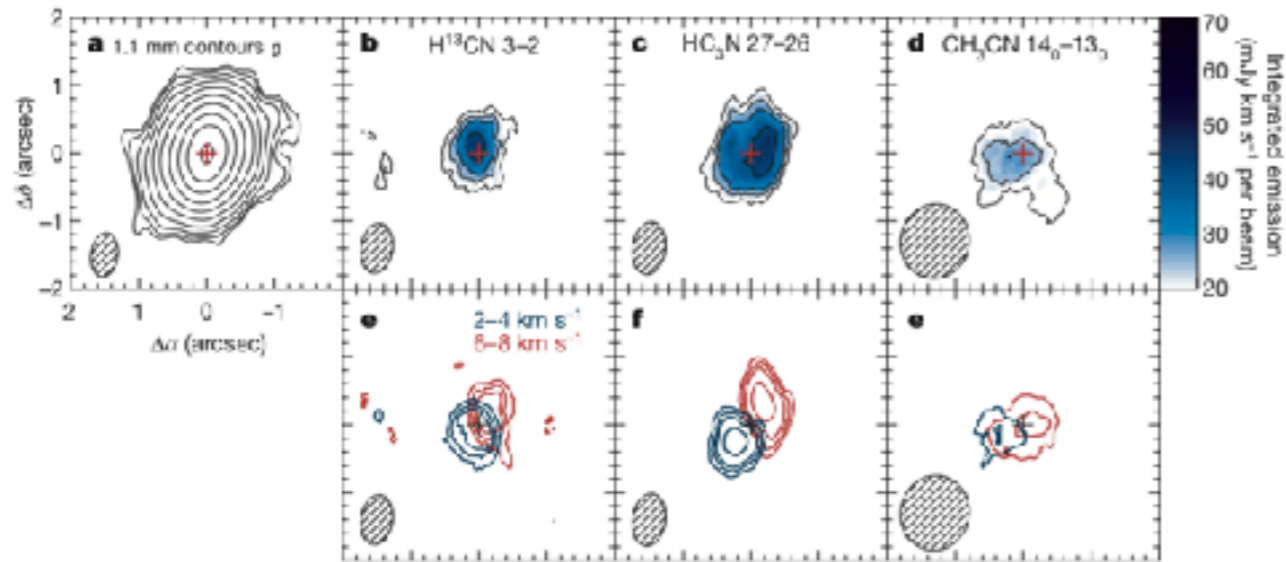
Rotational diagram:
high T => surface layer



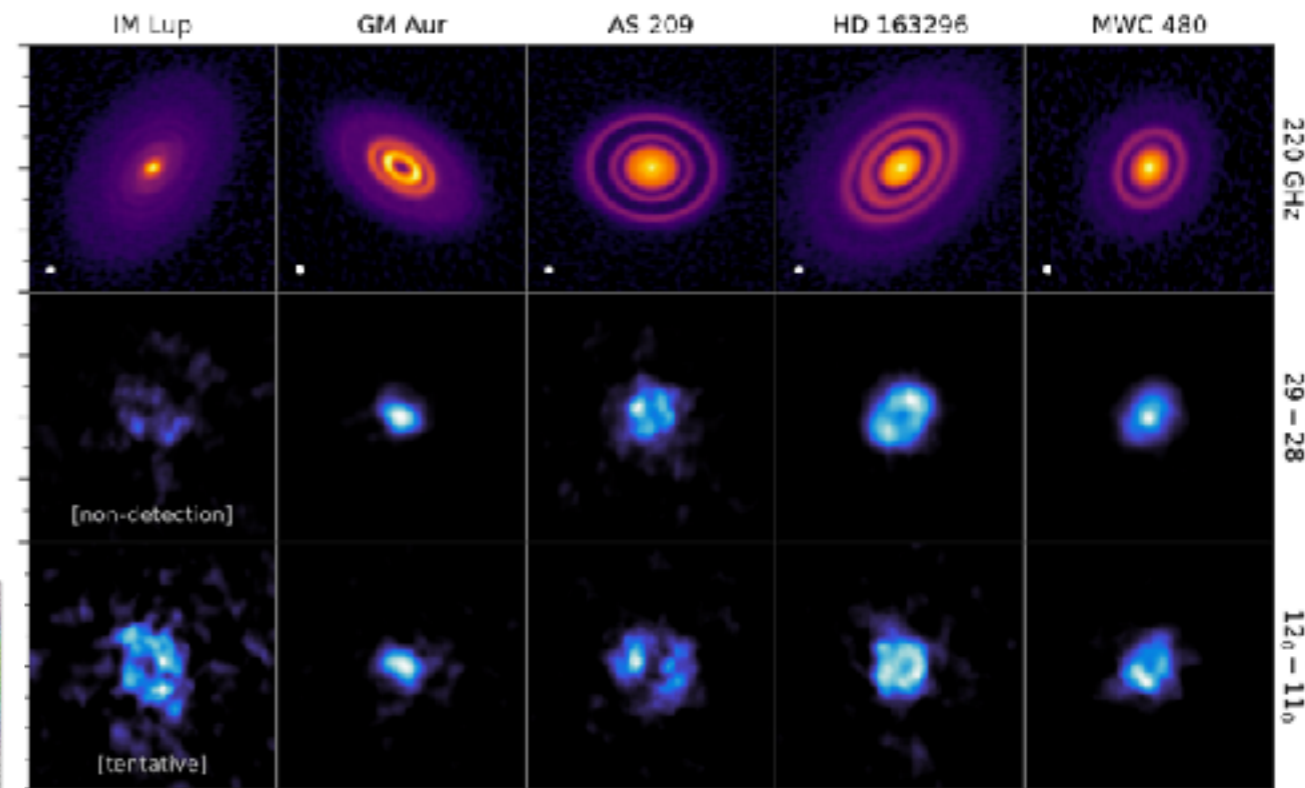
**Scenario: icy dust gets trapped,
vertical turbulence brings icy
grains to surface and ice desorbs**



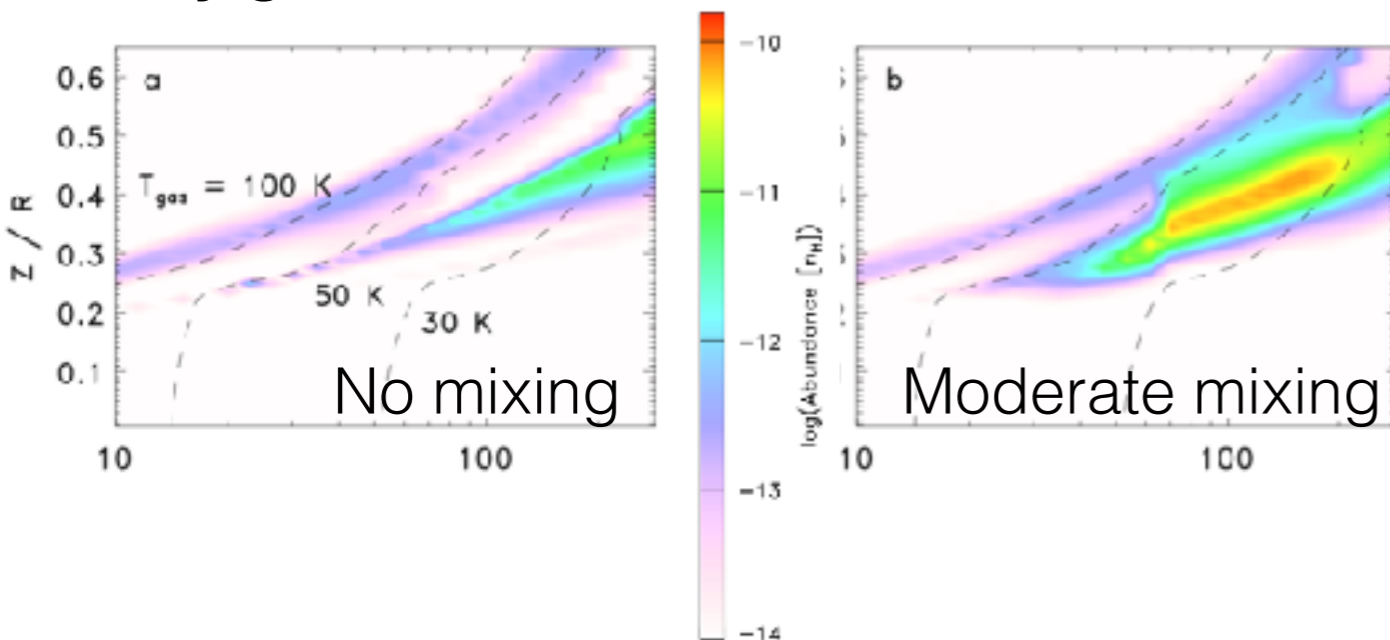
CH₃CN and HC₃N



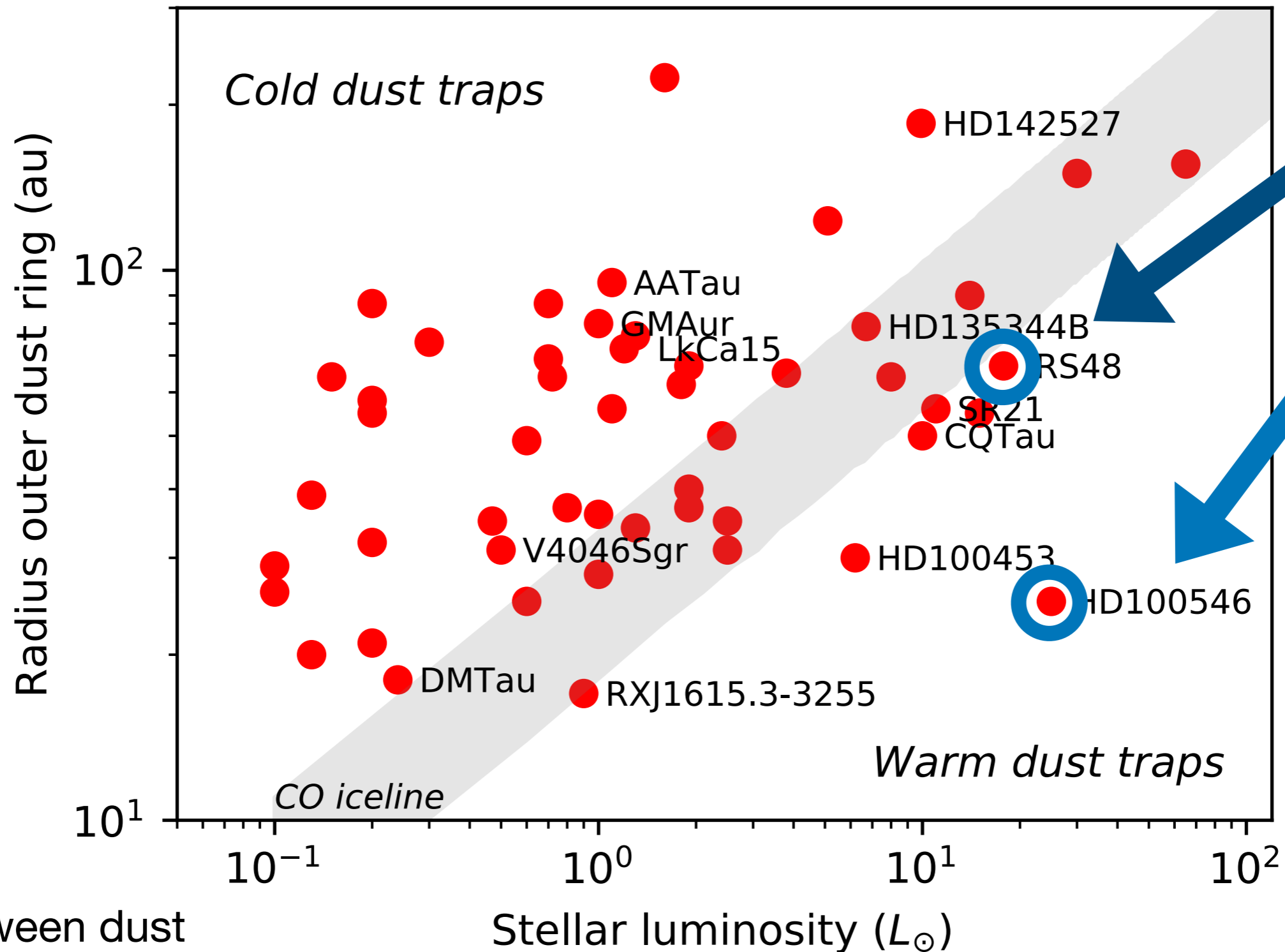
Also detected in MAPS disks



Also here: vertical mixing required to bring icy grains to surface and sublimate

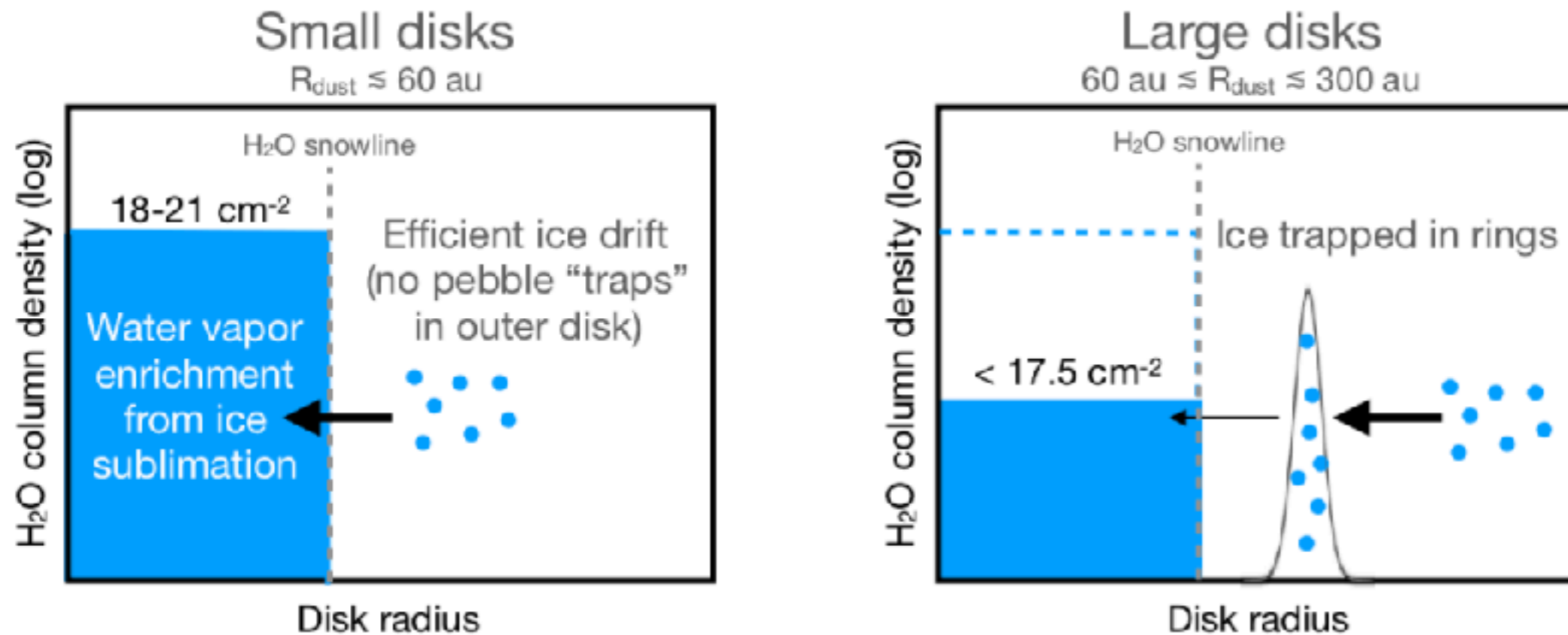


Why these two disks for CH₃OH?

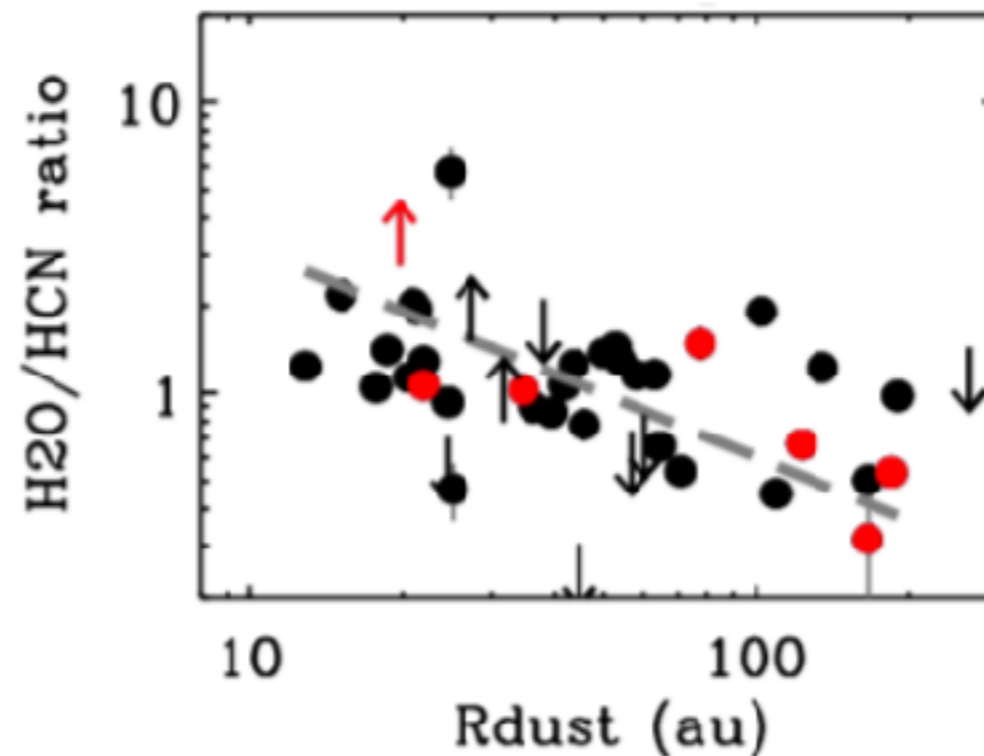


Link between dust transport and chemistry

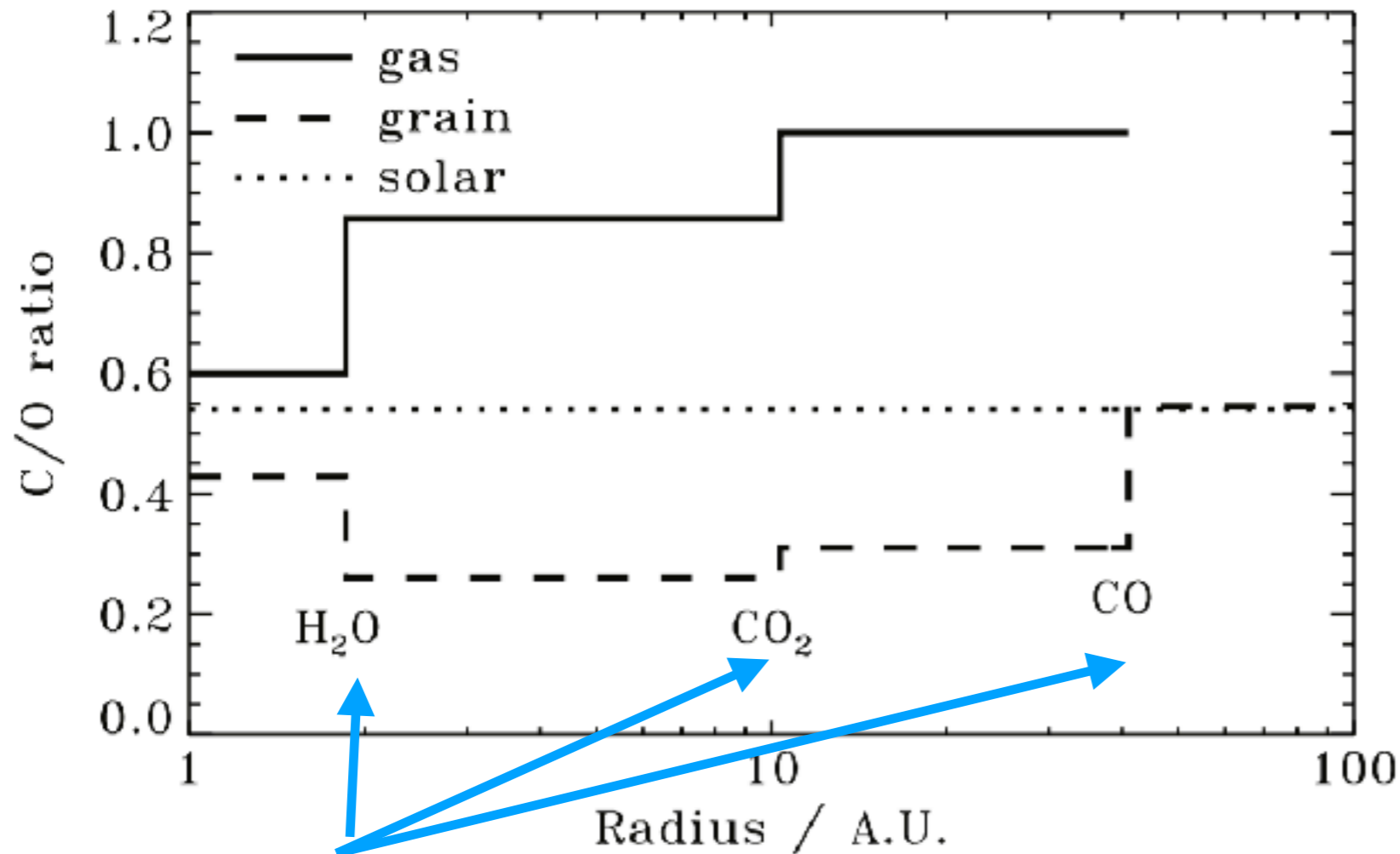
Link between dust drift and chemistry?



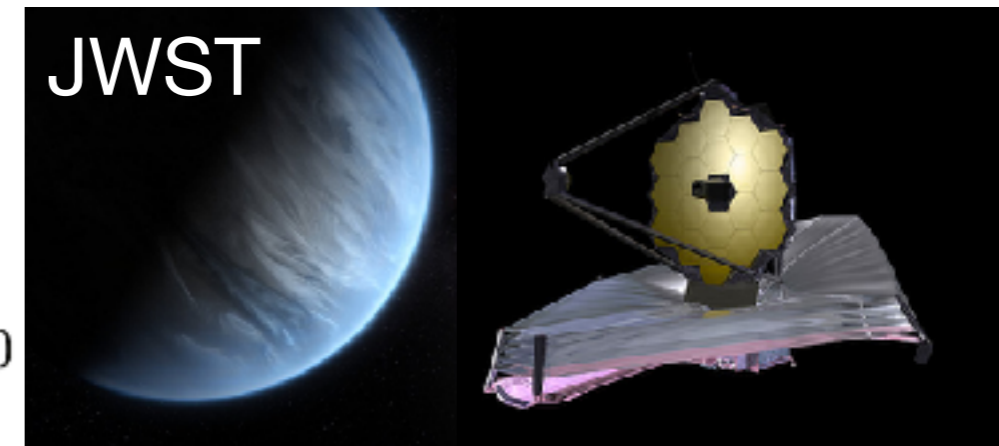
Two types of disks:
possible explanation
for elevated warm H₂O
in compact disks



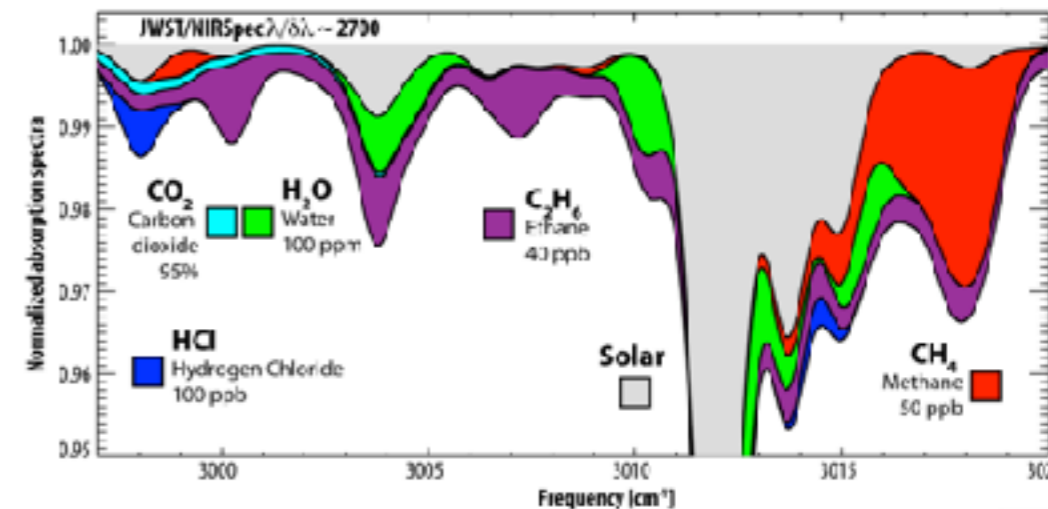
C/O ratios in disks



Classical picture of C/O in disk: snowlines

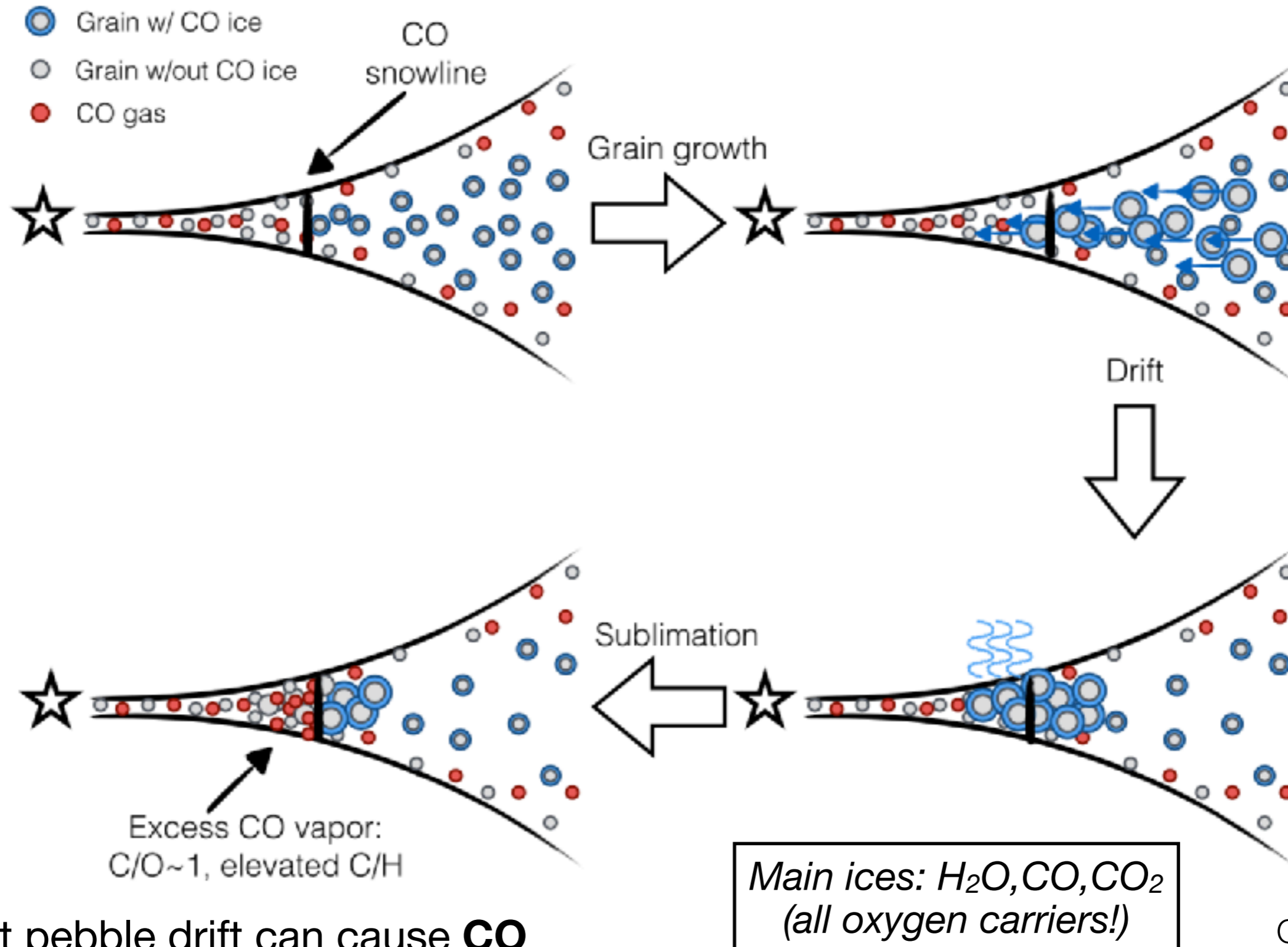


Snowlines



Link exoplanet atmospheric composition to formation location

Dust transport regulate (ice) chemistry?

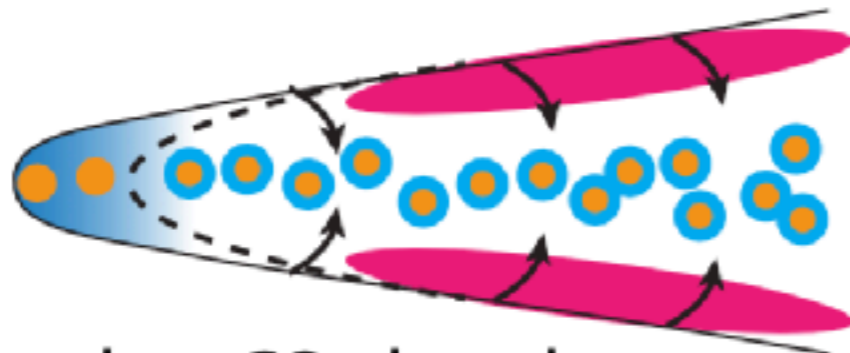


Dust pebble drift can cause **CO depletion and increase C/O > 1**

Link between C/O and dust drift?

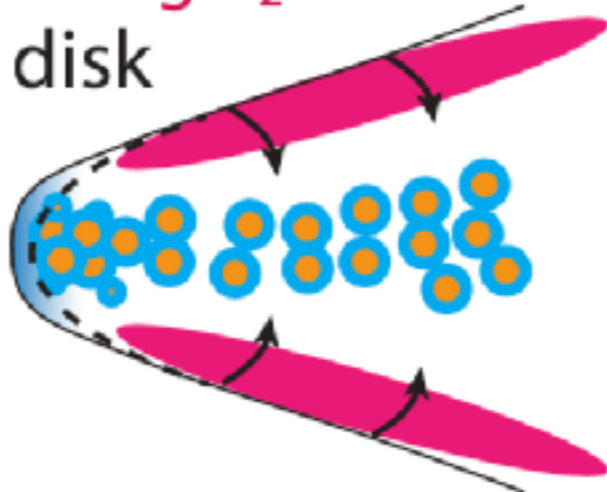
Cold disks: high C/O

Ring disk



low CO abundance
strong C_2H emission

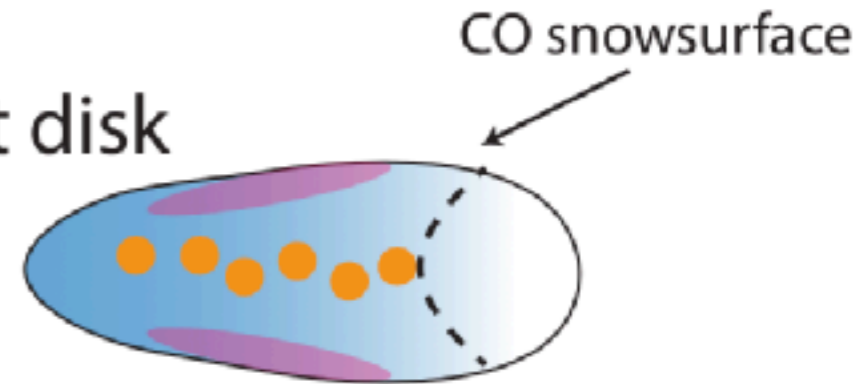
Cold transition disk



C_2H detection

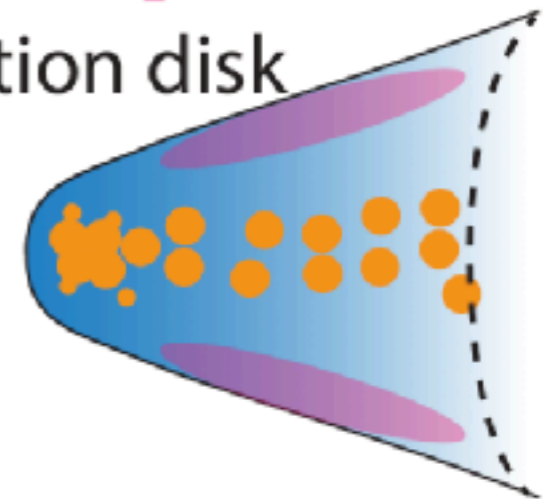
Warm disks: low C/O

Compact disk



high CO abundance
weak C_2H emission

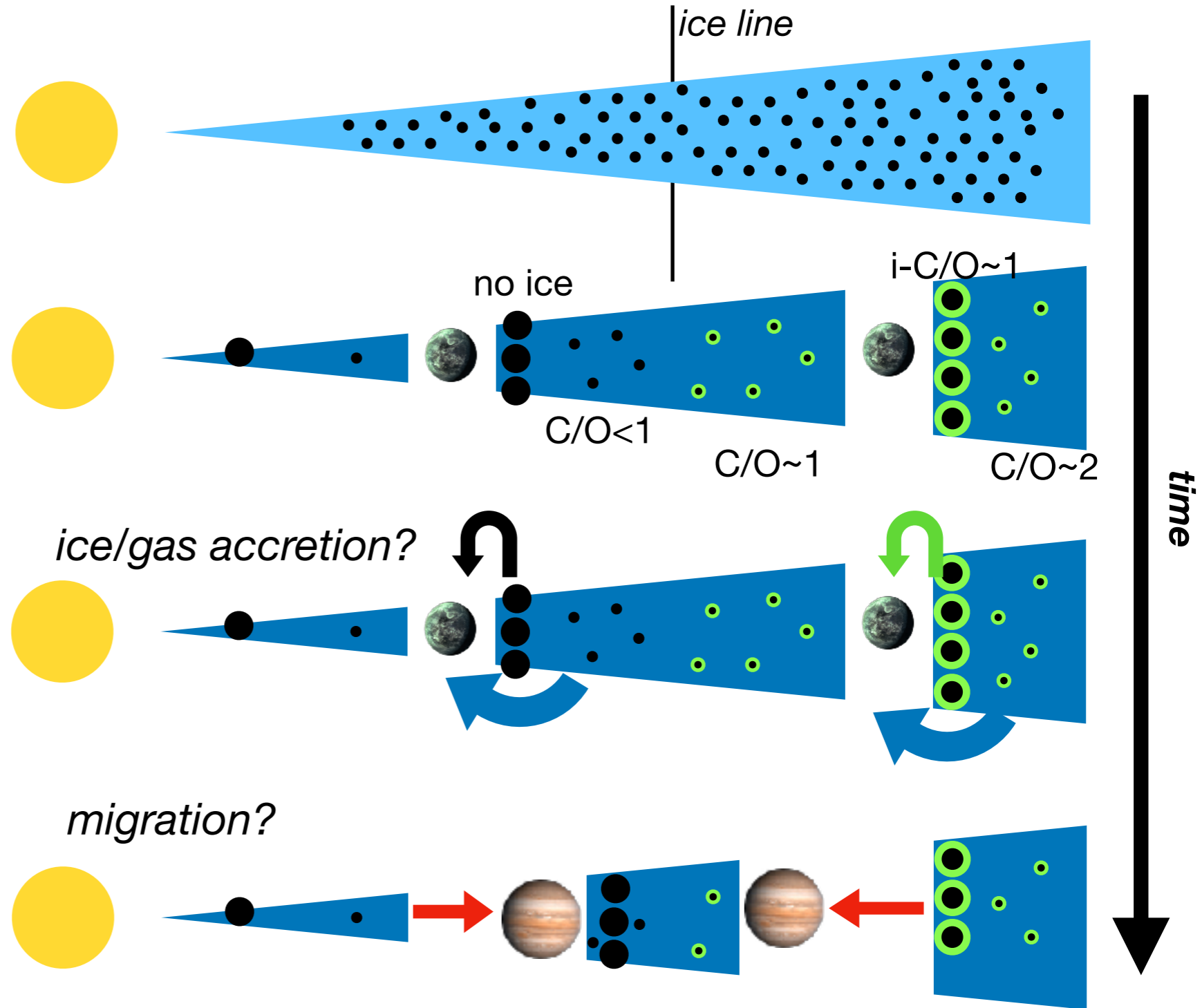
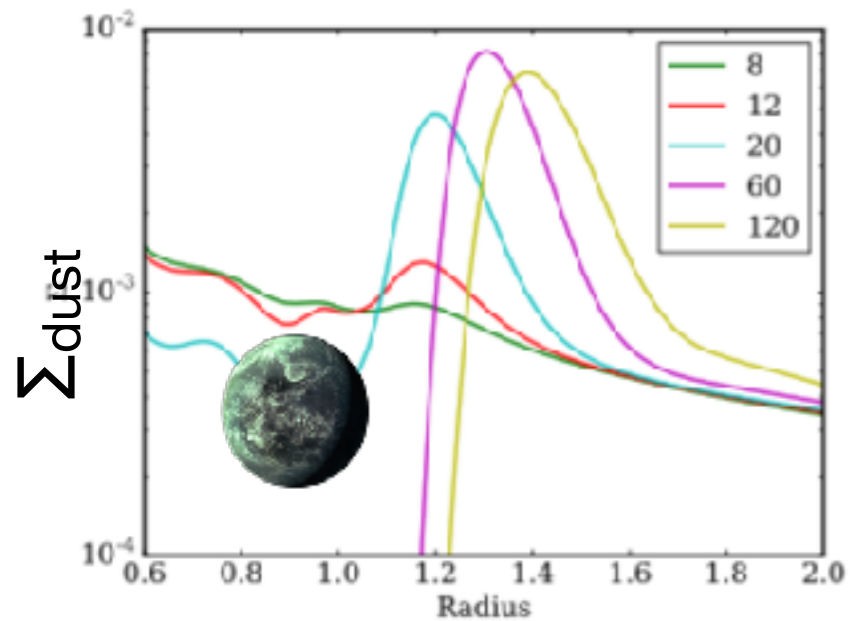
Warm transition disk



**CO mostly evaporated:
 C_2H non-detection**

Impact on exoplanet atmospheres?

Recall:
Minimum core mass to
create dust trap



**Planet formation models need
to take icy pebble drift into account to
figure out what gets accreted where**

C/O ratios in disks

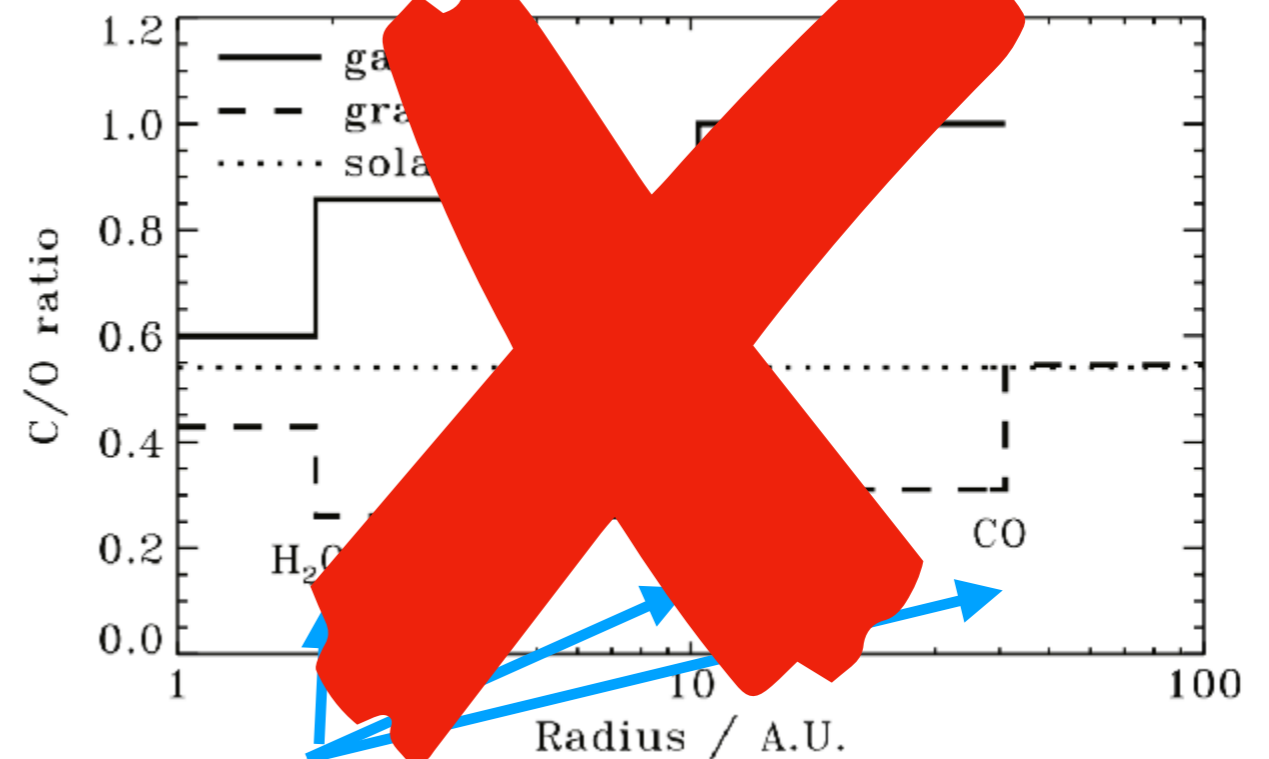
LETTER TO THE EDITOR

If you like C/O variations, you should have put a ring on it

Nienke van der Marel¹★, Arthur D. Bosman², Sebastiaan Krijt³, Gijs D. Mulders^{4,5}, and Jennifer B. Bergner⁶



Needs an update



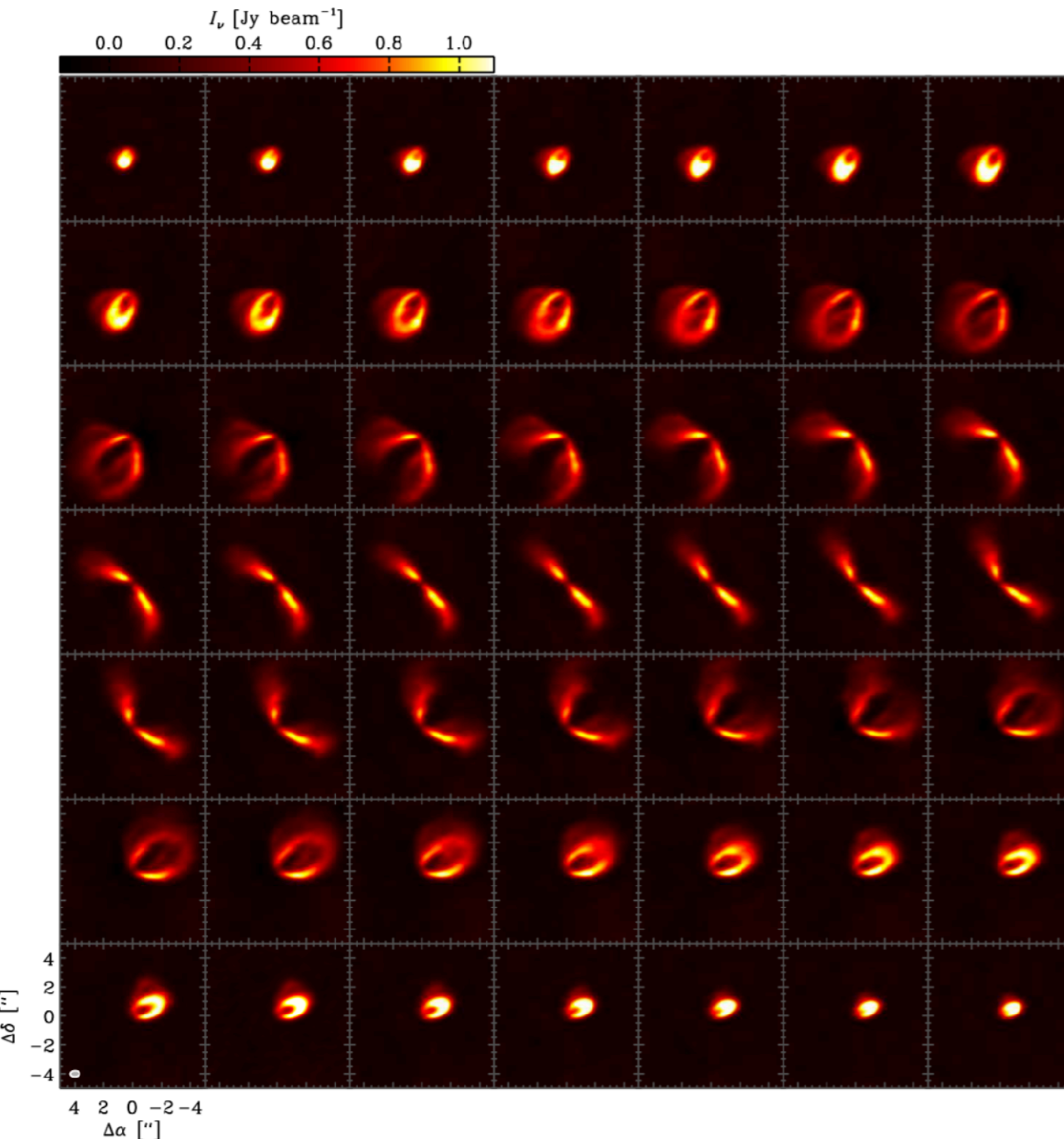
Summary

- Astrochemistry can help to constrain physical conditions and mechanisms in a disk
- Disk chemistry is particularly complex/interesting because of the strong temperature/radiation gradients
- Snowlines play a key role in determining temperature structure in the disk
- The detection of complex organic molecules in two disks proves inheritance and transport of ices
- The C/O ratio in the disk (and therefore in the planet) may be more complex due to dust trapping



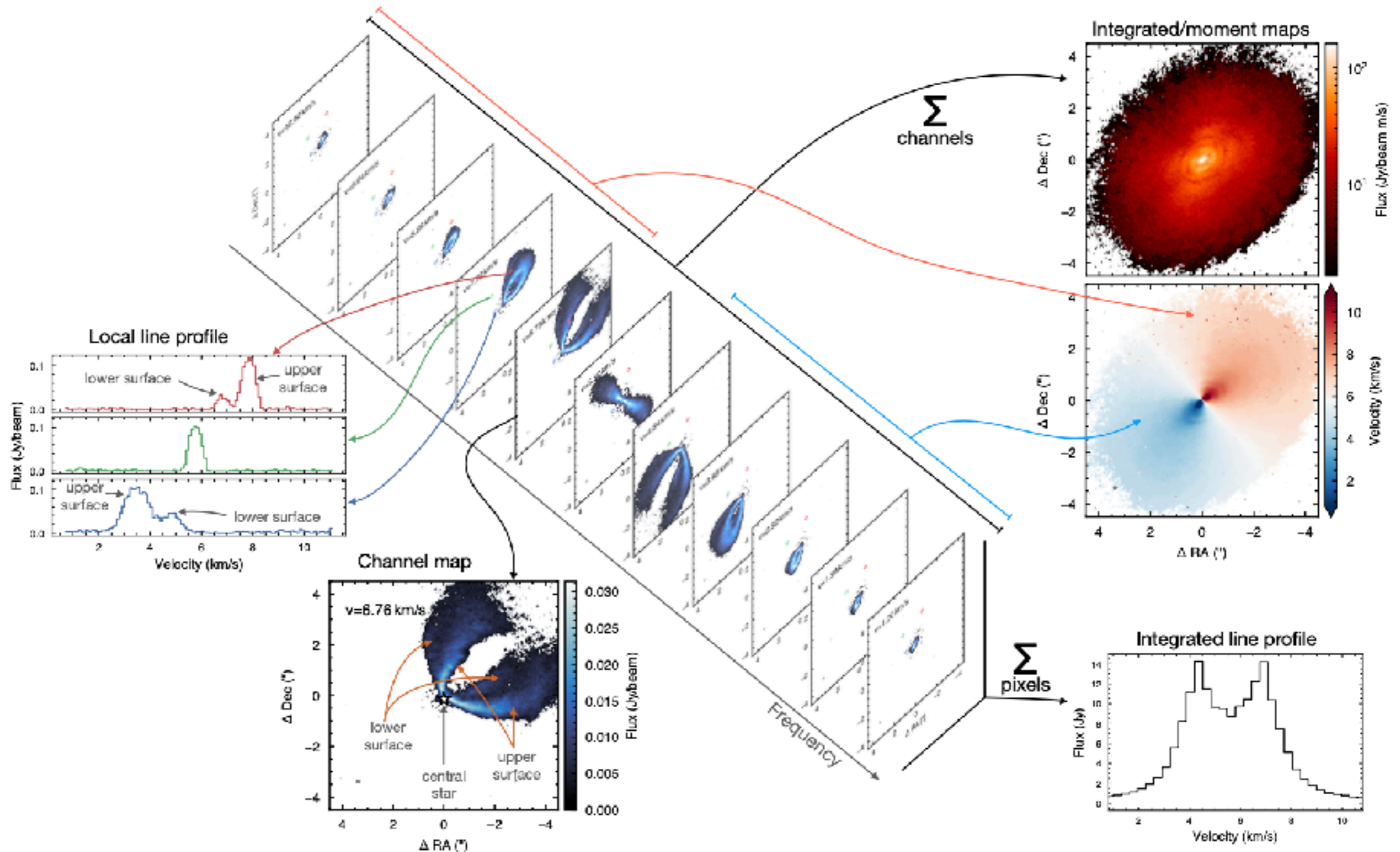
Disk kinematics

Channel maps

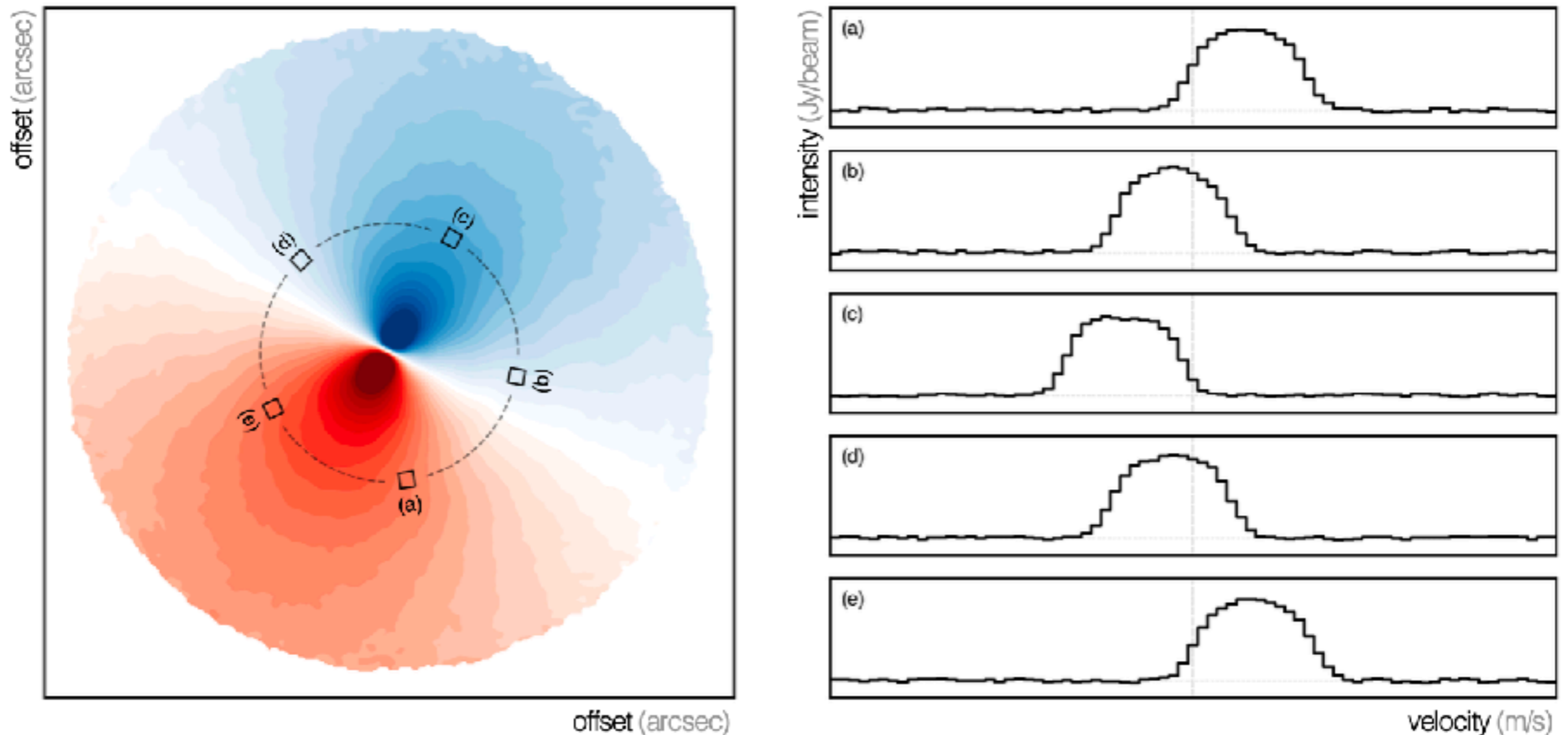


A picture is worth a thousand words.
An ALMA observation is worth **3.8 million**.
(almost 8 copies of War & Peace)

Channel maps

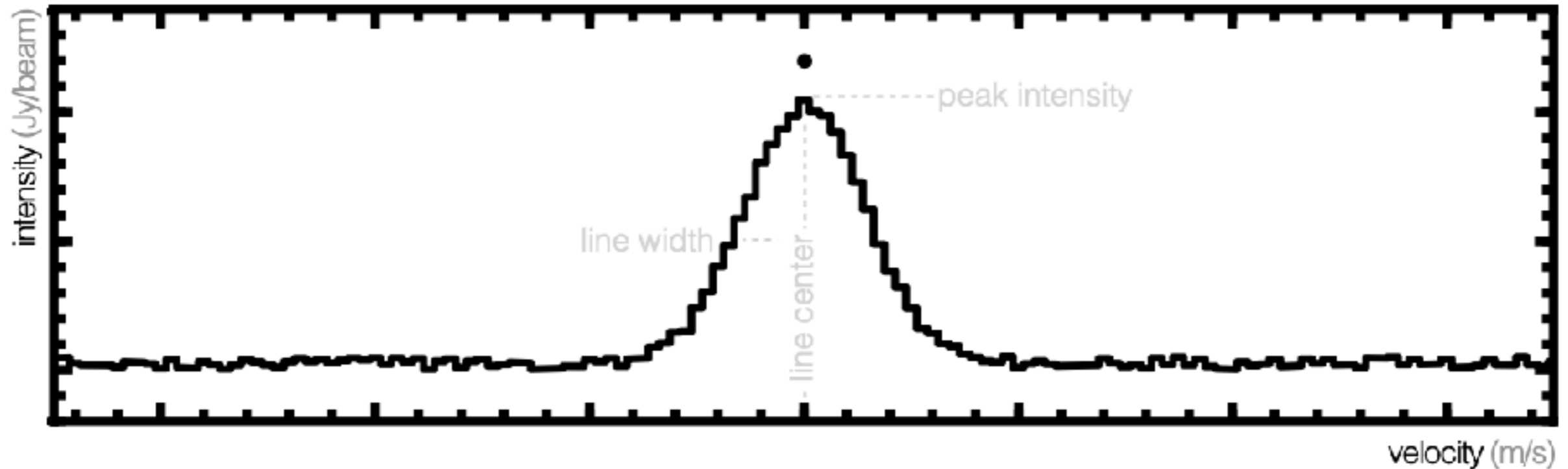


Channel maps



Each pixel is an emission line that has been Doppler shifted relative to the systemic velocity.

Line profile

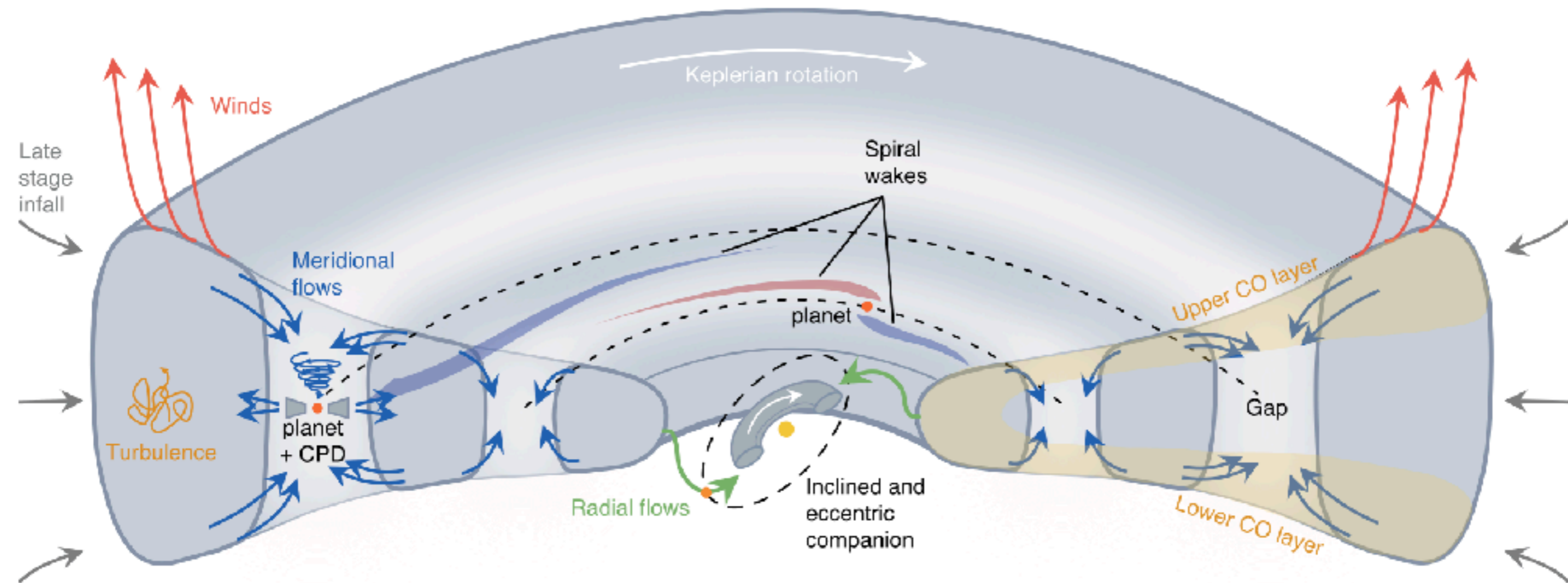


Peak Intensity: gas temperature, molecular column density.

Line Center: (coherent) velocity structure.

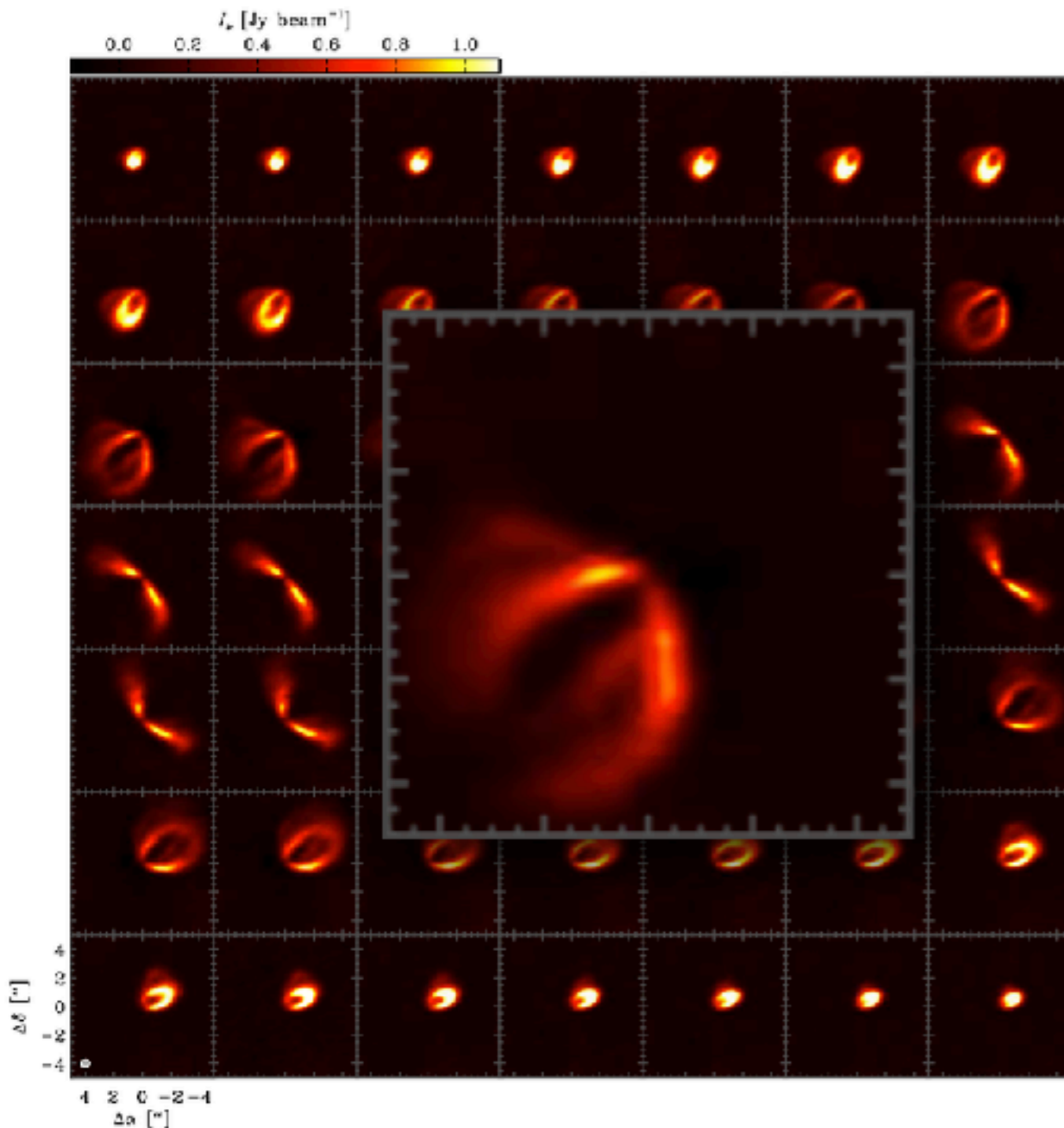
Line Width: velocity dispersions.

Expected kinematics in a disk



Much more than just Keplerian rotation!

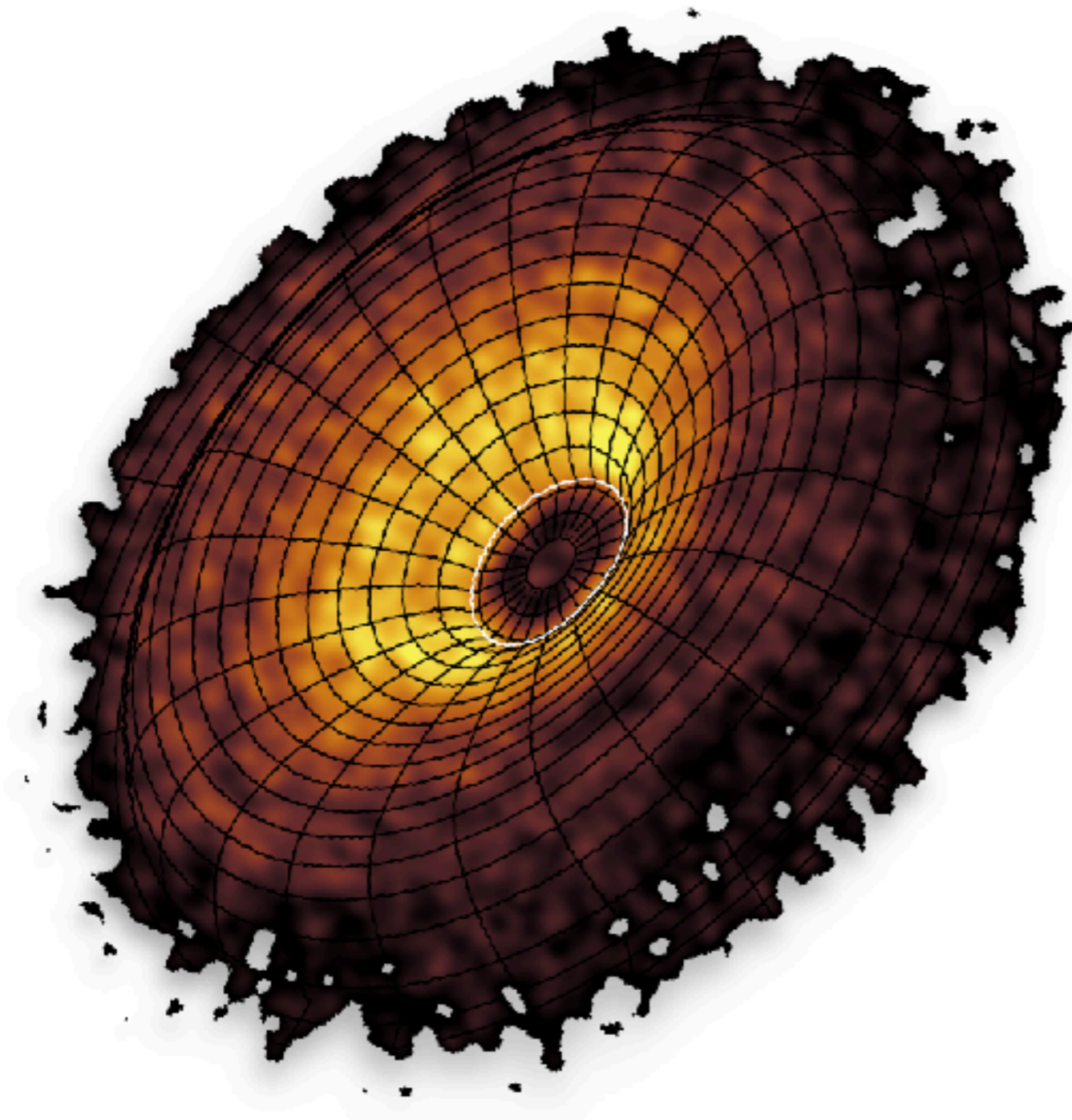
Channel maps



We're actually tracing *two* sides of the disk and we can start to map out the 3D structure of the disk.

Pinte et al. (2018), Teague et al. (2019), Keppler et al. (2019), Rich et al. (2021), Casassus et al. (2021), Law et al. (2021c)

Channel maps

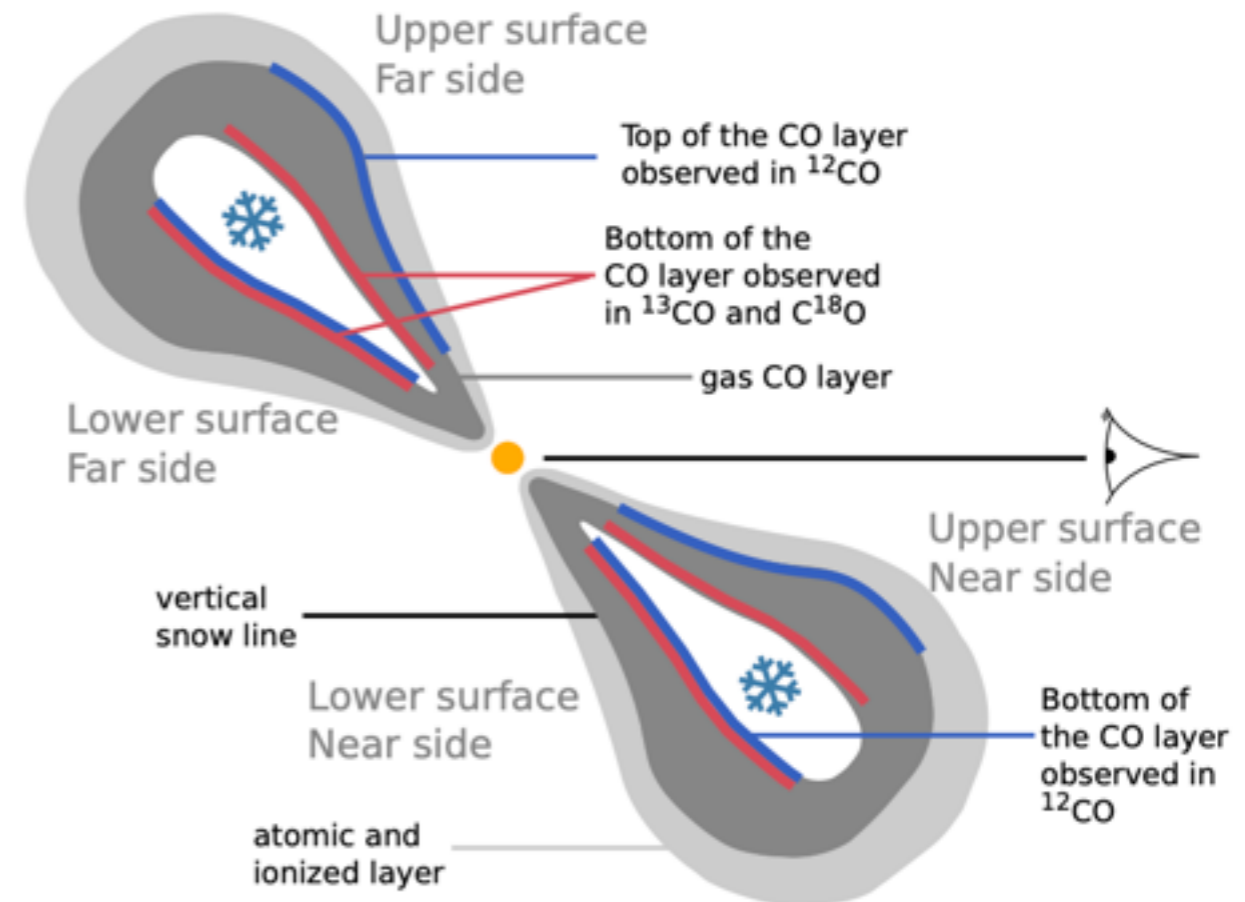
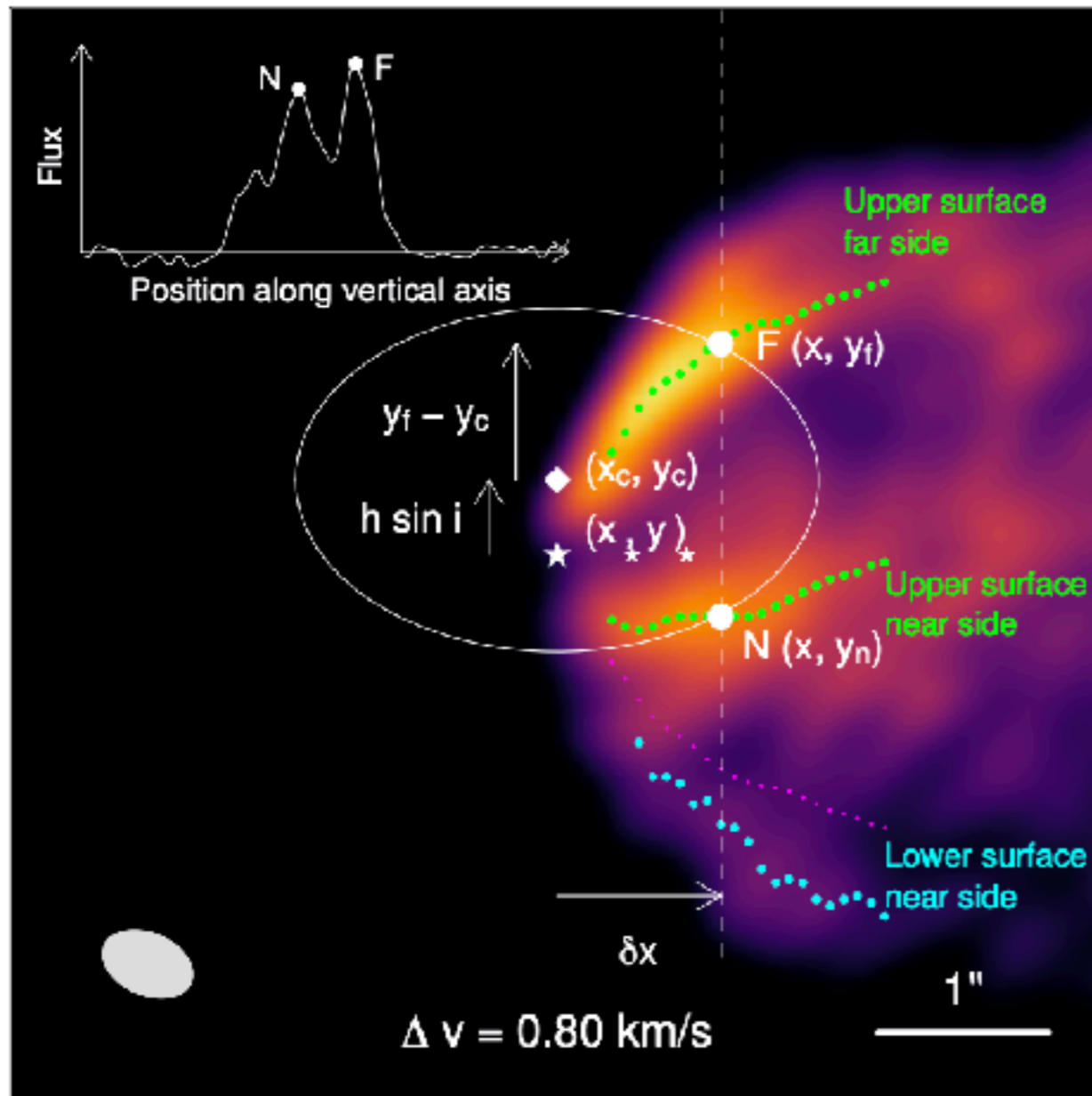


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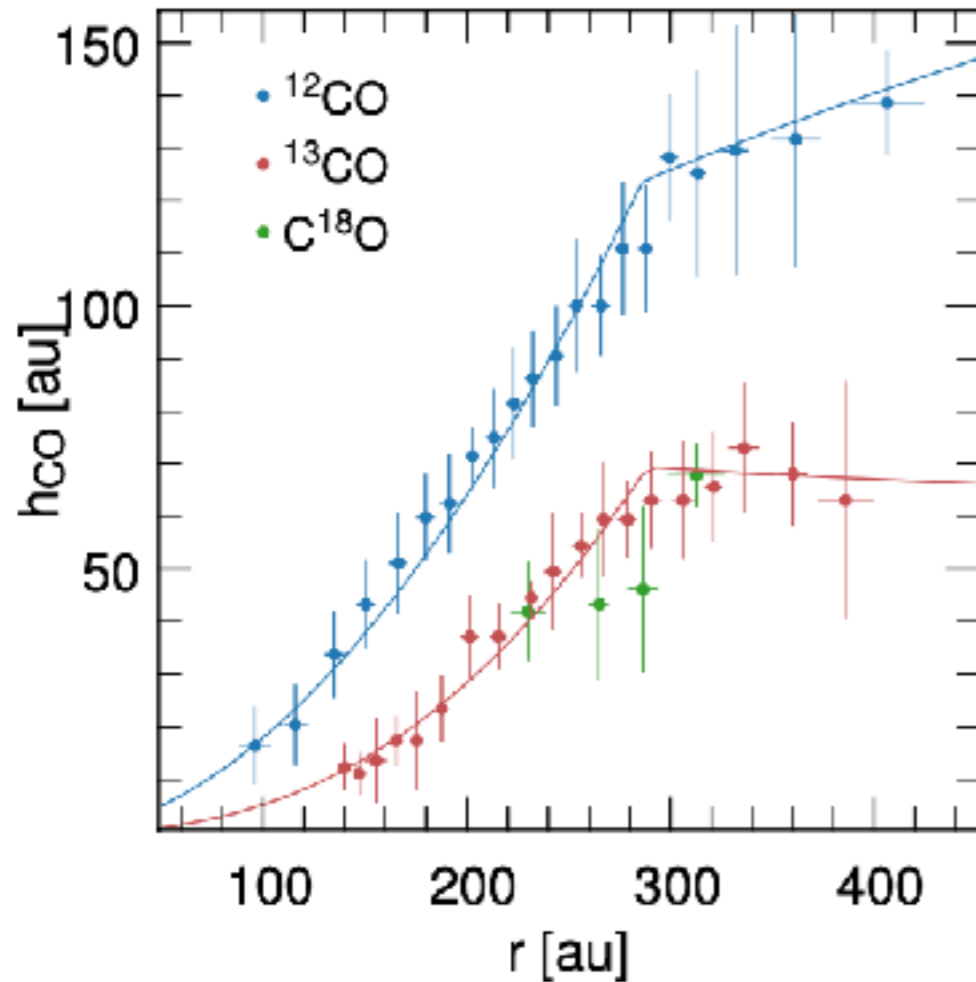
Vertical height

With high spatial and spectral resolution, it is possible to extract the emitting surface height directly from the peak emission in each channel

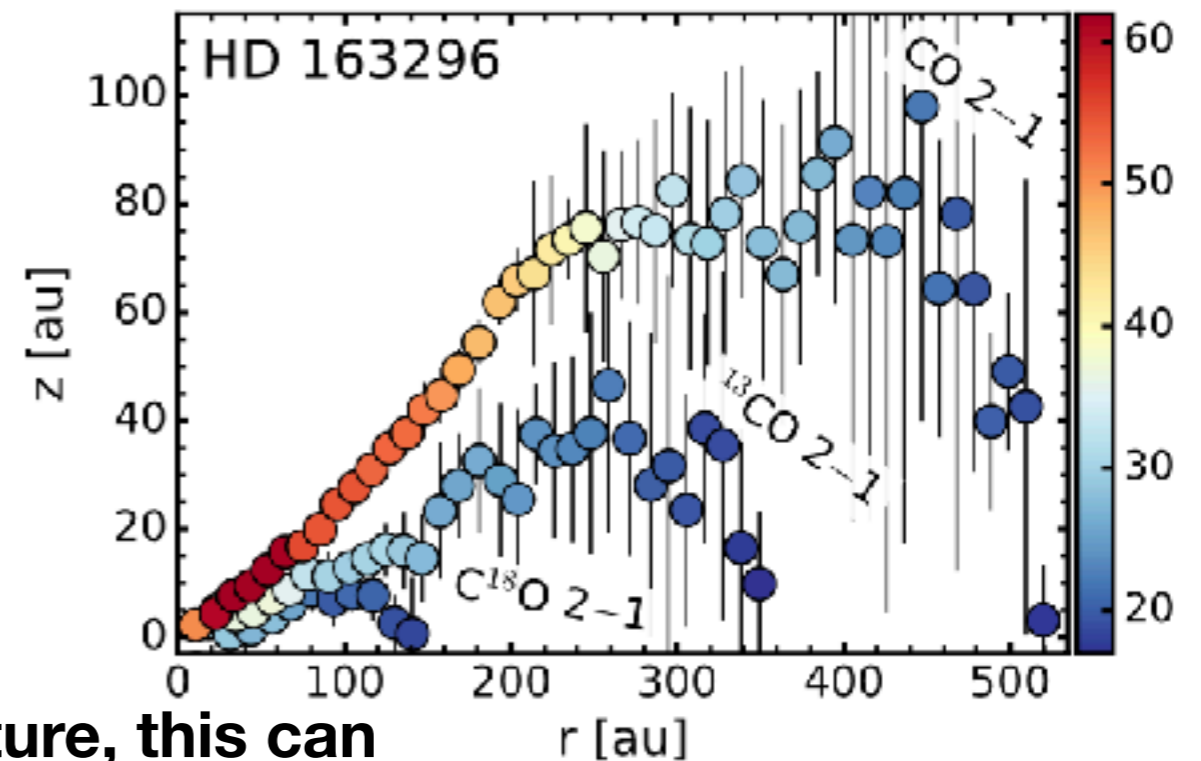
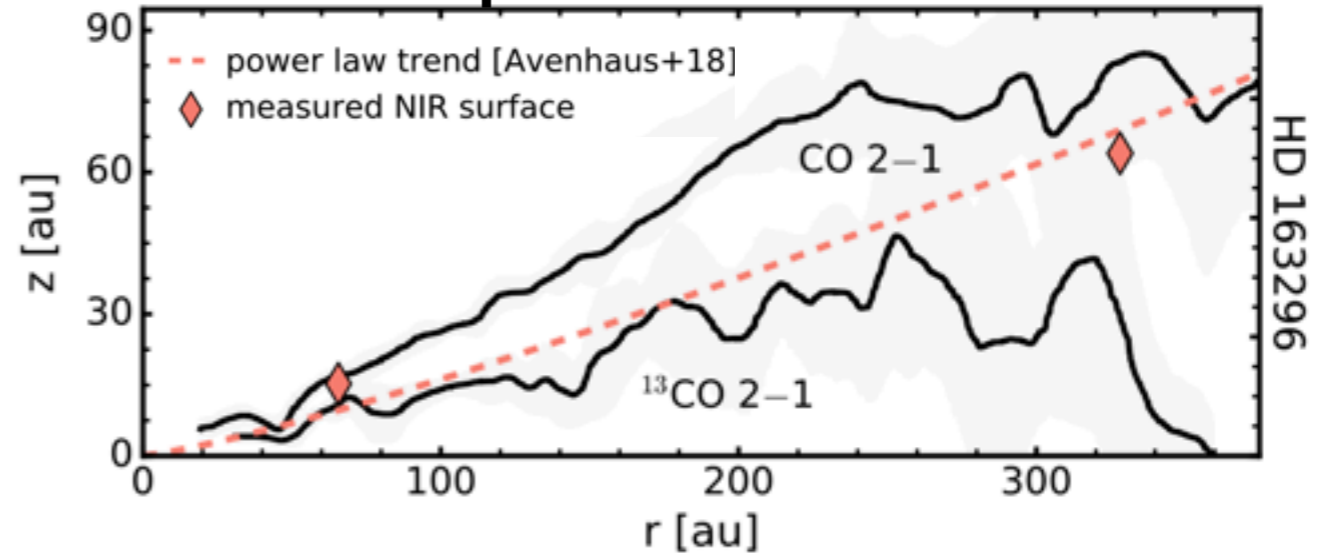


Vertical height

Different CO isotopologues show different heights (optical depth)



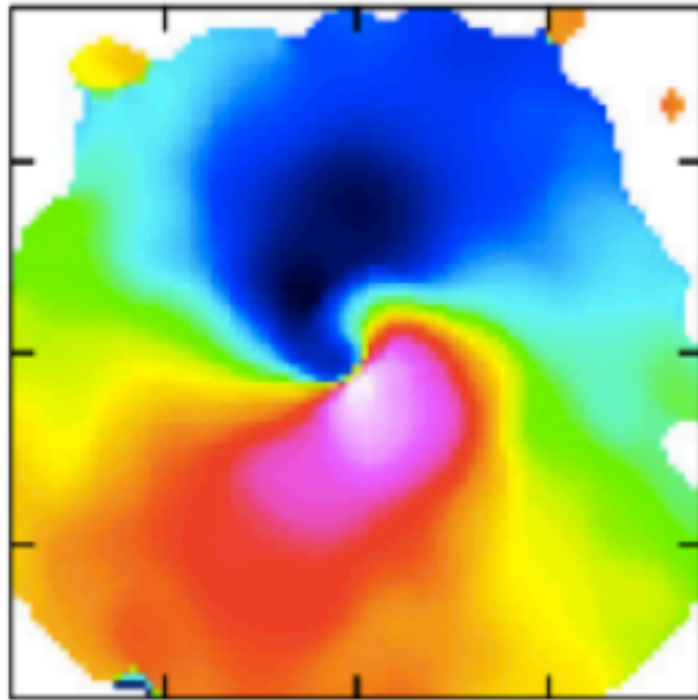
Comparison with NIR surface



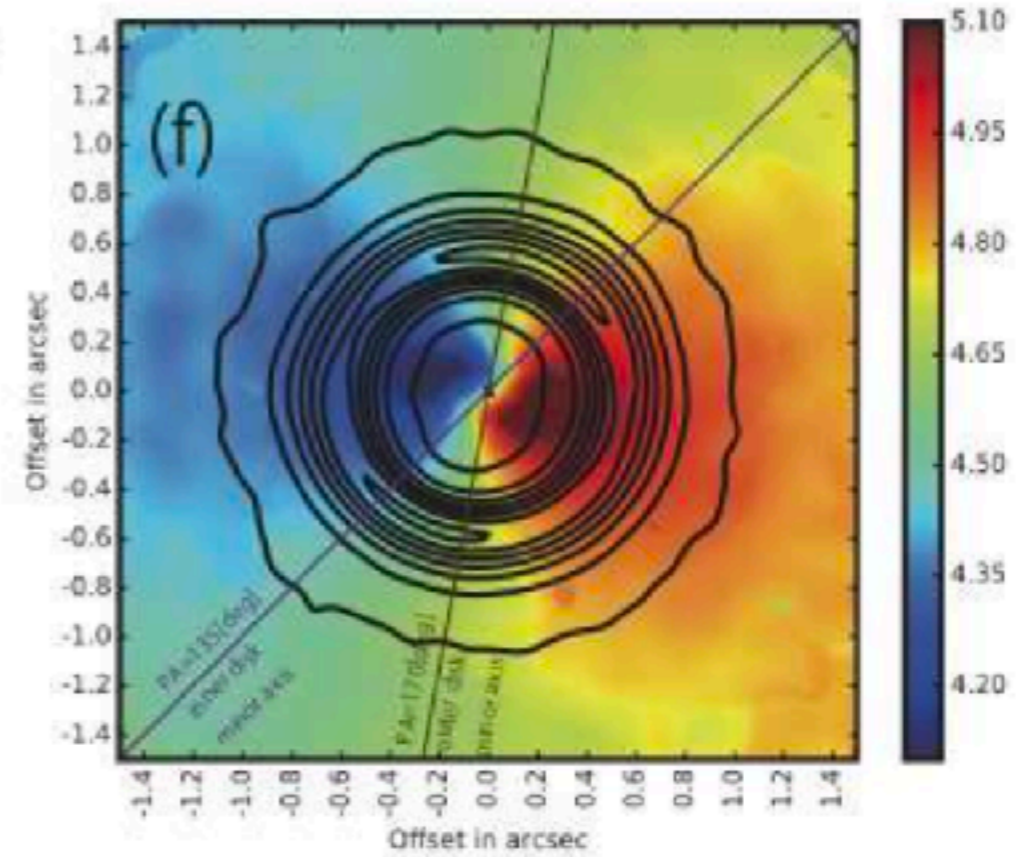
In combination with fits to the temperature, this can constrain the temperature structure in the disk, rather than calculating it with a radiative transfer model

Warps

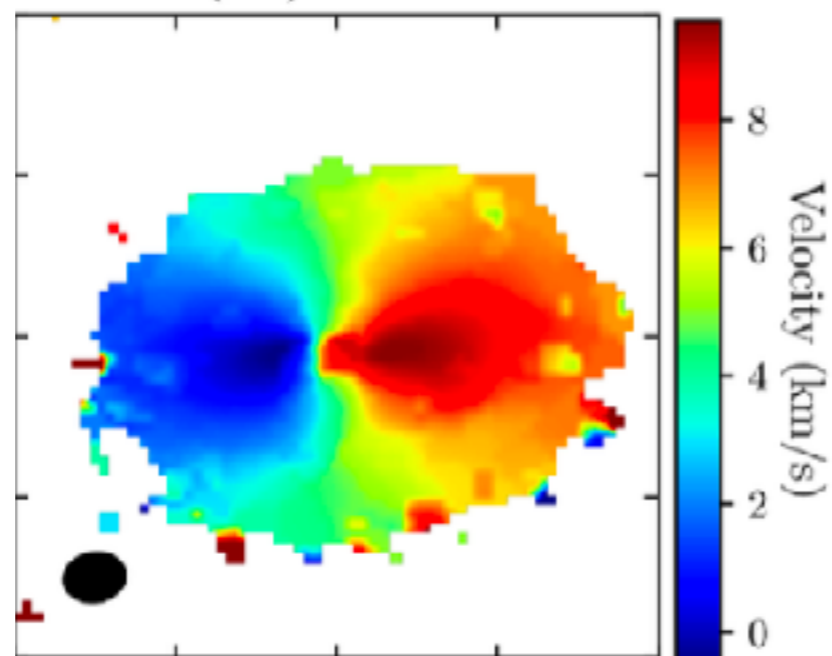
HD142527



J1604-2130

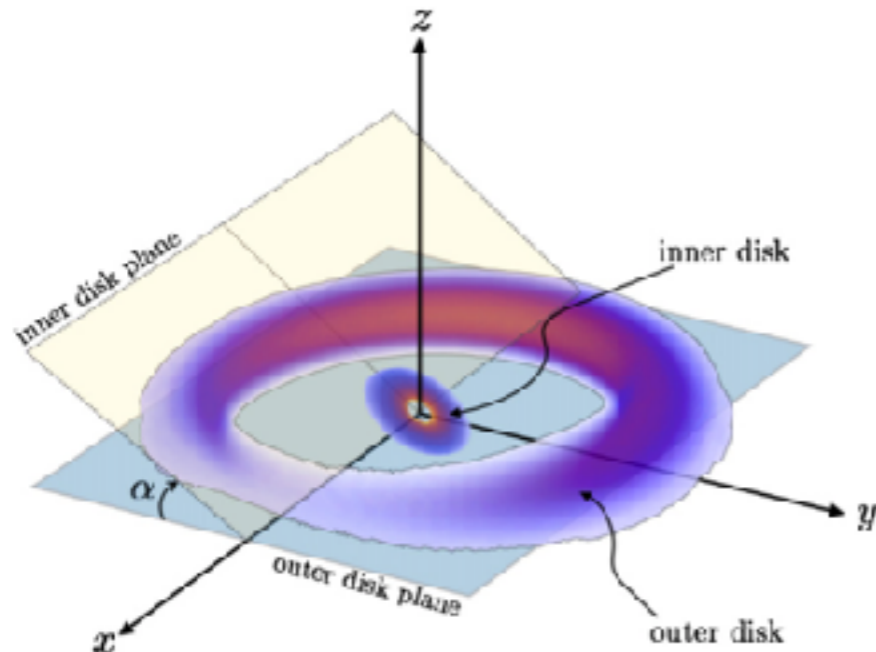


IRS48



Origin warps

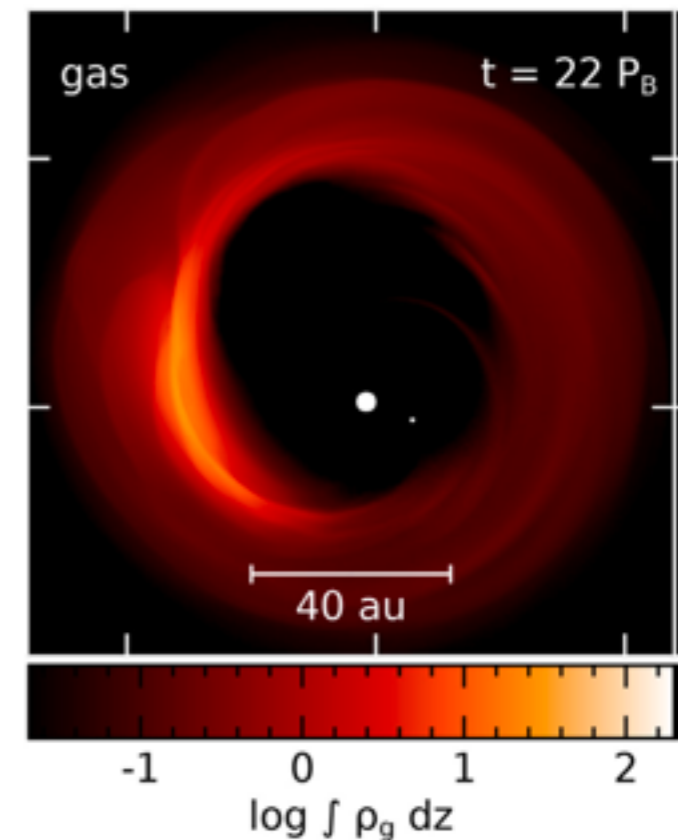
Misalignment between
inner and outer disk



Infalling material
through gap
(‘radial flows’)

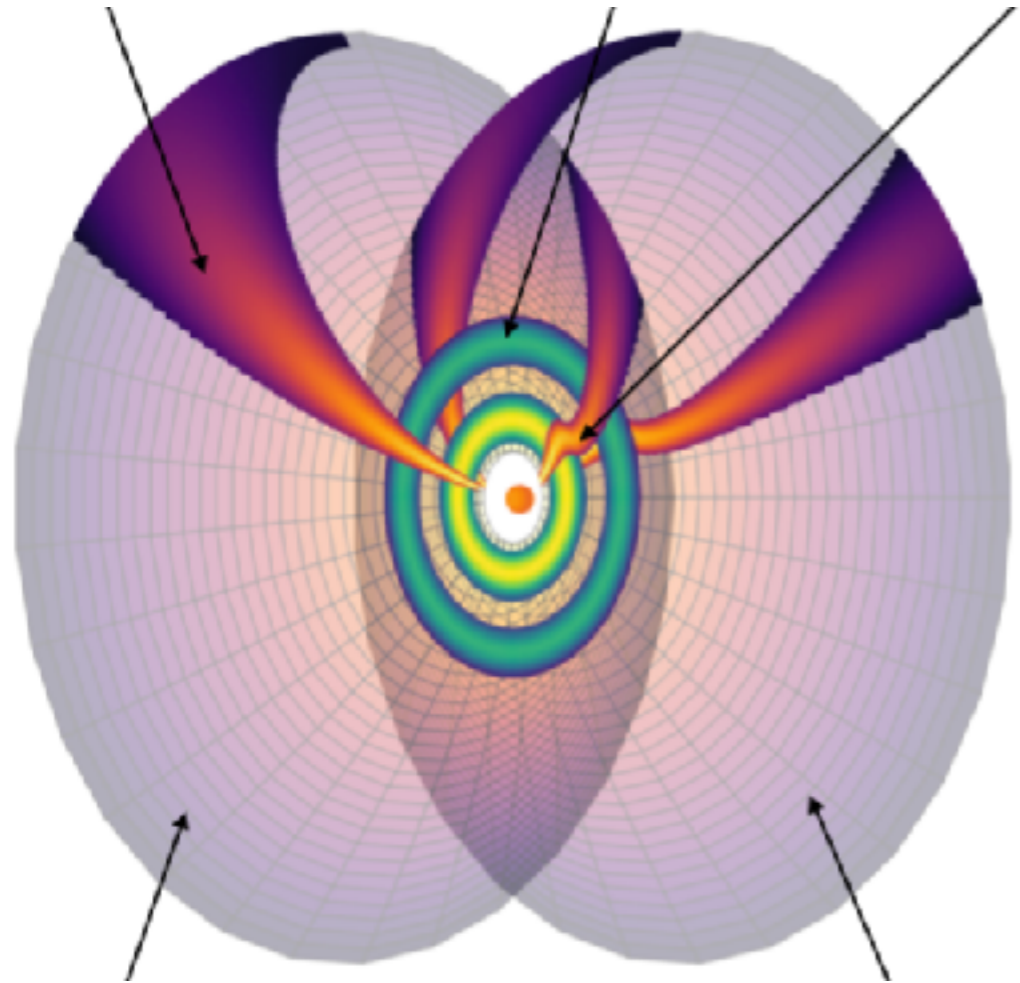


Eccentric disk



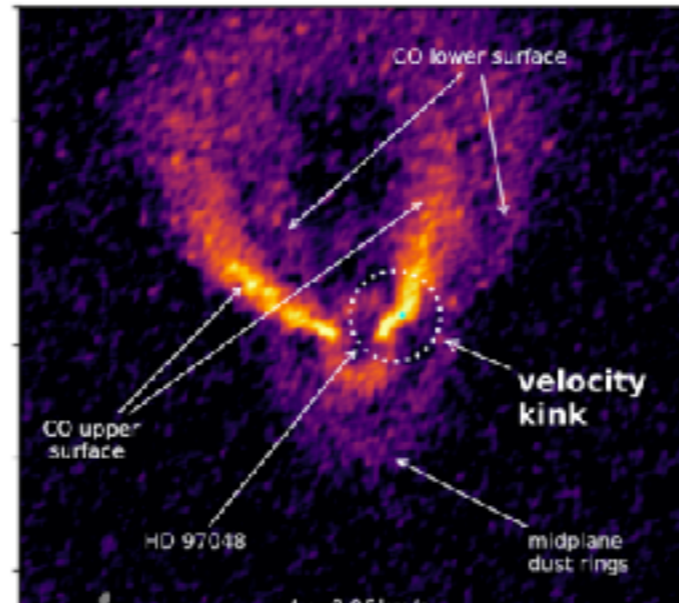
Marino et al. 2015
Zhu 2019
Calcino et al. 2019
Casases et al. 2013
Rosenfeld et al. 2014

Kinks in channels

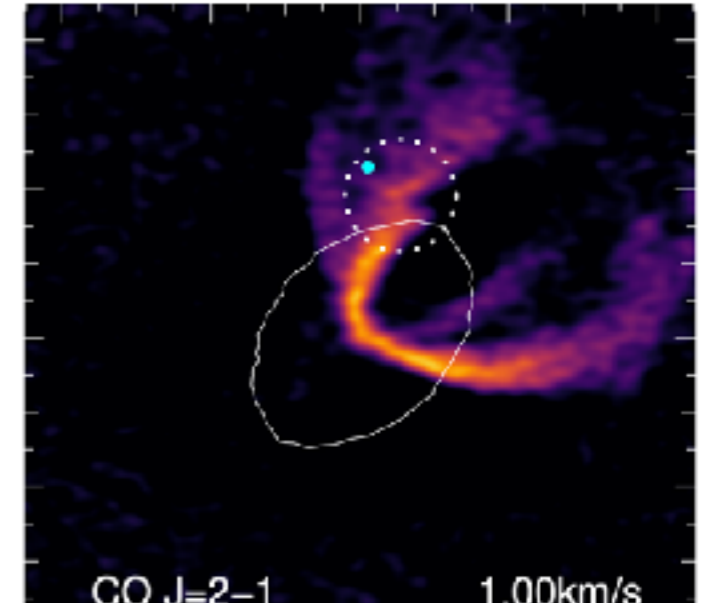


Deviations from Keplerian rotation in CO are thought to be velocity perturbation in the gap caused by the planet

HD97048



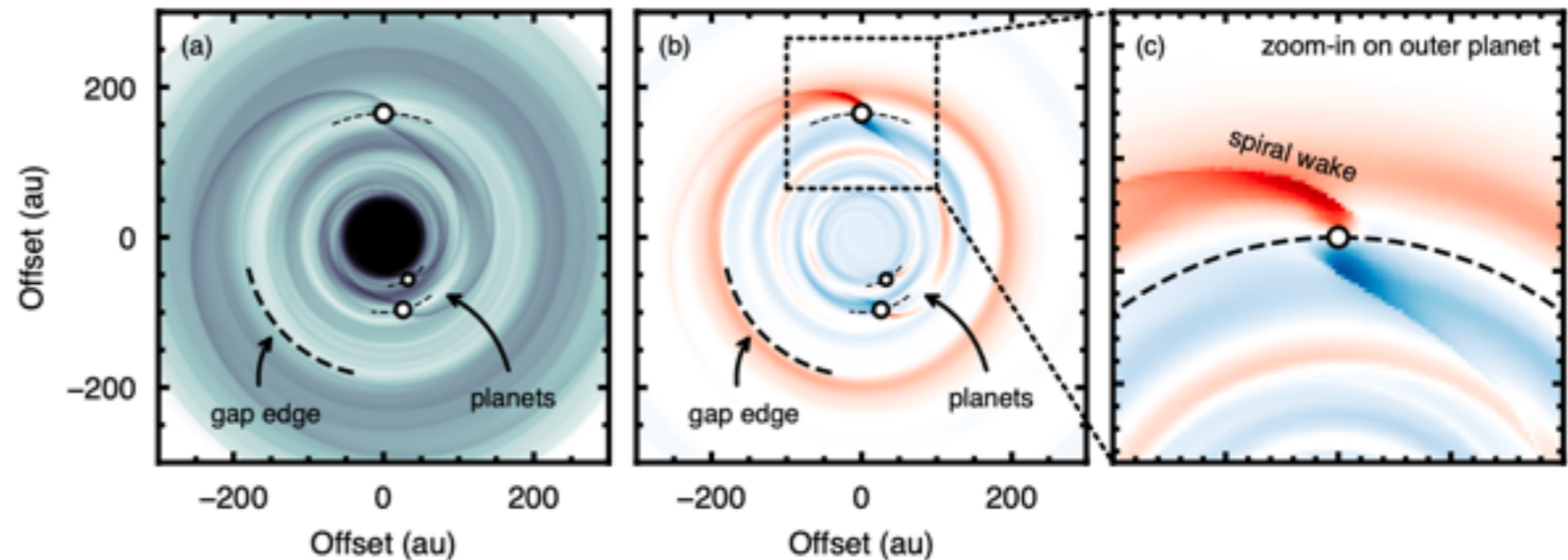
HD163296



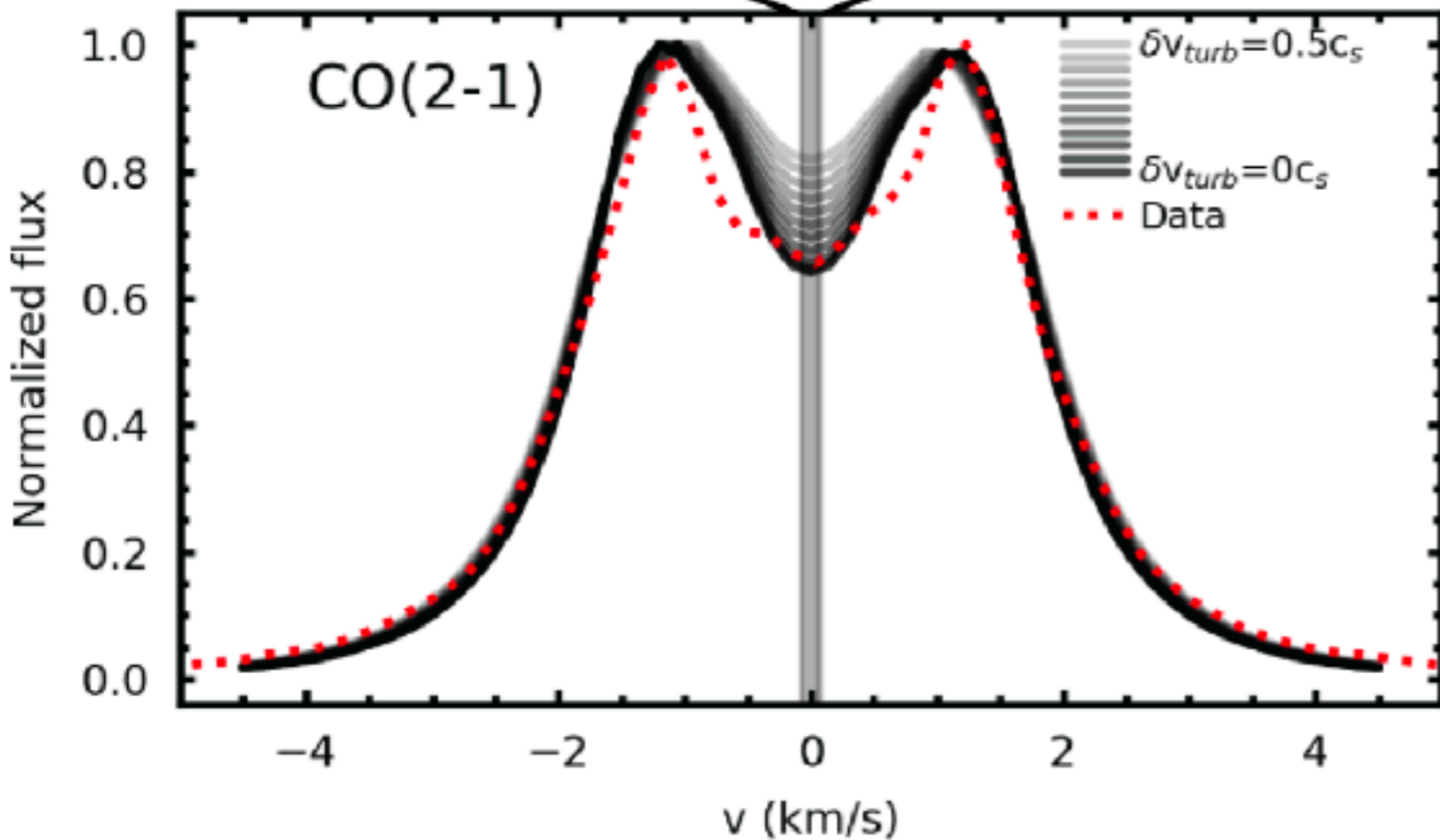
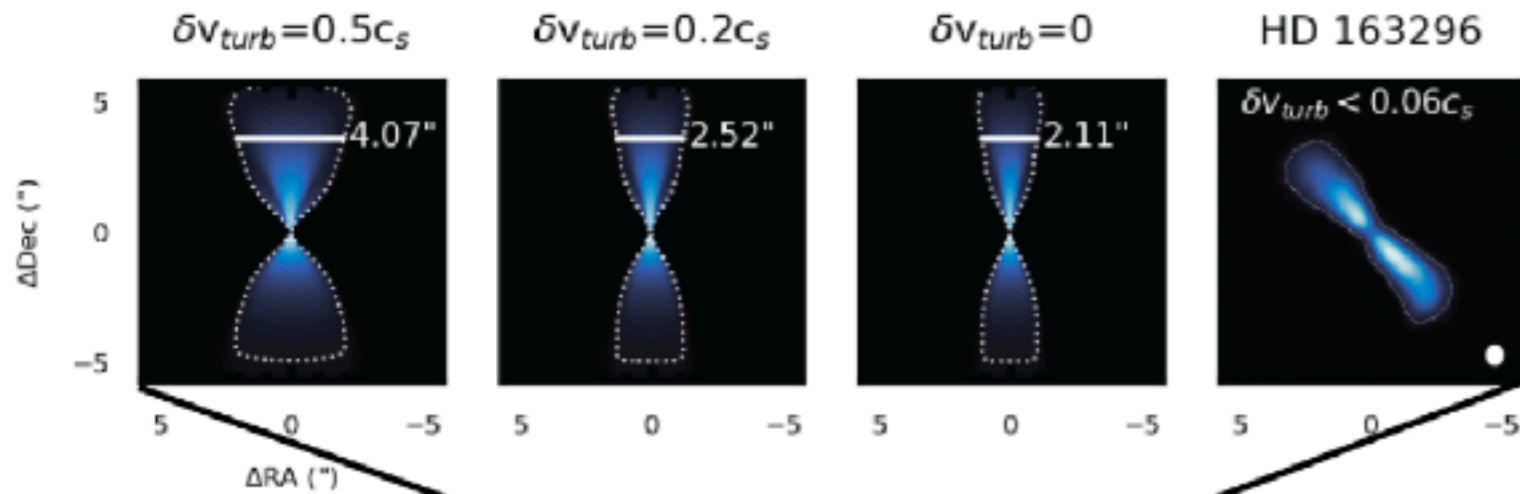
Surface Density ($\log_{10} \text{cm}^{-2}$)
-0.5 0.0 0.5 1.0



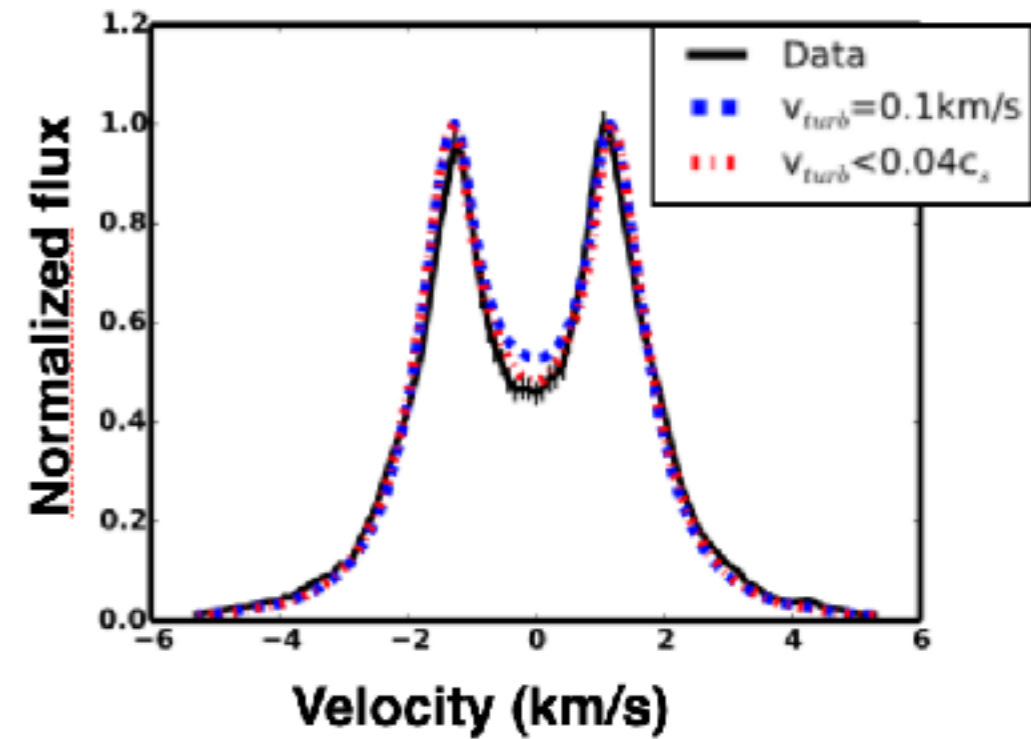
v_{ϕ} Deviation (%)
-5 0 5



Turbulent broadening

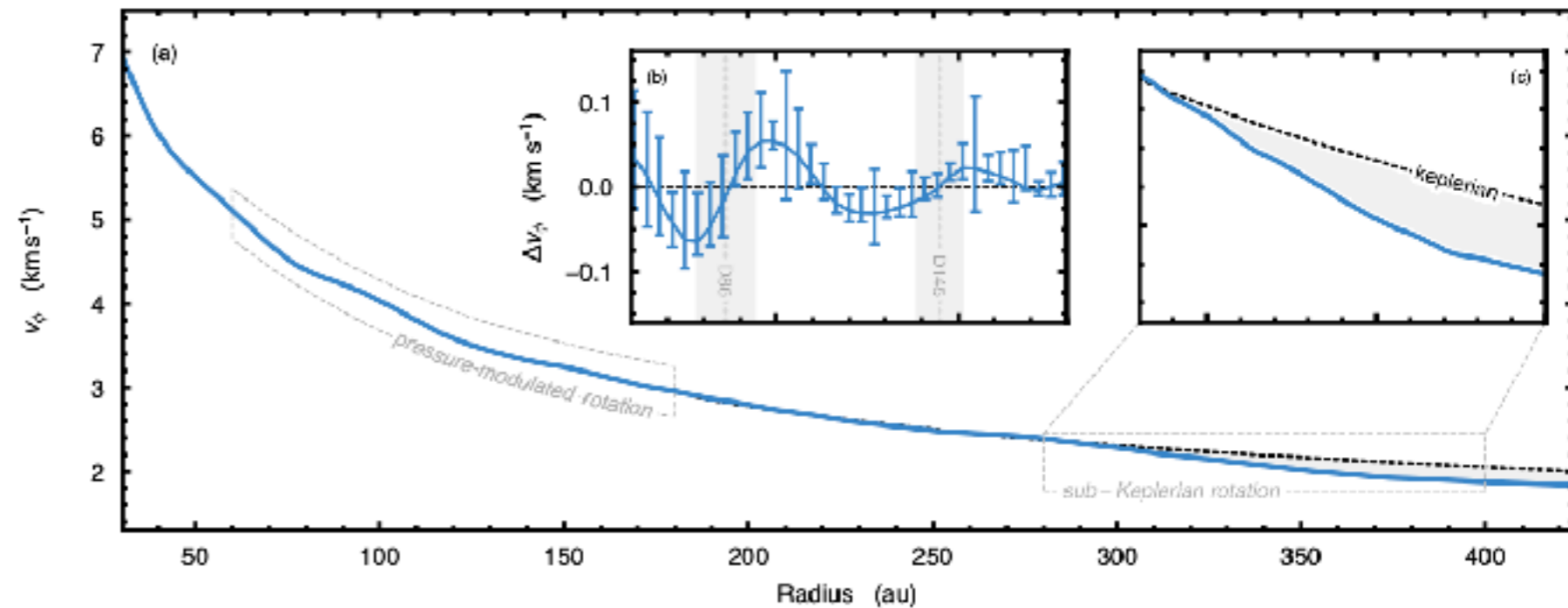
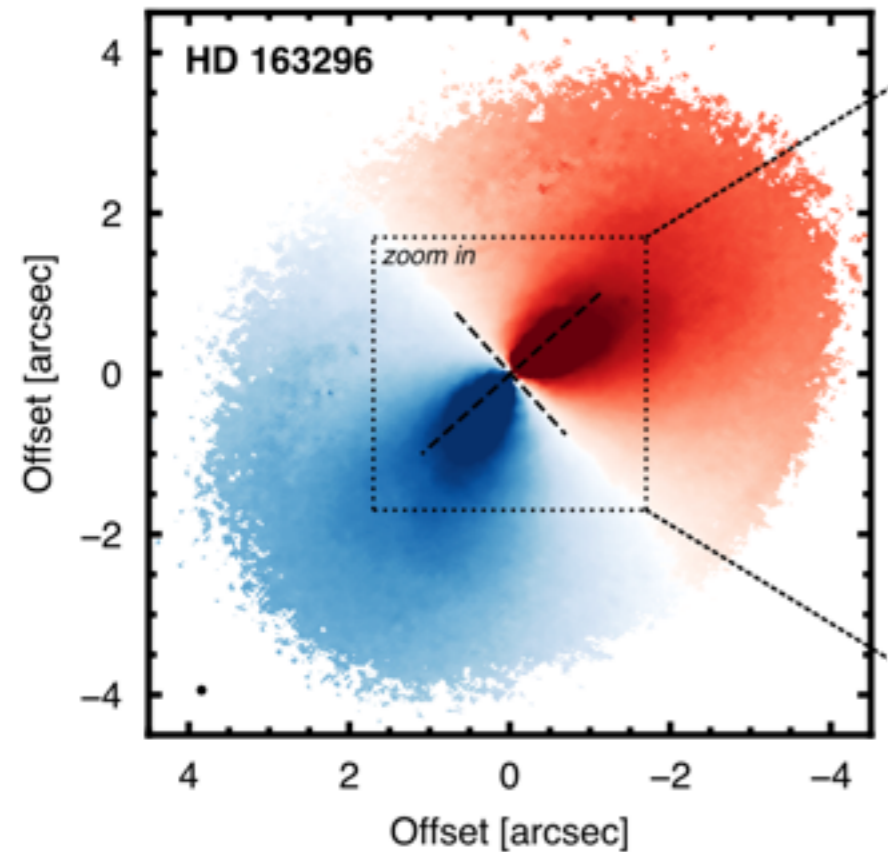


CO line profile: very little pressure broadening



Line profiles and channels allow to measure the turbulent broadening: alpha very low!

Rotation curve



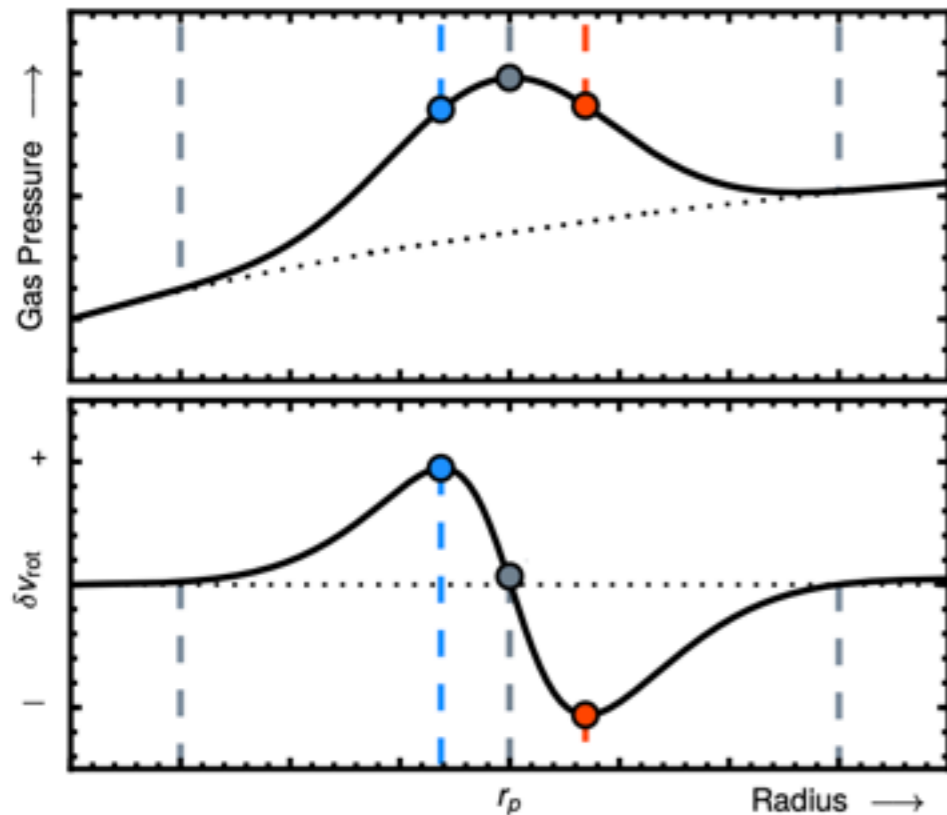
From a first moment map it is possible to extract a rotation curve: azimuthal velocity as function of radius

By assuming azimuthal symmetry, we can extract a rotation curve achieving a precision of less than 10 ms^{-1} .

conerot (Casassus et al., 2021) // eddy (Teague 2019)

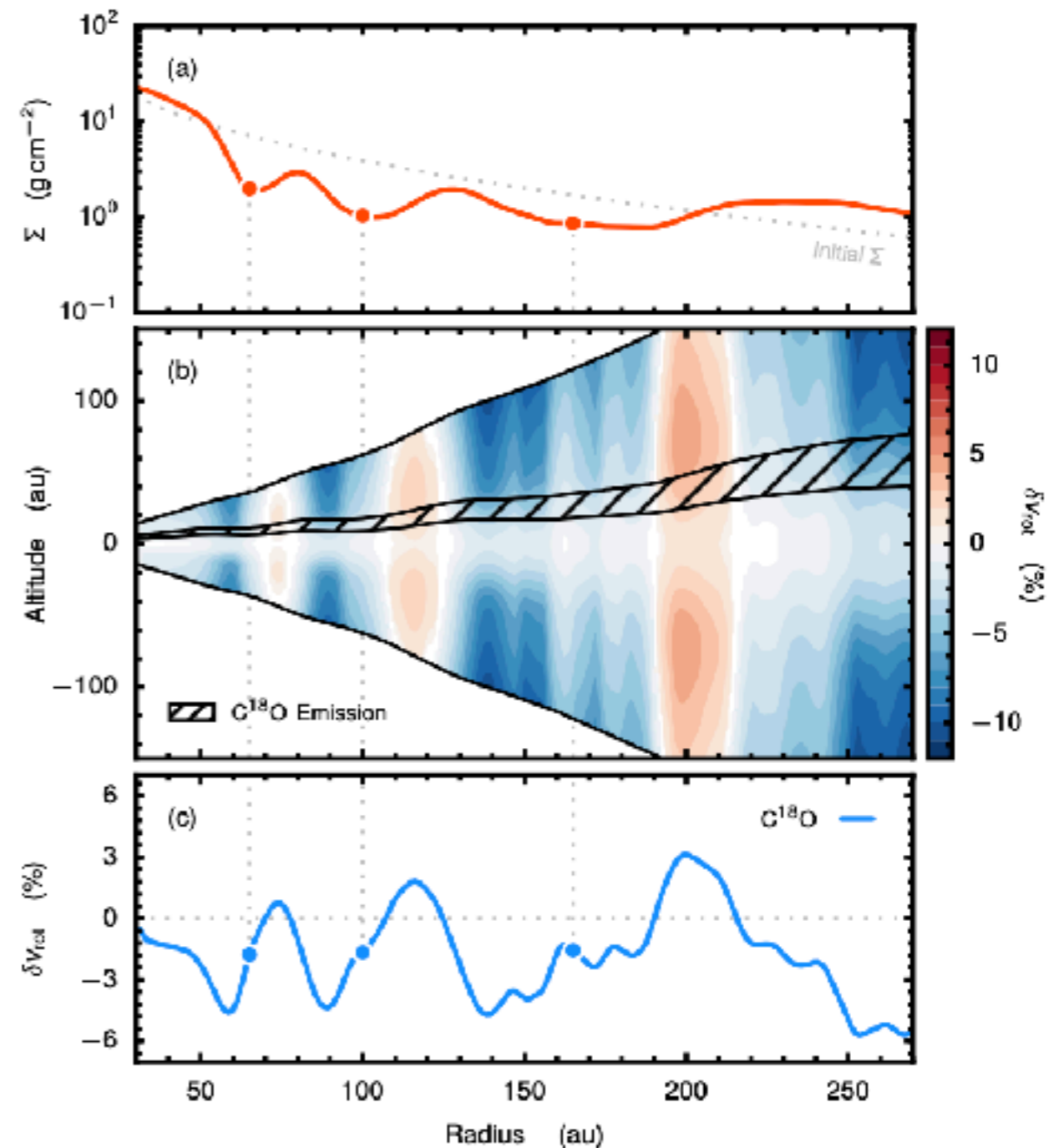
Github tool 'eddy' allows to do this yourself!

Rotation curve



Localized changes in the rotation velocity allow to infer the presence of substructure in the gas pressure.

Changes in dV_{rot} can be converted to pressure => gas surface density gaps

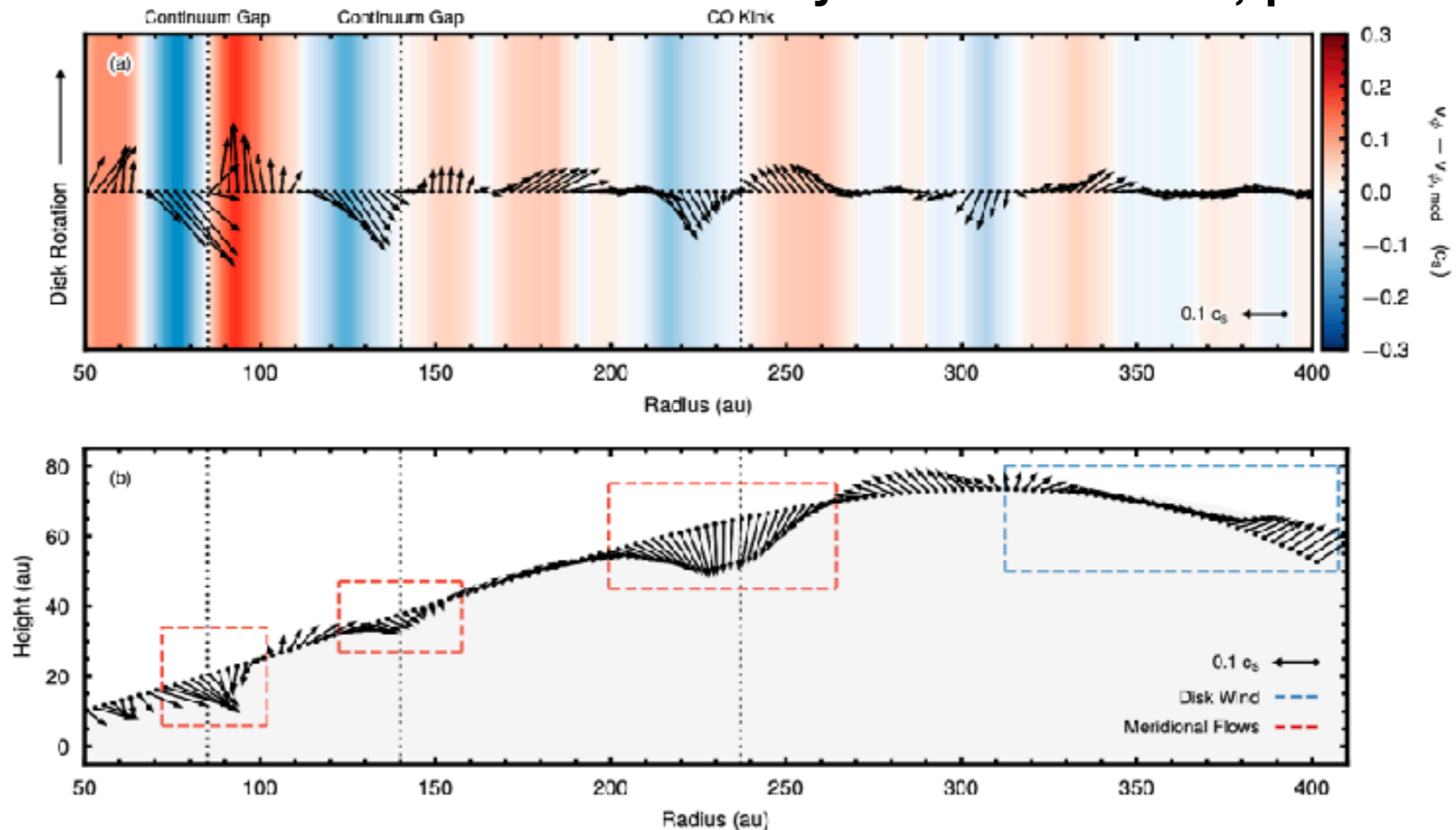


Decomposition

Velocity profile can be decomposed in three dimensions:

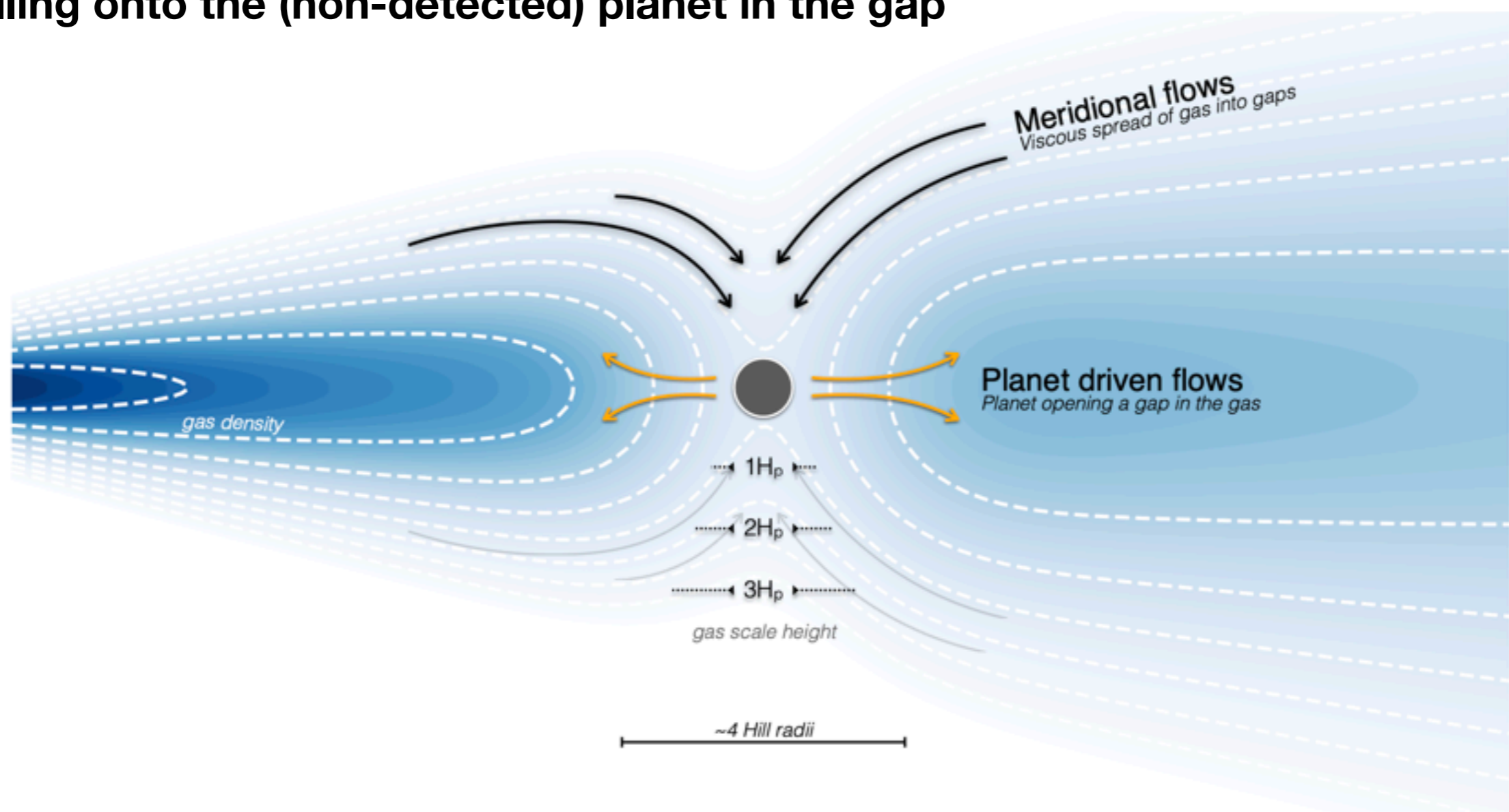
$$v_0 = v_\phi \cos(\phi) |\sin(i)| + v_r \sin(\phi) \sin(i) + v_z \cos(i) + v_{\text{LSR}}$$

So now one can measure the azimuthal velocity variations in the r,-plane



Meridional flows

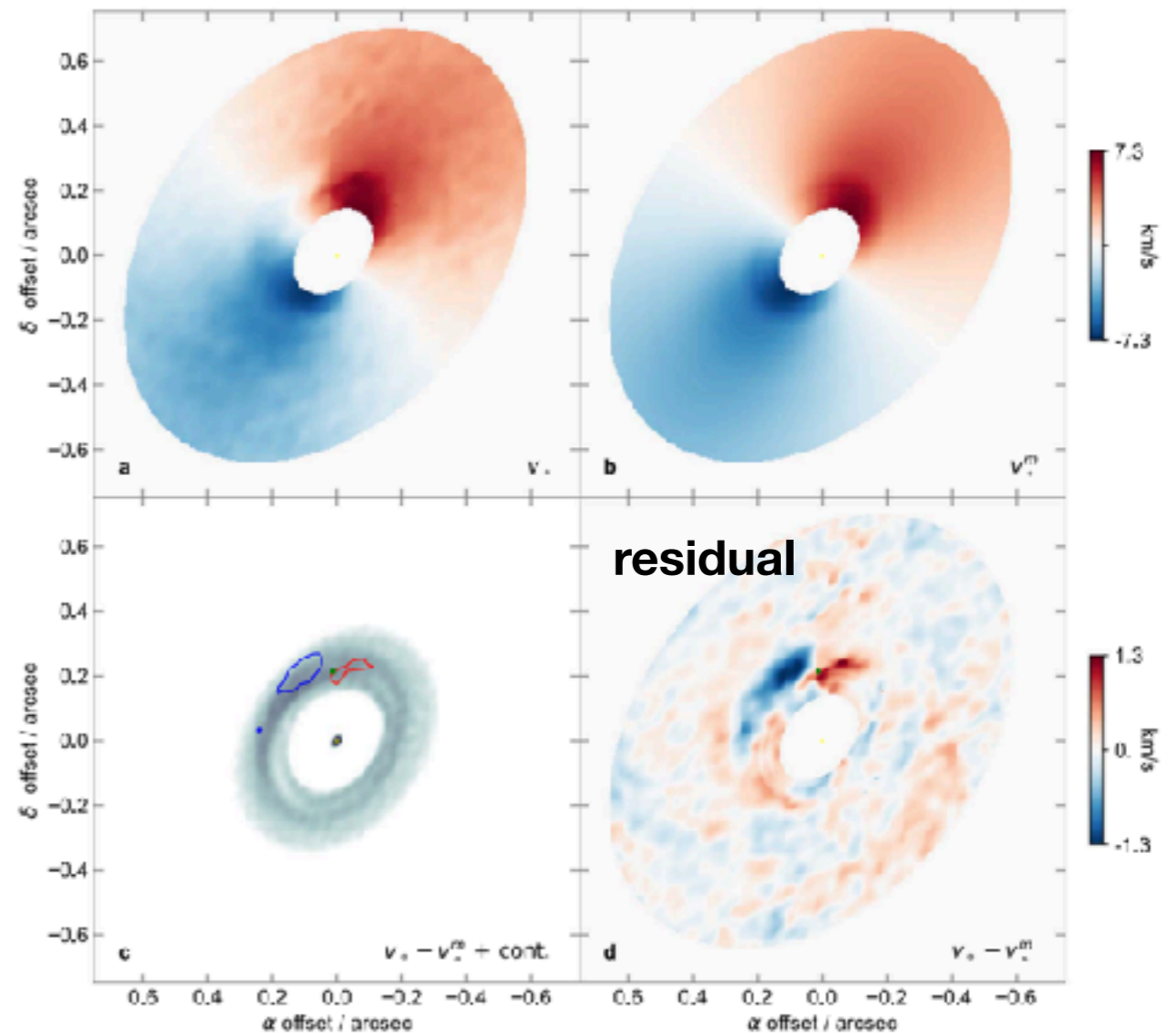
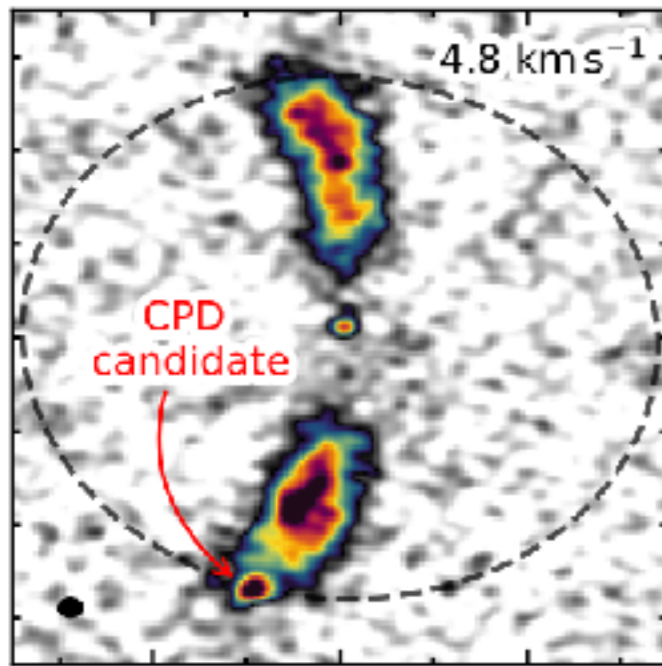
The variations are interpreted as flows of material falling onto the (non-detected) planet in the gap



Circumplanetary disks

HD100546: 'Doppler flip' in ^{12}CO in residual

AS209: ^{13}CO 2-1 blob: CPD because of morphology



But Doppler flip could also be due to a spiral...

Bae et al. 2022

Casassus & Perez 2019

Norfolk et al. 2022

What's next in kinematics?

- Kinematic studies generally rely on high-resolution line cubes in both velocity and spatial resolution (bright disks only)
- Features are generally detected by subtracting a (perfect) model of Keplerian velocity structure in the disk and look in the residuals
- Will have to be careful with imaging artefacts, continuum absorption, spiral structures, low SNR features before making claims
- Several tools publicly available to analyse cube data (GitHub): eddy, bettermoments, discmminer...
- ALMA Large Program exoALMA (PI: Teague): 15 disks at 0.1" resolution and 0.026 km/s velocity resolution

Questions?

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astro@nienkevandermarel.com
<http://www.nienkevandermarel.com>