

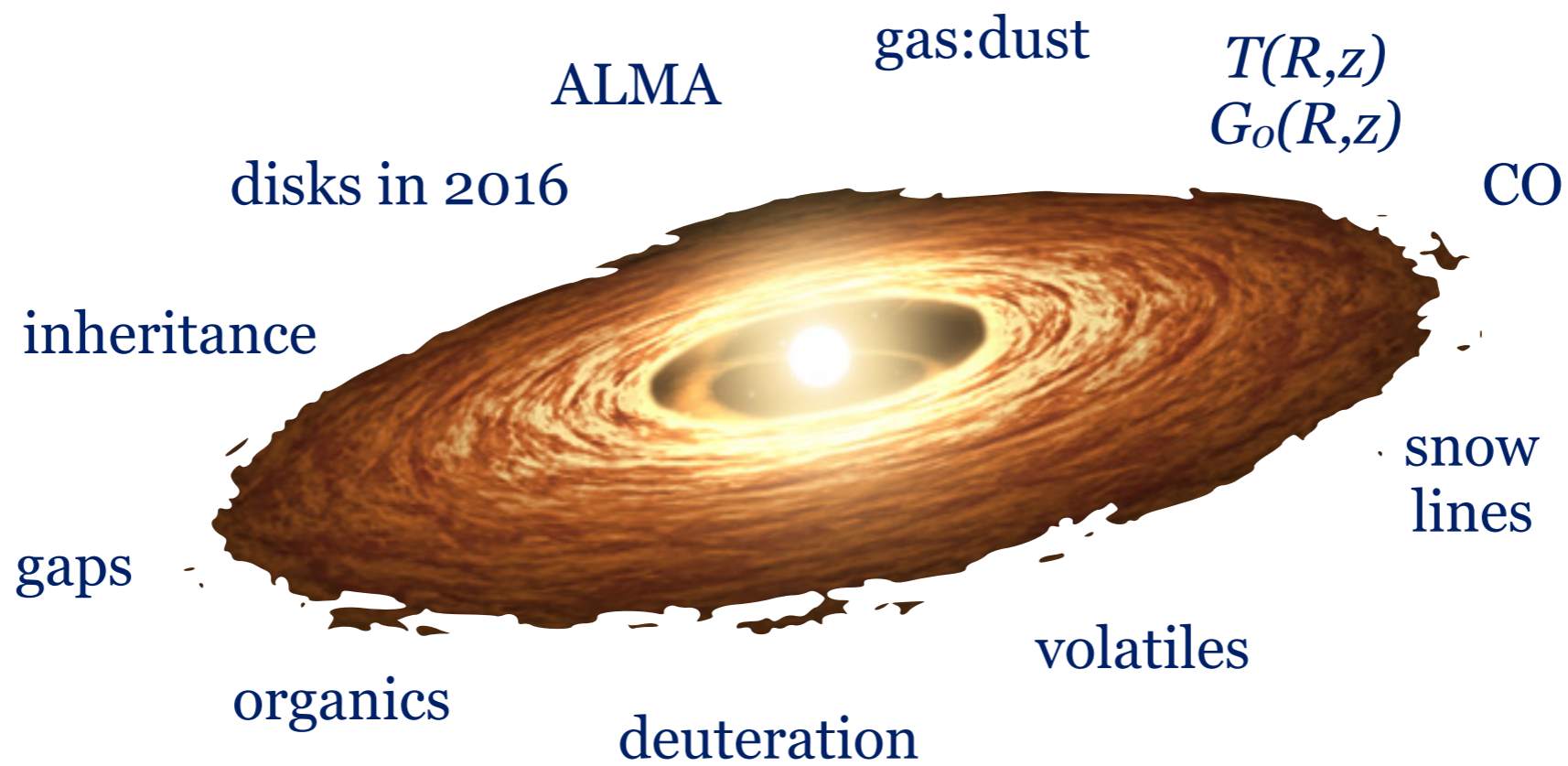
Chemical conditions of gas in planet-forming disks



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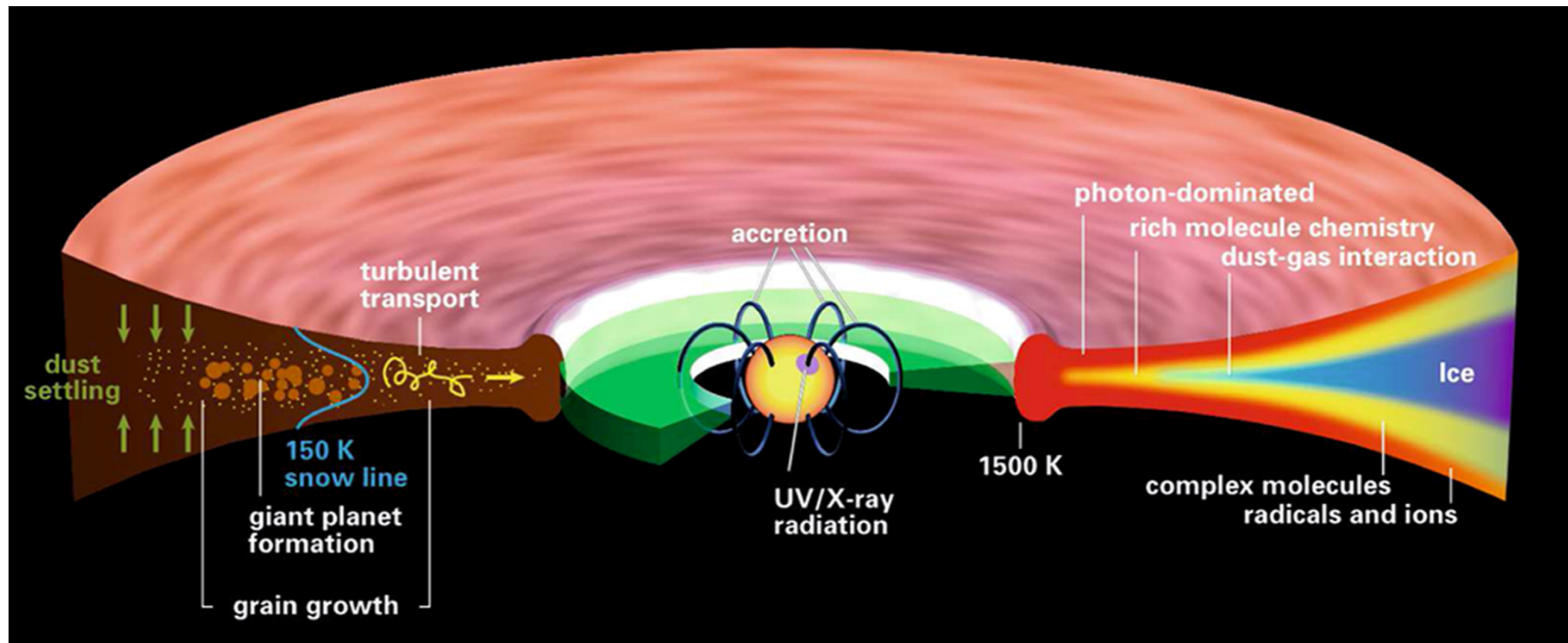
Big questions

- What is the gas mass and the gas:dust ratio?
- What is the chemical inheritance for the ISM & star formation process?
- What is the balance between ice and gas? What is the role of snow lines?
- Where do the elements like C,O,N reside?
- Where/how do organics form?
- (How) does the chemistry reflect the underlying disk structure?



Disk structure

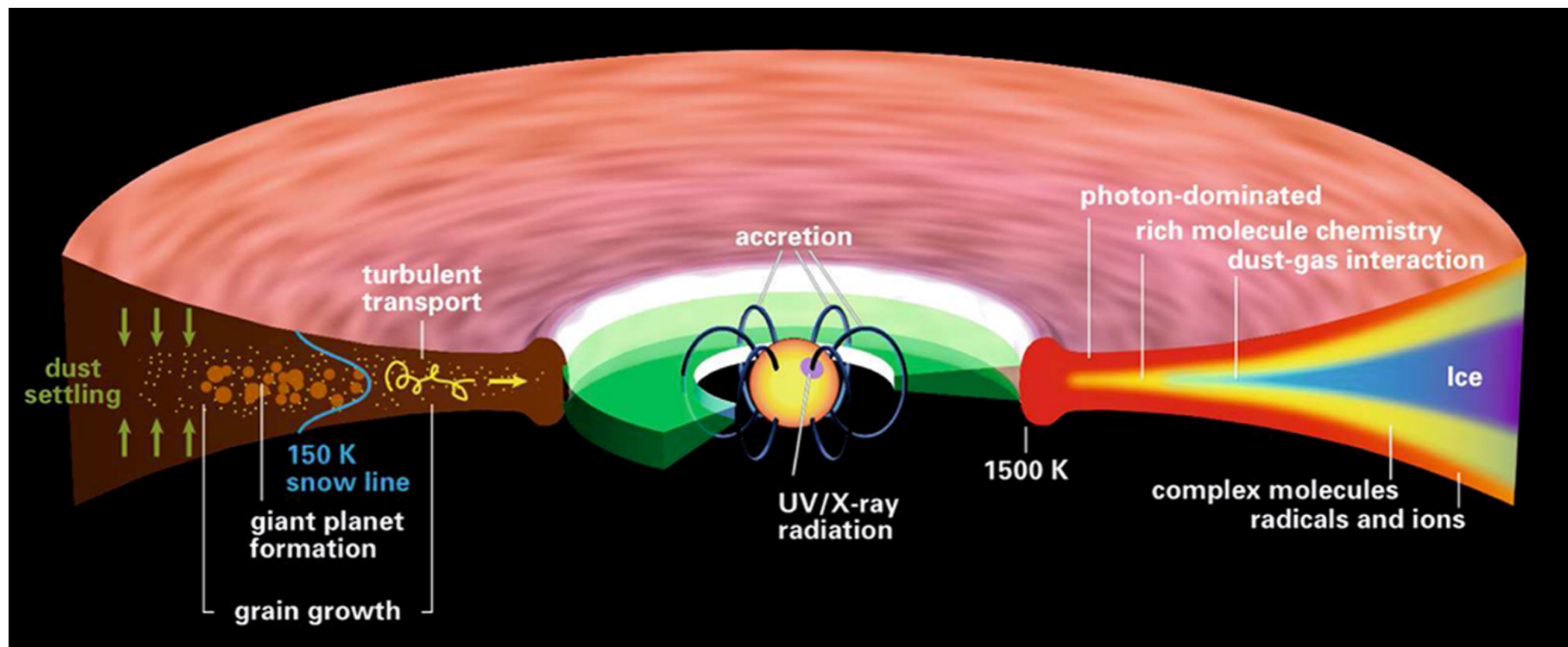
- *Basic* structure of the disk
 - Radial surface density profile (gas, dust)
 - Vertical hydrostatic scale height
 - Irradiation by stellar spectrum
- Assumption: small ($\sim\mu\text{m}$) grains coupled (thermally, hydrodynamically) to gas
- \Leftrightarrow Spectral Energy Distribution fitting provides overall disk structure



$T(R,z), G_o(R,z)$

- Radial and vertical temperature gradient
- (Inter)stellar ultraviolet radiation attenuated by small grains → photo-dissociation layer
- Stellar X-rays, cosmic rays penetrate to midplane → secondary ionization
 - Do stellar winds shield Cosmic Rays effectively from the disk?
 - Short-lived radioactive nuclei also (may) provide secondary ionization

Cleeves et al. (2013, 2014, 2015)

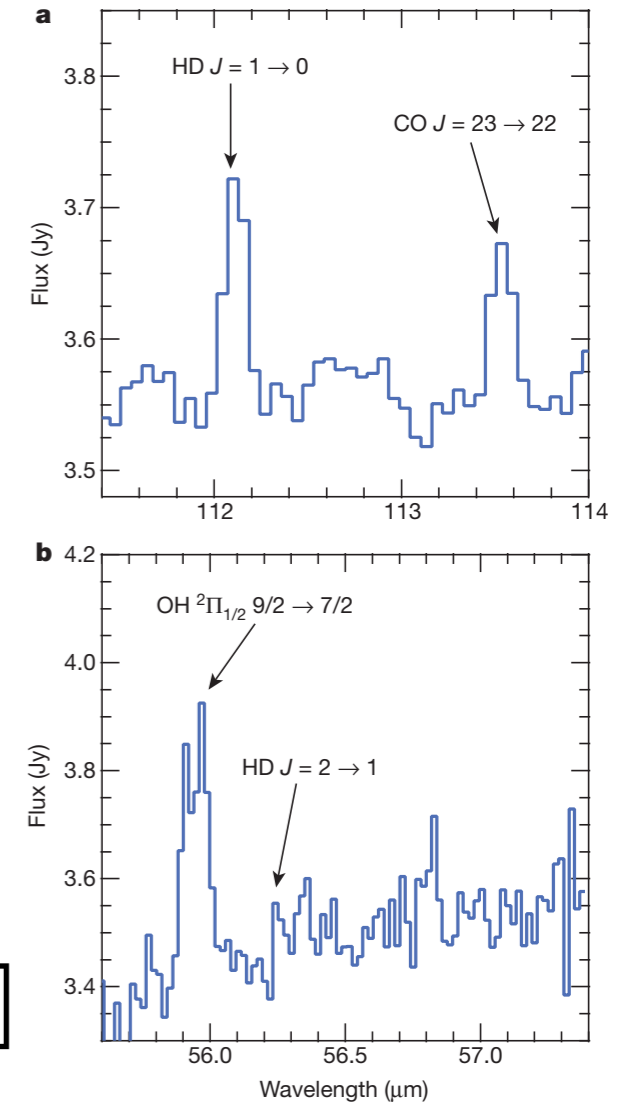


Henning & Semenov (2013)

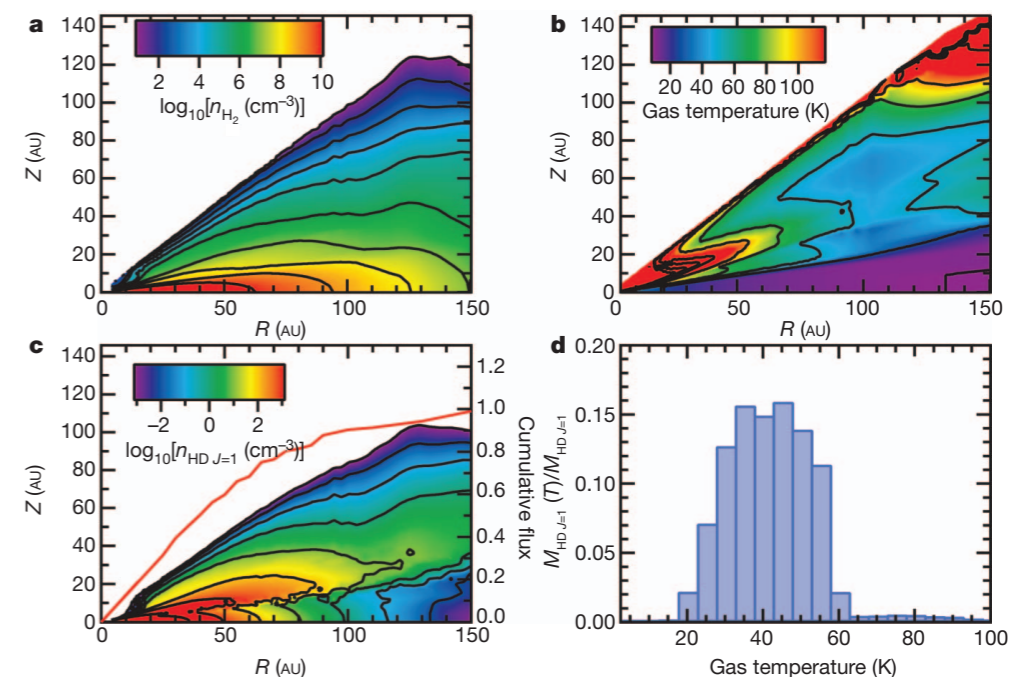
Gas:Dust

- Dust mass estimates good to ~factor of a few
 - Complications: dust evolution, migration
- Gas mass estimates uncertain
 - CO generally observed to be depleted (... see next slides...)
 - H₂ only observable in warm/hot surface, inner disk (weak lines)
- HD detected in TW Hya

- With thermal structure (+chemistry) → large gas mass estimates (0.05 M_{sun}), gas:dust~100:1 (~ISM)
- Model uncertainties? Unresolved contributions from hot material? Generalization to other disks?



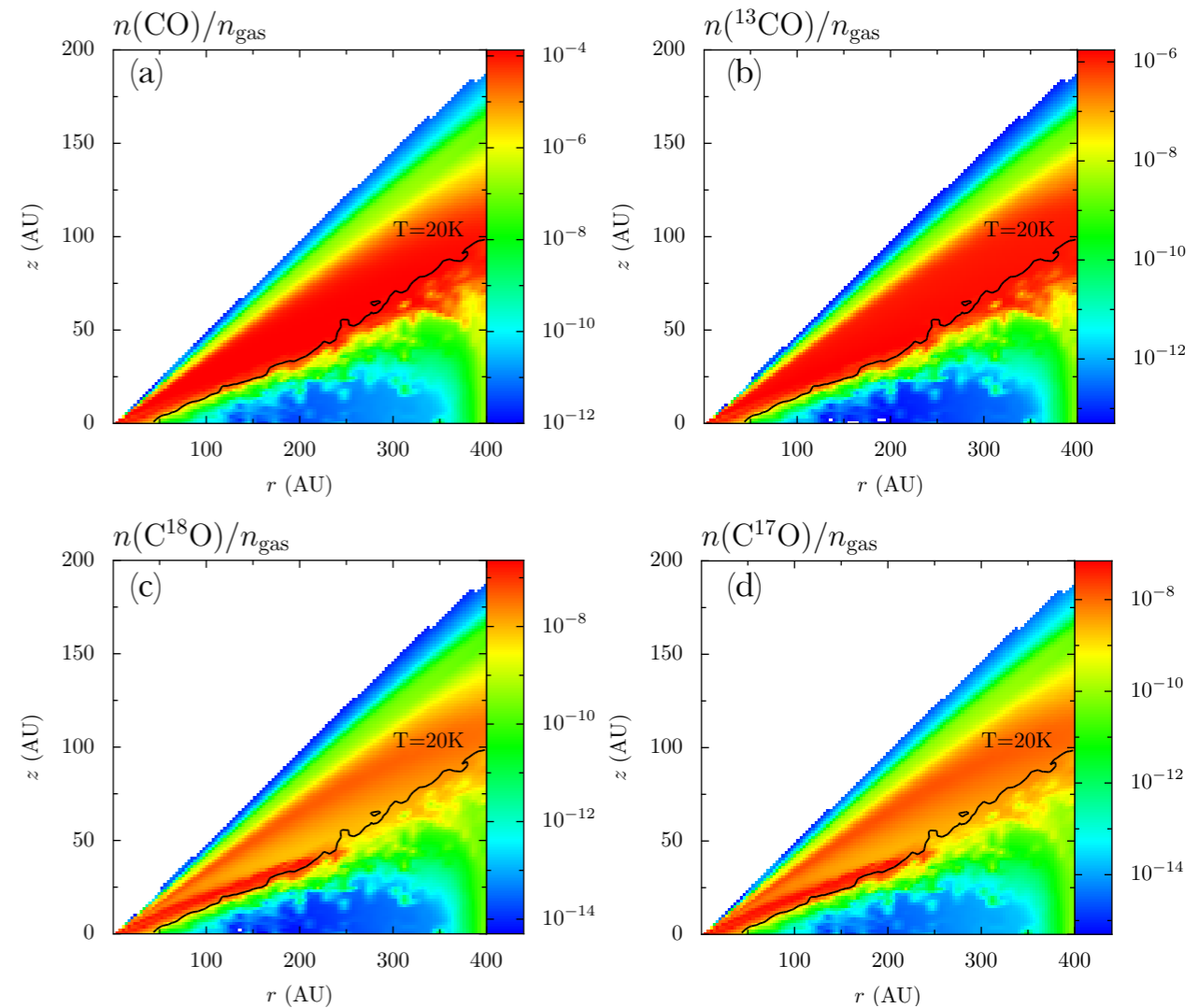
TW Hya



Bergin et al. (2013)

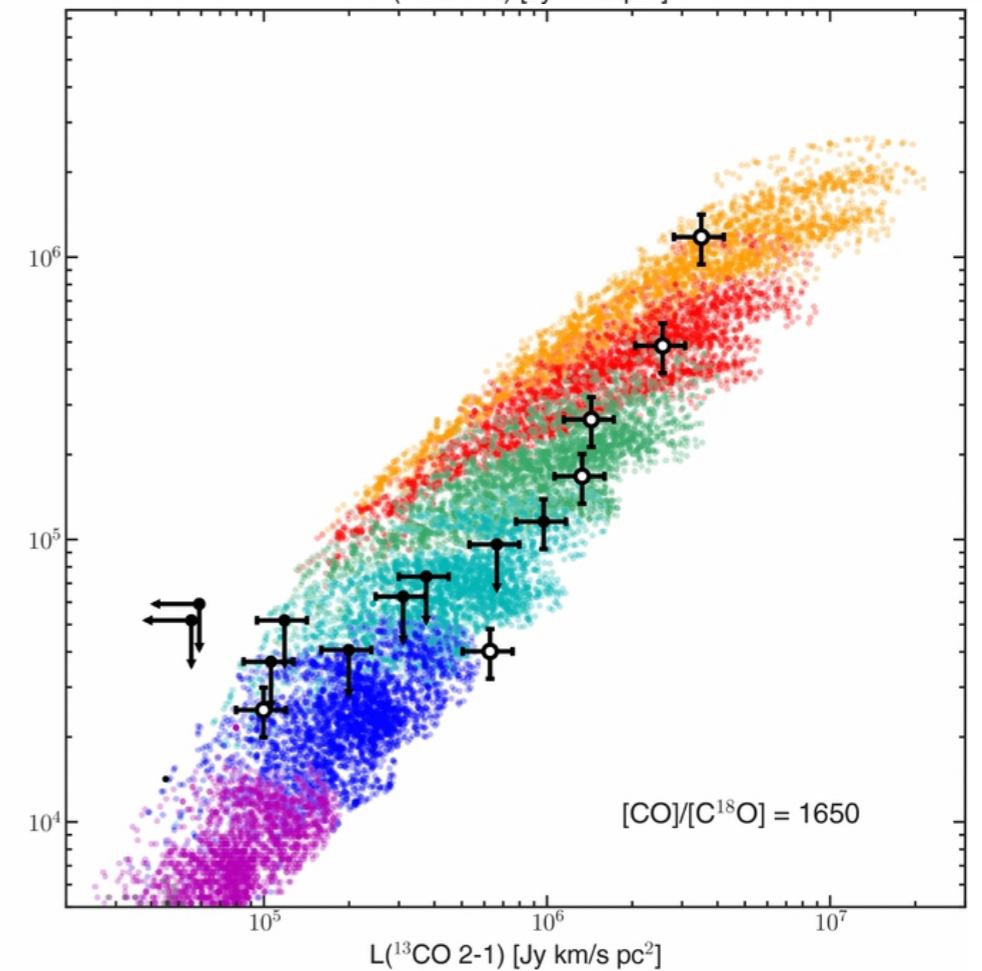
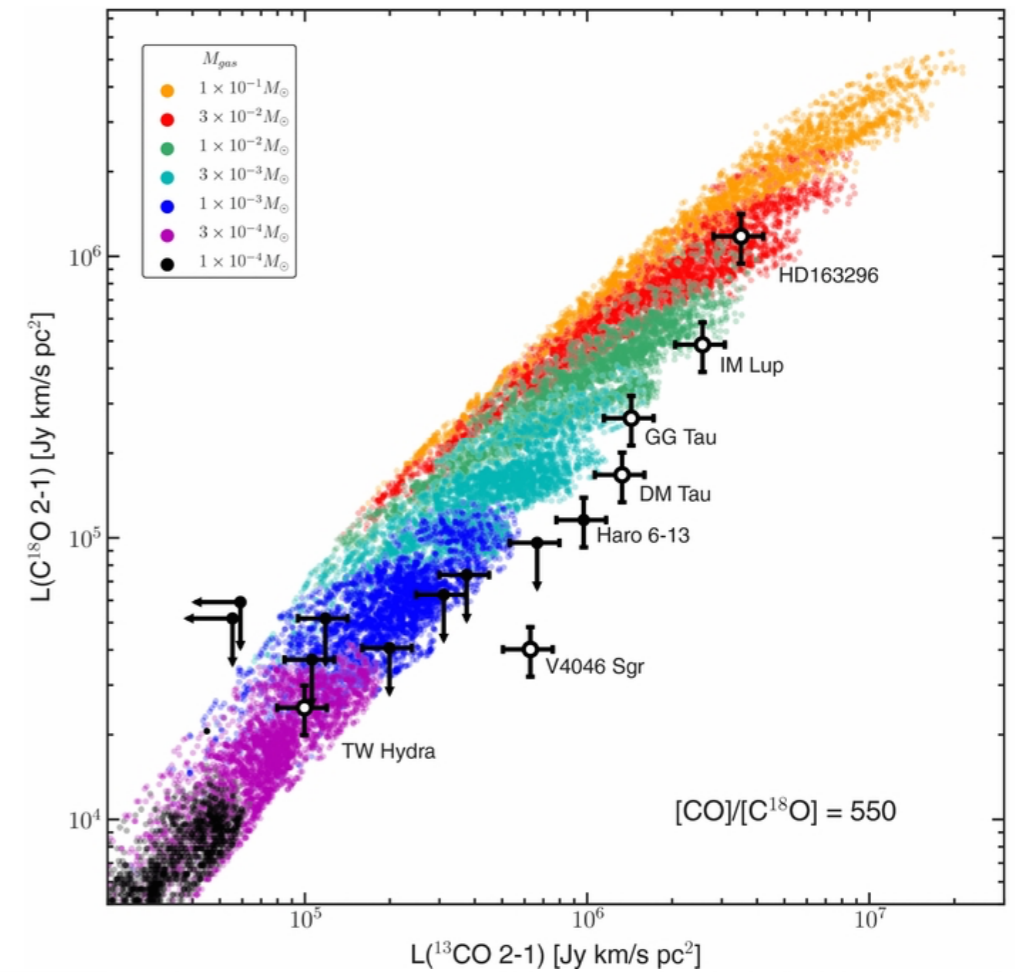
CO depletion

- Consistently observed to be depleted (Dutrey et al. 1997, ...)
- Freeze out in cold disk interior
- Photodissociation of CO in UV-irradiated surface, outer region
 - Isotope-selective photodissociation: ^{13}CO , C^{18}O , C^{17}O
- With appropriate model: reliable gas masses
 - e.g., Lupus survey gas:dust <100 (Ansdell et al. 2016)



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Snow lines

- Radial temperature gradient → snow lines for major volatiles: H₂O, CO, N₂?
- Directly traced via CO isotopes

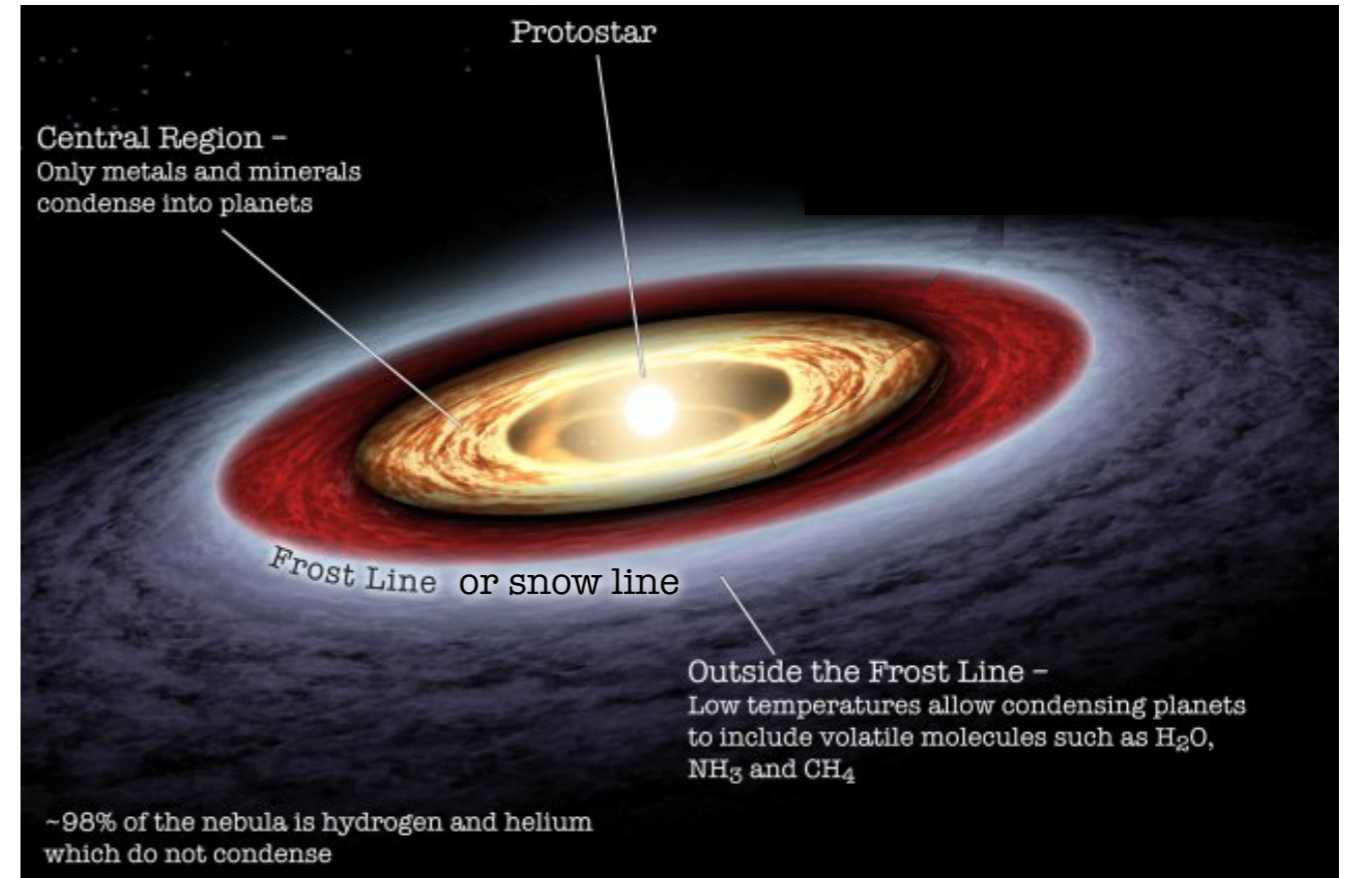
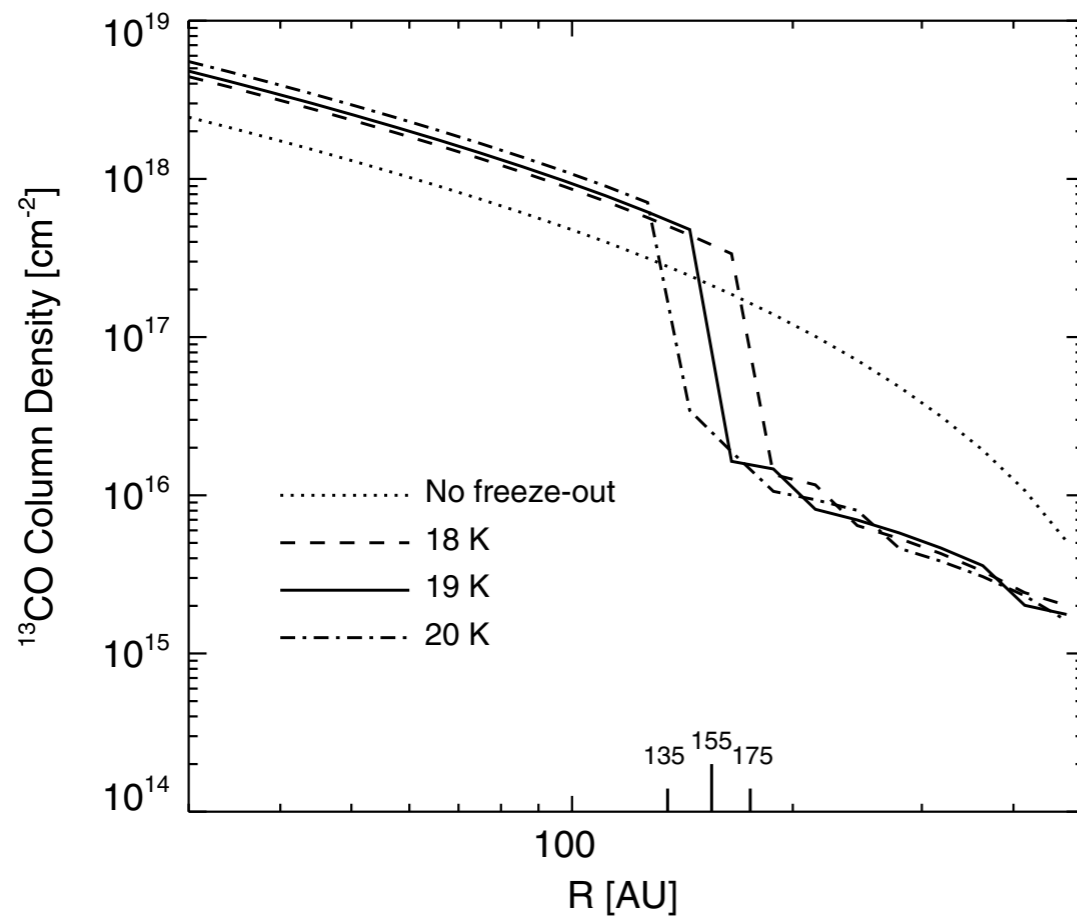
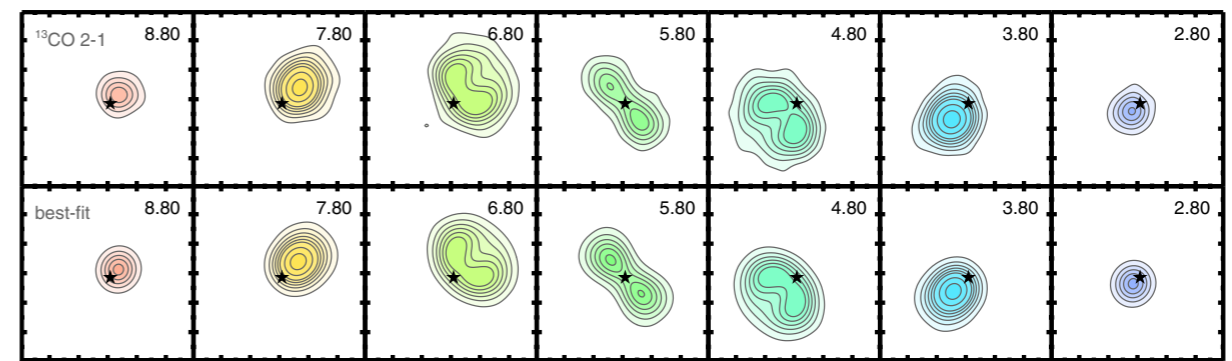


Image credit: NASA/JPL

HD163296



Qi et al. (2011)

Snow lines

- Radial temperature gradient → snow lines for major volatiles: H₂O, CO, N₂?
- ...or indirectly via N₂H⁺

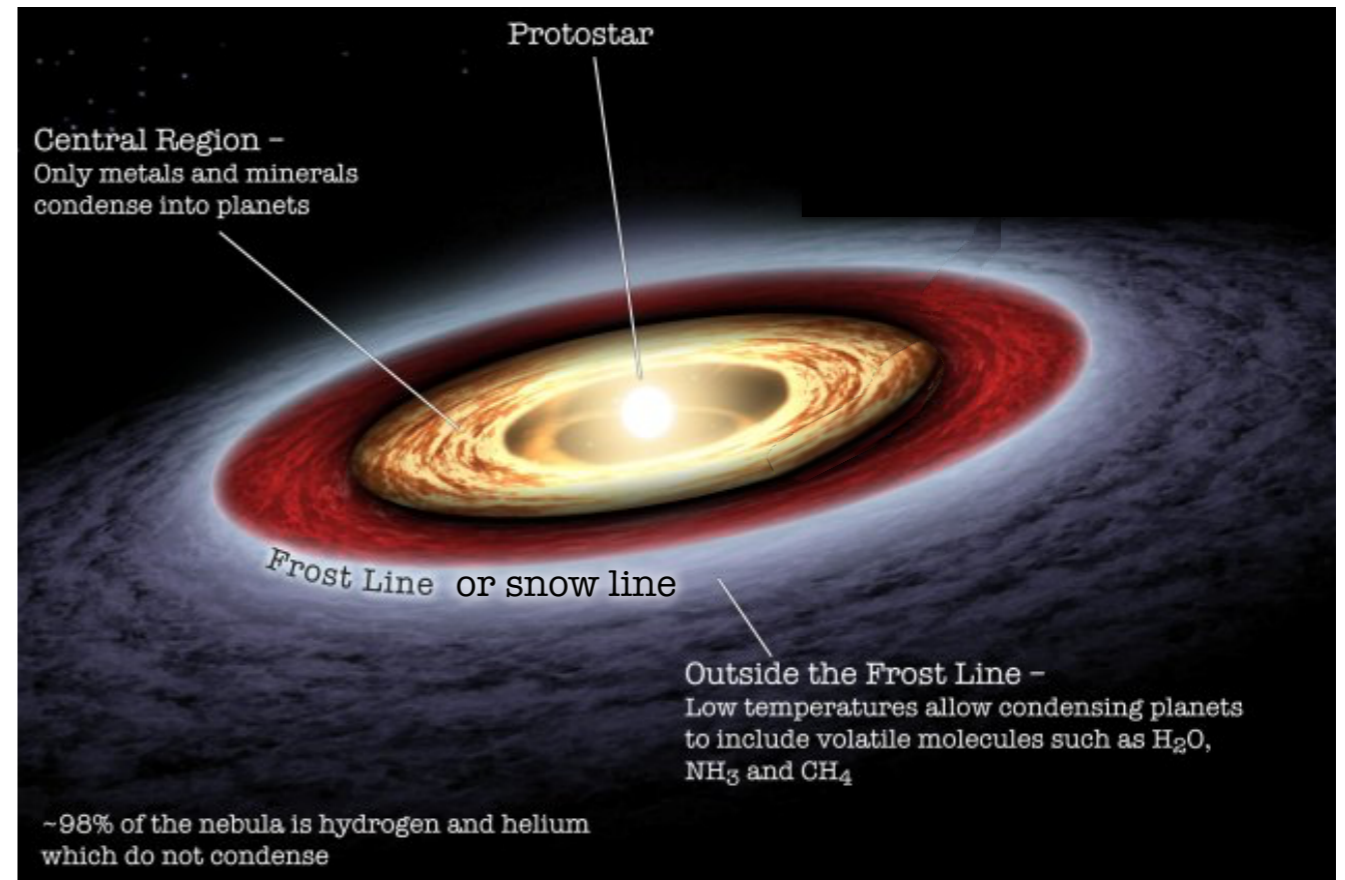
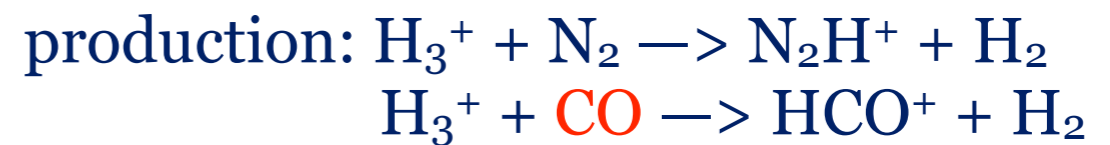
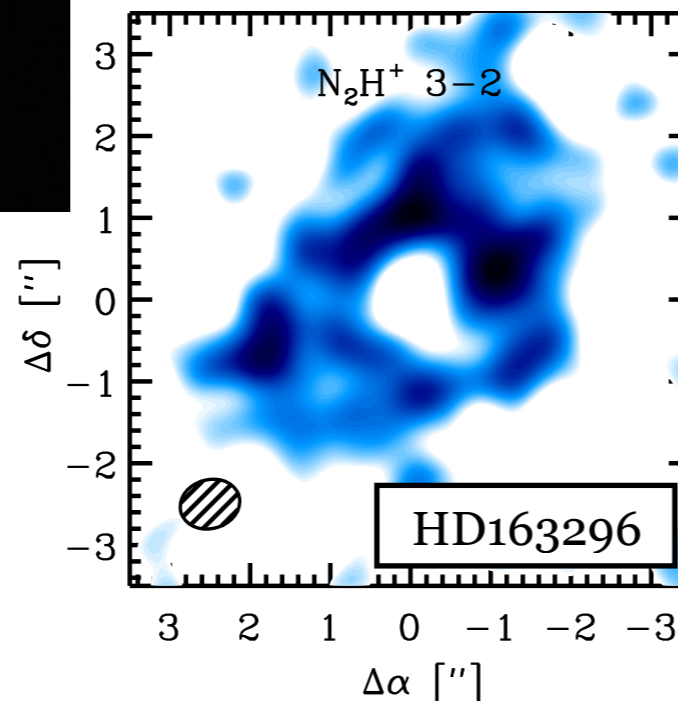
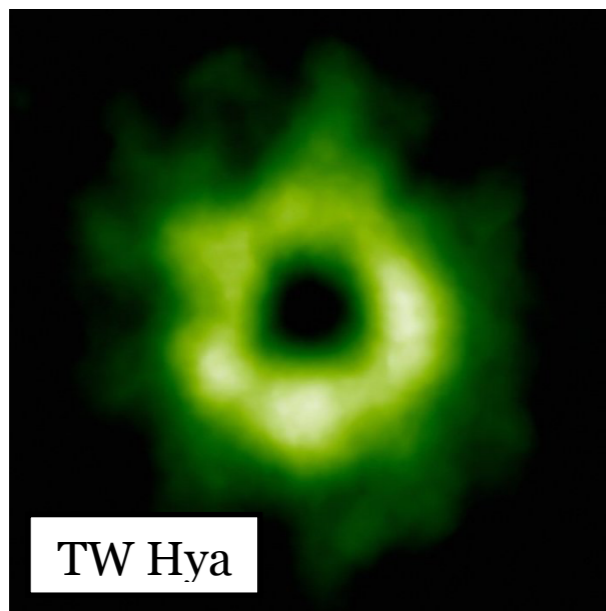


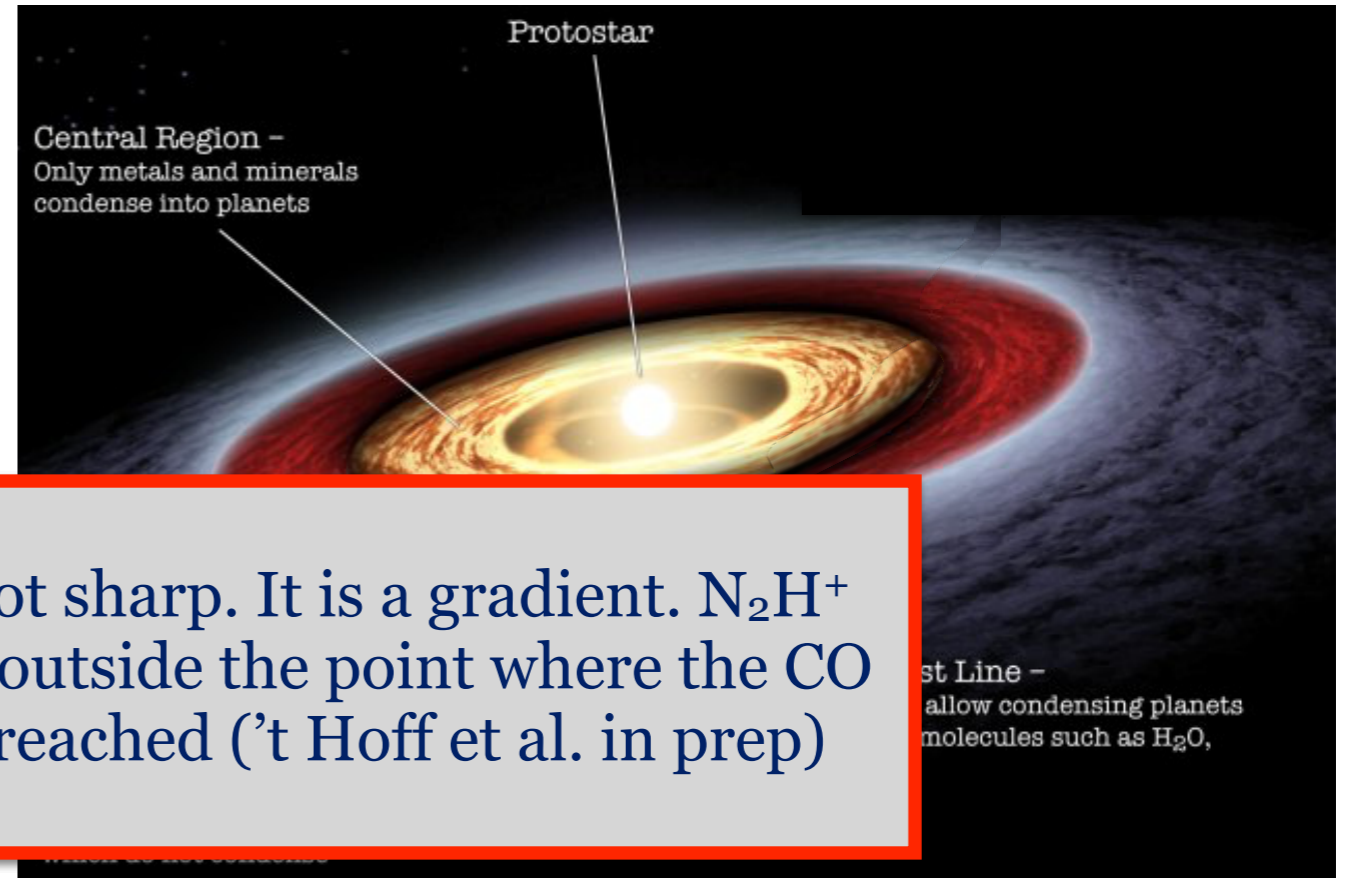
Image credit: NASA/JPL



Qi et al. (2013, 2015)

Snow lines

- Radial temperature gradient → snow lines for major volatiles: H₂O, CO, N₂?
- ...or indirectly via N₂H⁺



Caution: CO snow line is not sharp. It is a gradient. N₂H⁺ may not show up until well outside the point where the CO freeze out temperature is reached ('t Hoff et al. in prep)

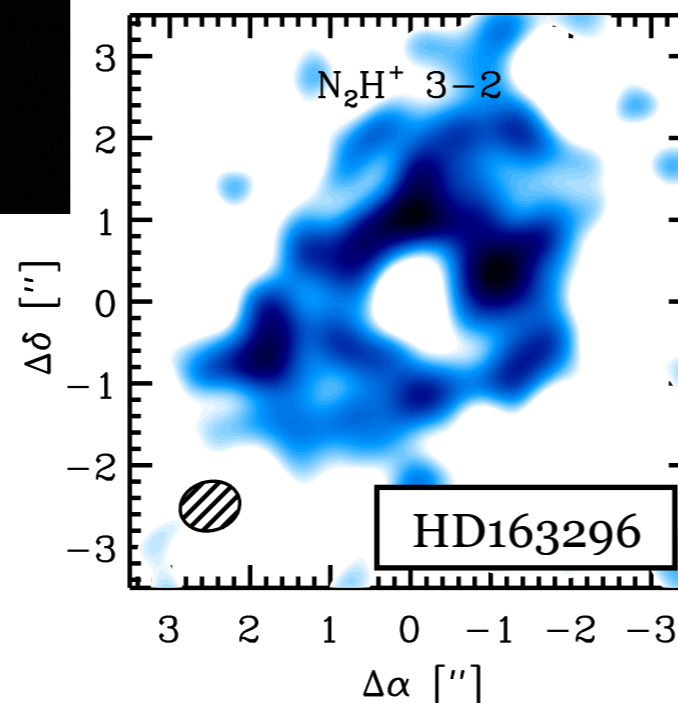
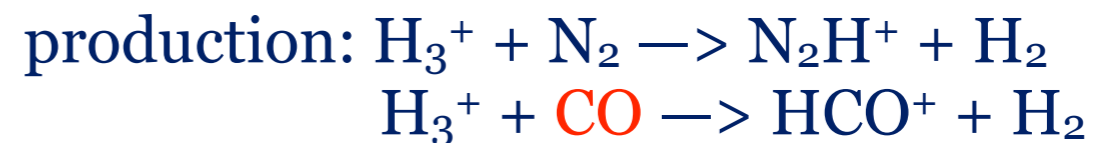


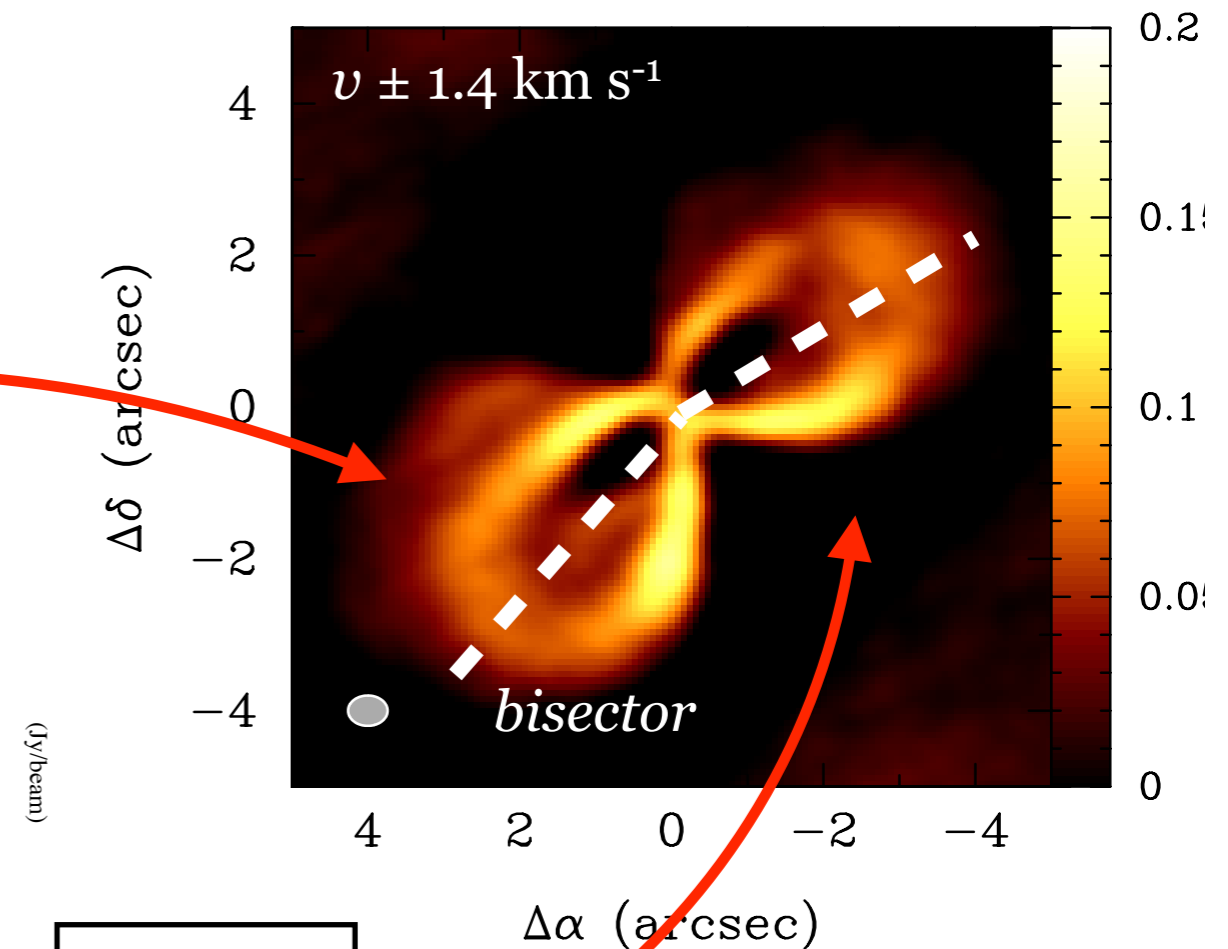
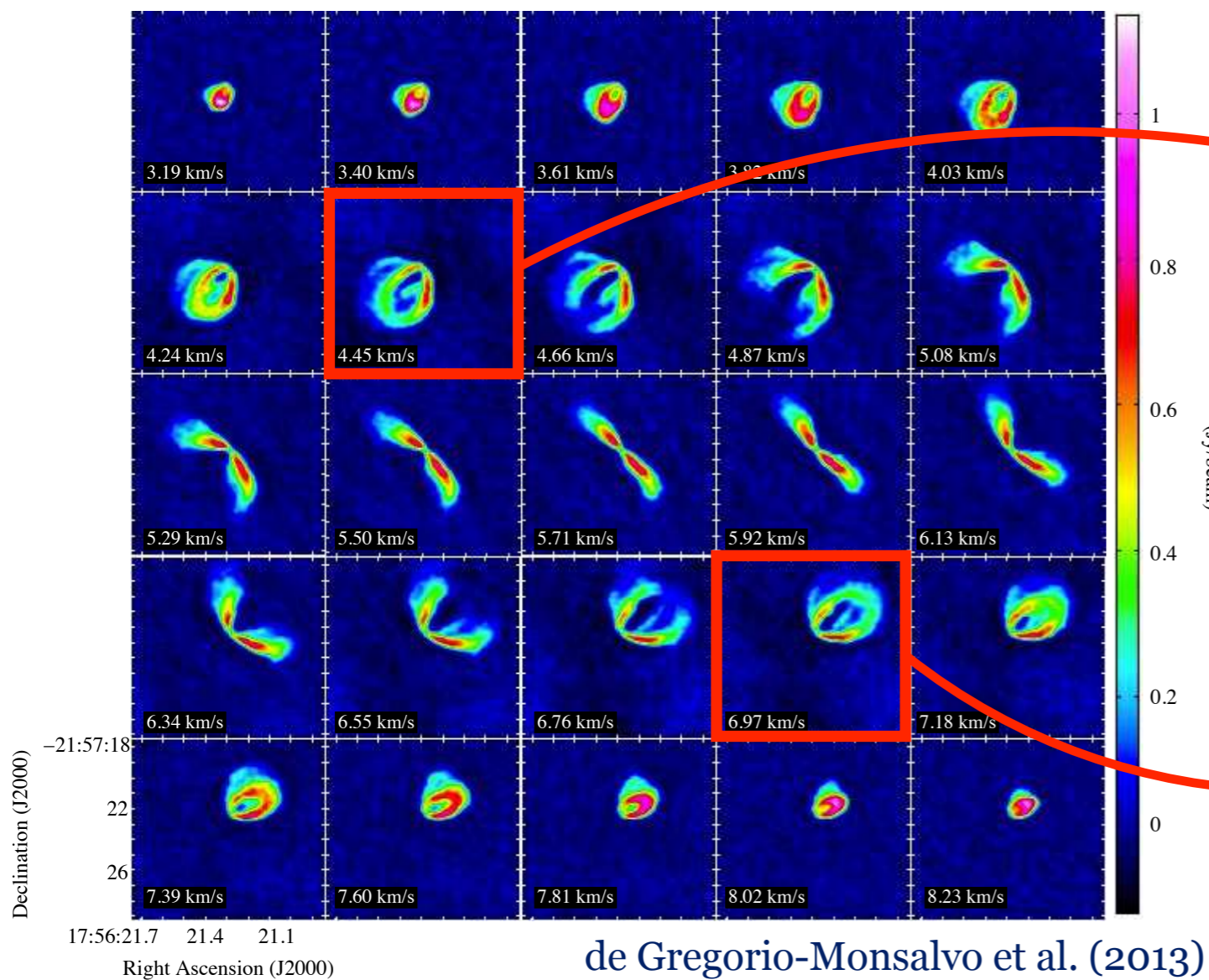
Image credit: NASA/JPL



Qi et al. (2013, 2015)

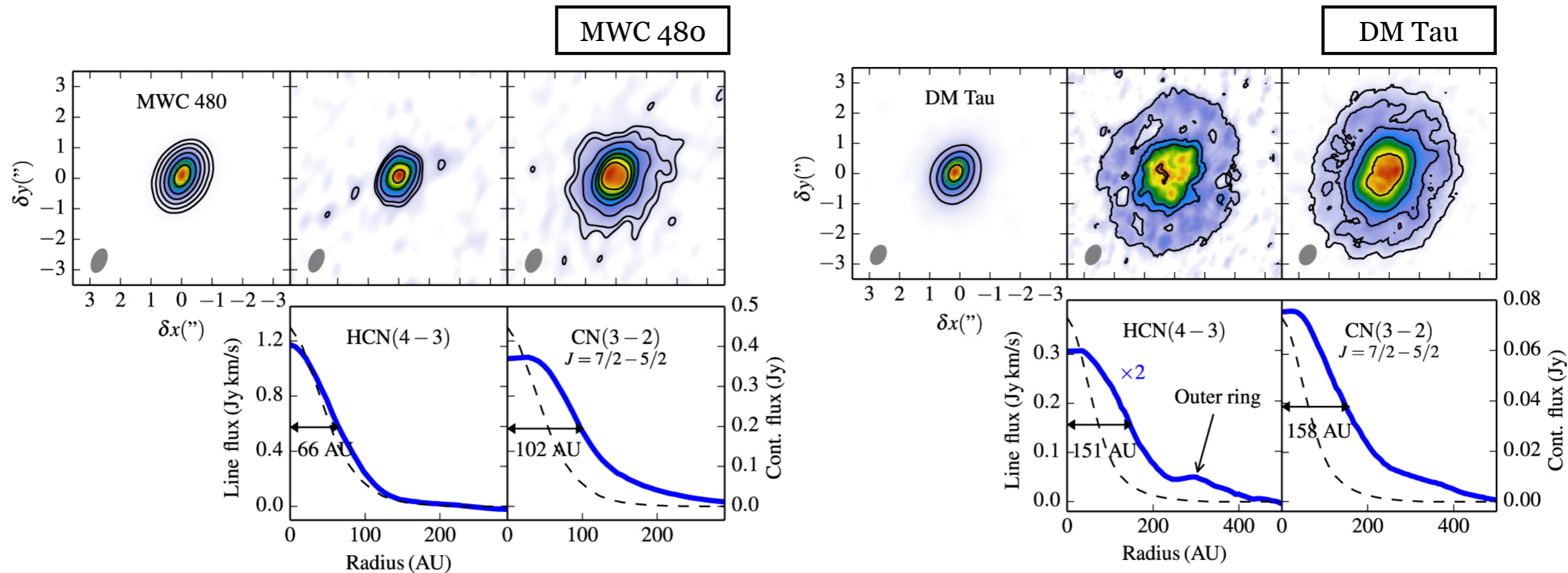
Snow surface

- Vertical temperature gradient \rightarrow snow surface
- Traced by
 - CO isotopes and different transitions
 - In channel maps for inclined disks



UV irradiated outer regions

- Interstellar radiation field penetrates outer disk
- Extended CN emission compared to HCN

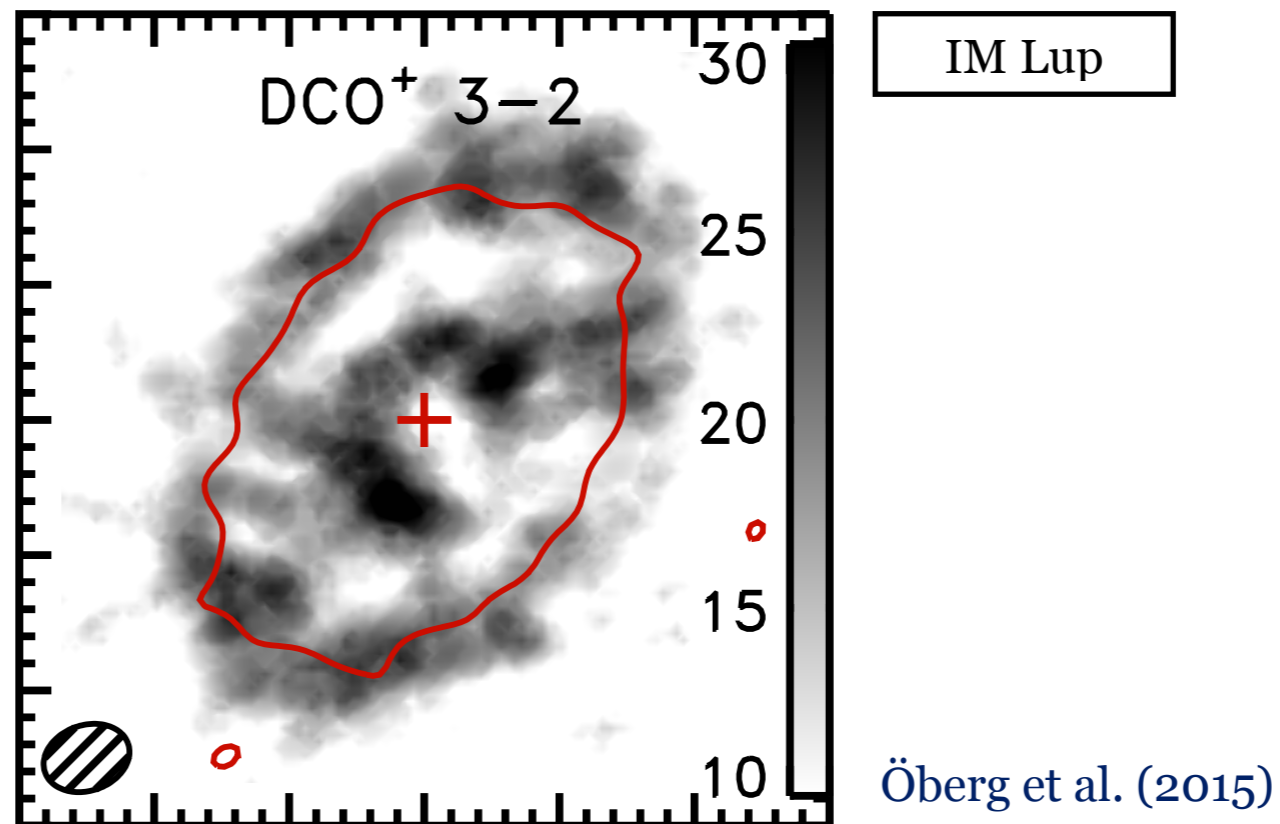


Guzmán et al. (2015)

See also Chapillon et al. (2012) for more results on HCN, CN, HC₃N

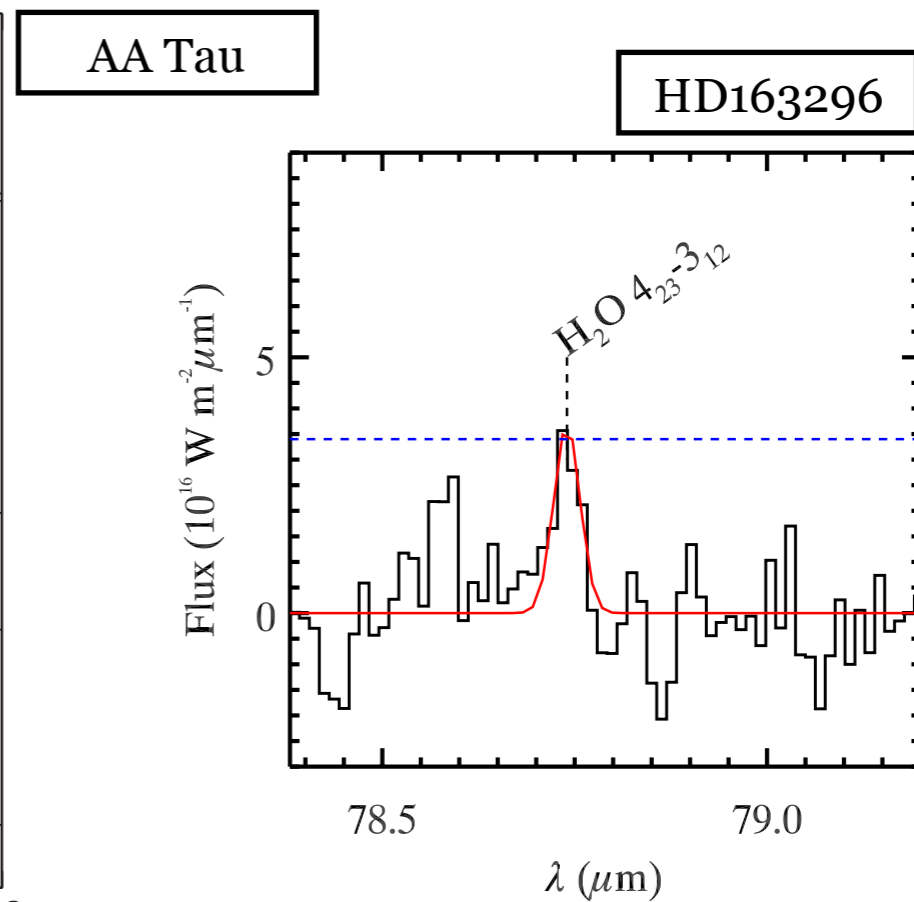
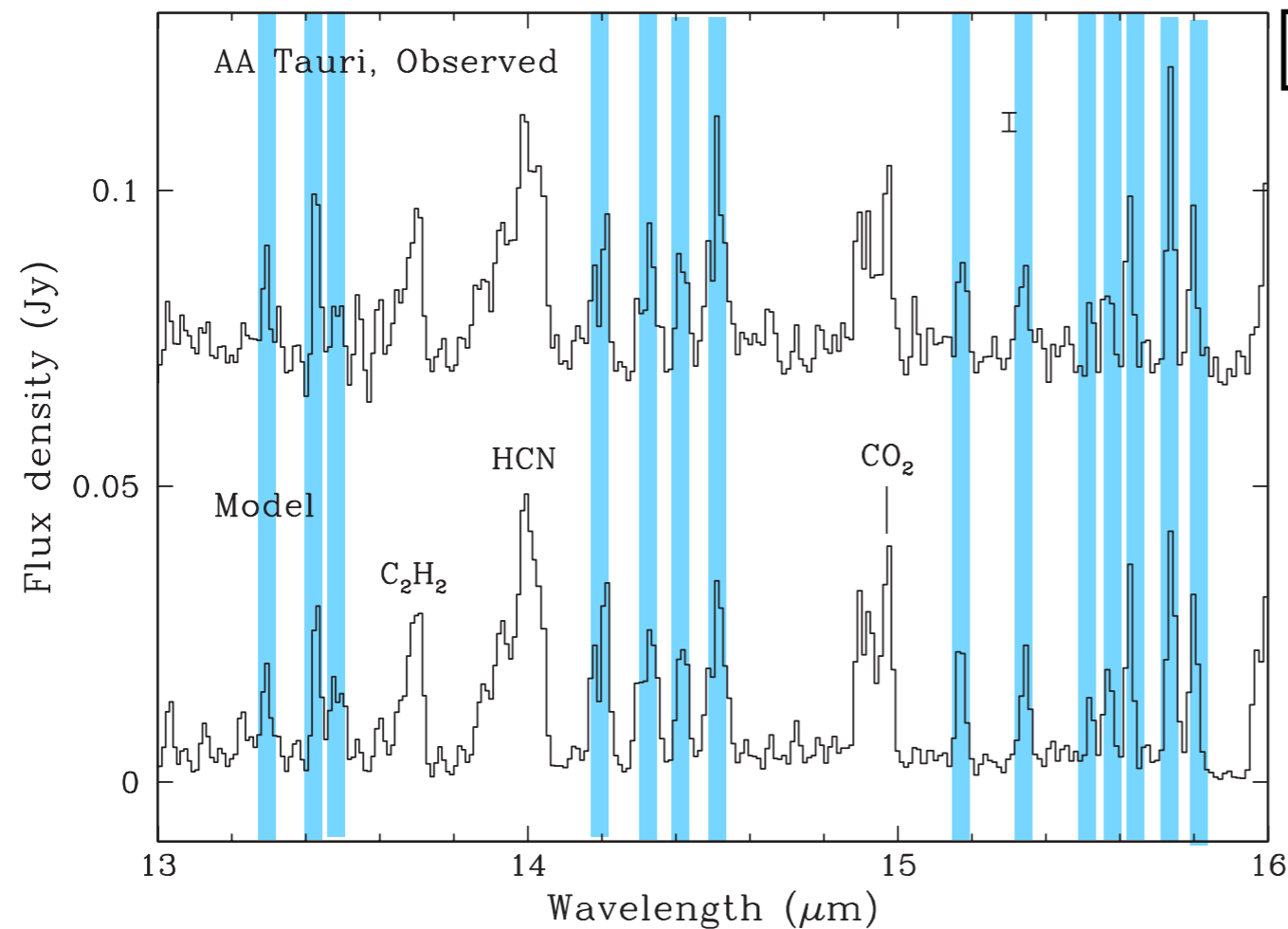
UV irradiated outer regions

- Interstellar radiation field penetrates outer disk
- Extended CN emission compared to HCN
- Photodesorption (rather than thermal desorption) sets up a second, outer snow line



Volatiles

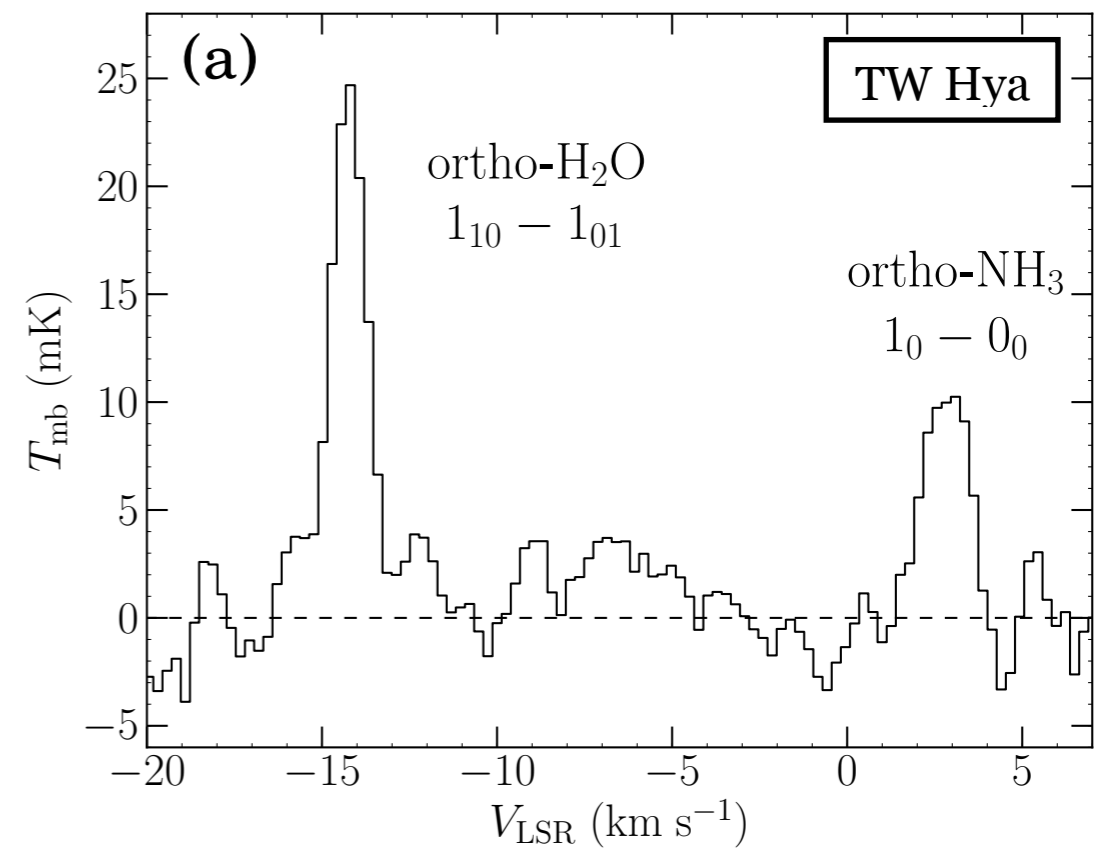
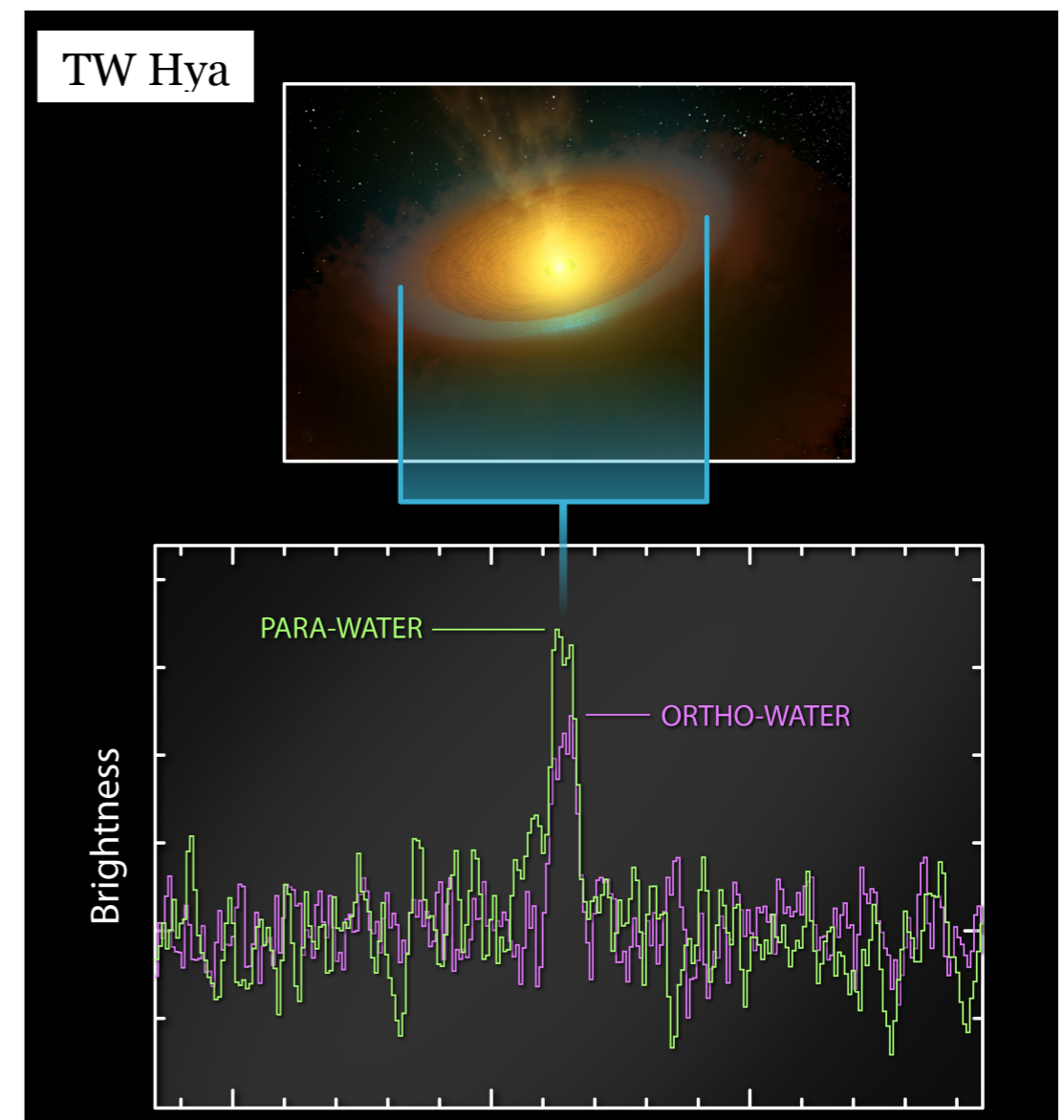
- Other detected volatiles
 - H₂O in several disks
 - gas-phase production / evaporation in inner disk



Carr & Najita (2008); Salyk et al. (2008, 2015);
Pontoppidan et al. (2010); Meijerink et al. (2009);
Zhang et al. (2013); Fedele et al. (2012); Riviere-
Marichalar et al. (2012)

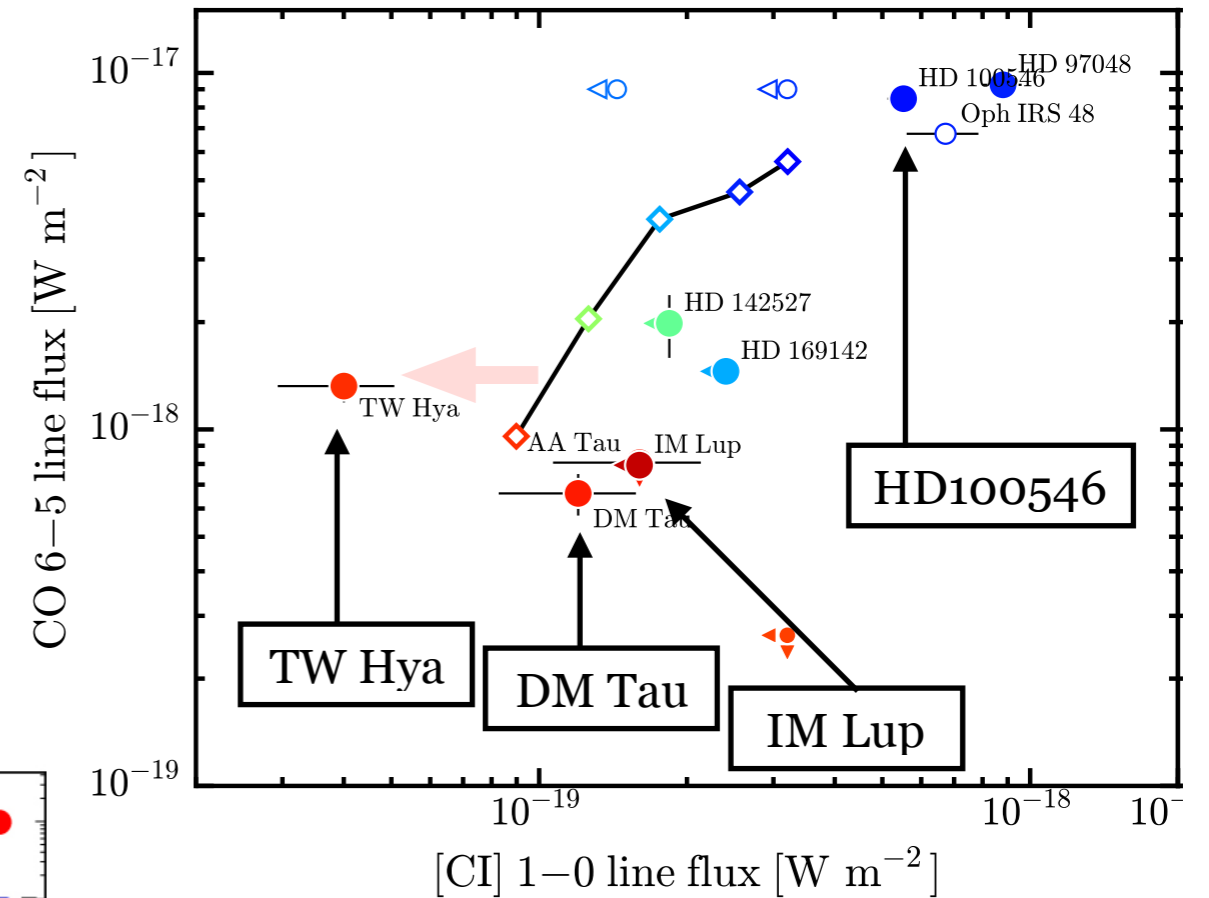
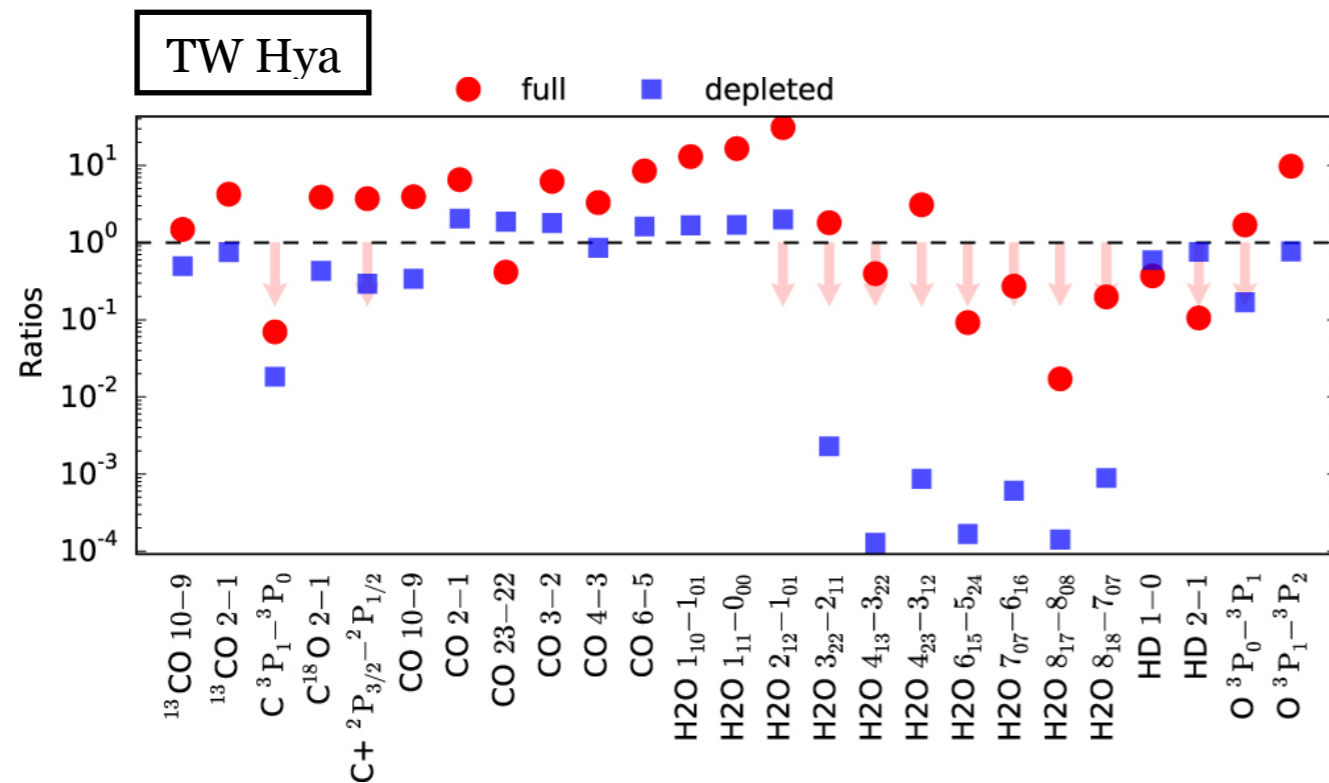
Volatiles

- Other detected volatiles
 - H₂O in several disks
 - gas-phase production / evaporation in inner disk
 - photodesorption in outer disk
 - much lower amount than expected
→ most ices settled in the midplane on larger grains?
- NH₃ in TW Hya



Depletion of volatiles

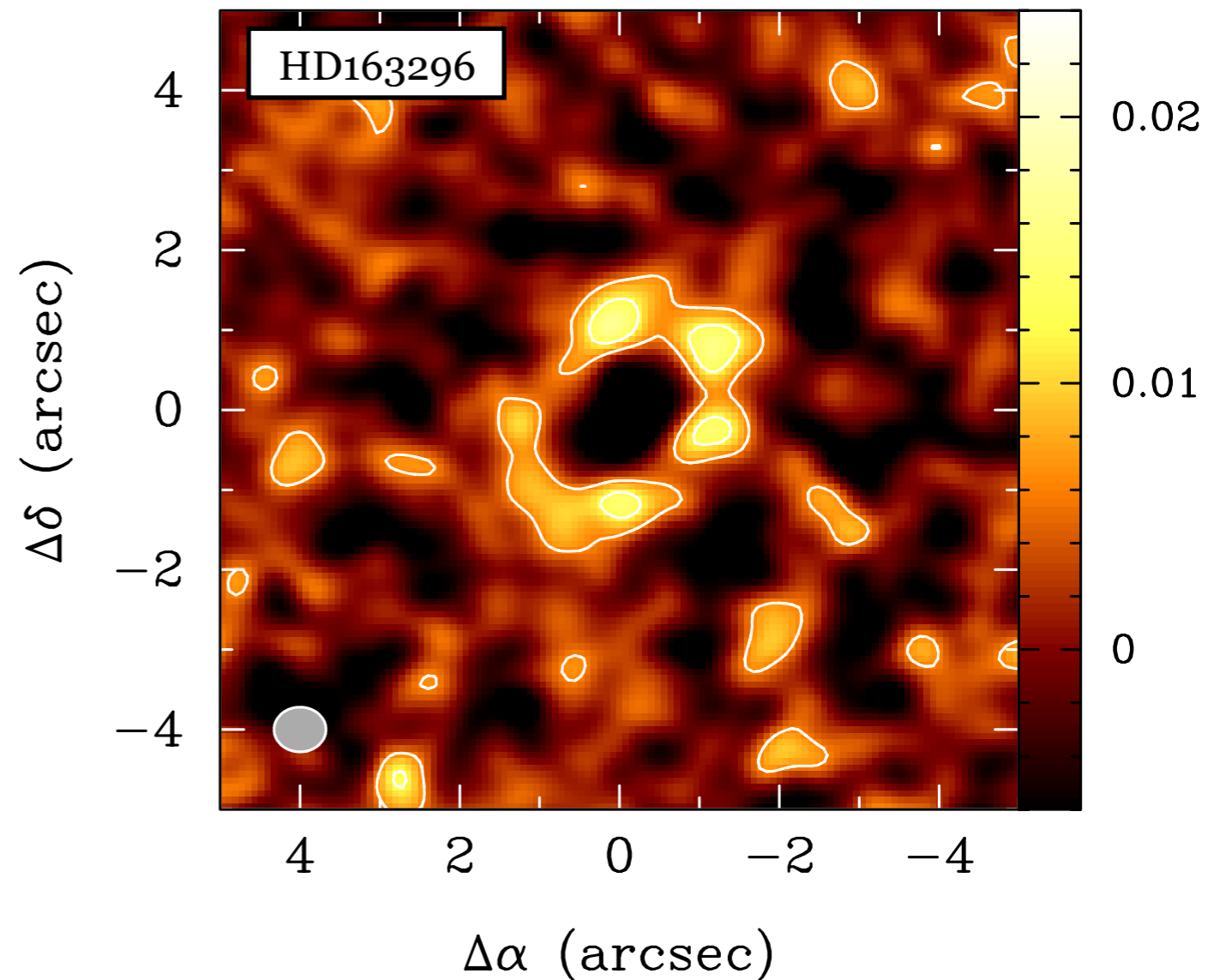
- CO, C, and H₂O depleted in many disks
- TW Hya in particular
- Locked up in the midplane



Deuteration

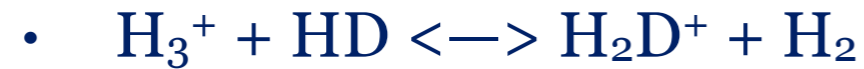
- Deuterated molecules are enriched in cold gas
 - $\text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2$
 - $\text{H}_2\text{D}^+ + \text{X} \rightarrow \text{XD}^+ + \text{H}_2$

N_2D^+ in HD163296

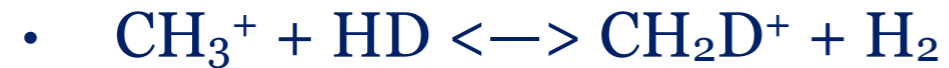


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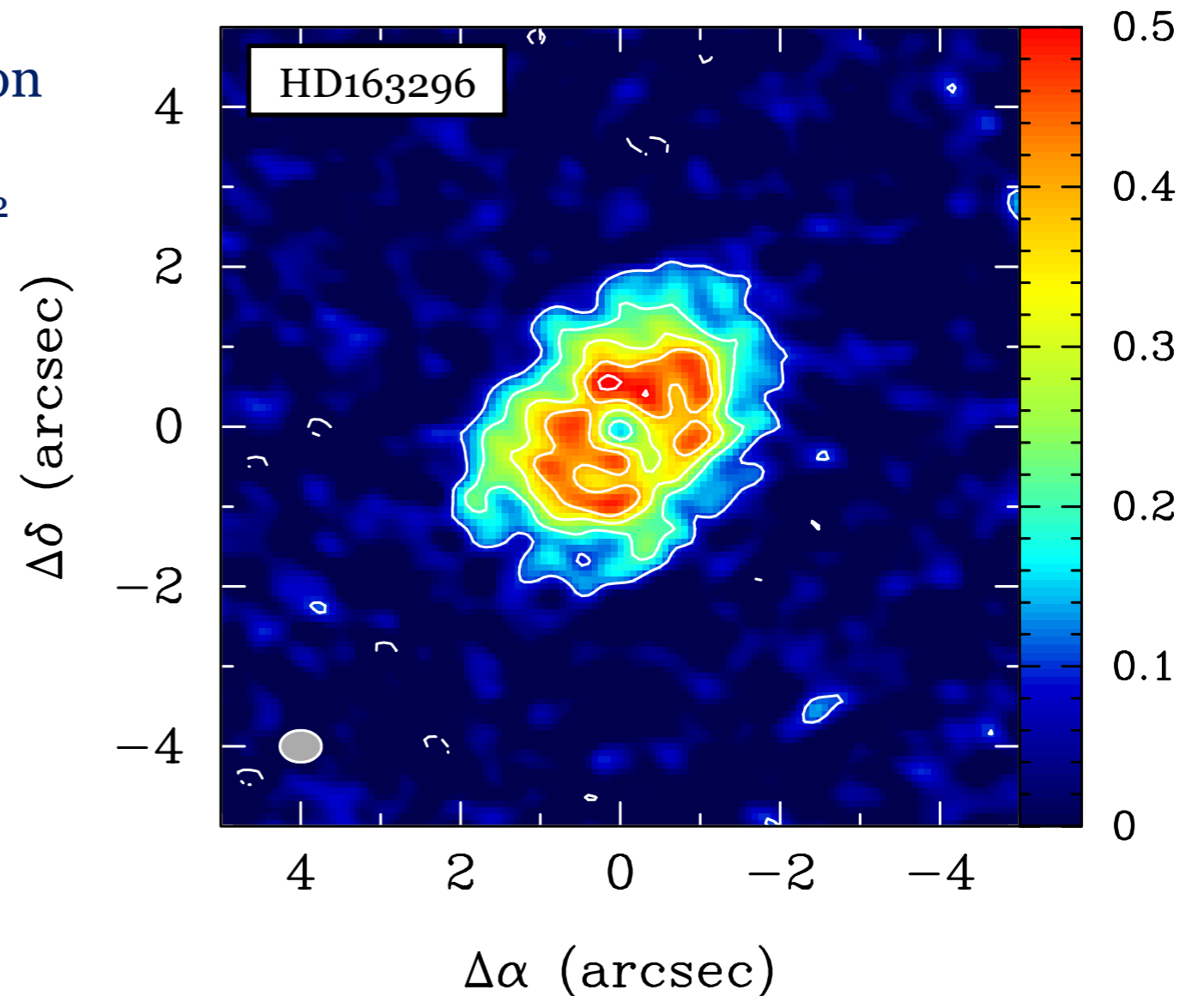
- Deuterated molecules are enriched in cold gas



- High(er) temperature deuteration



DCO⁺ in HD163296

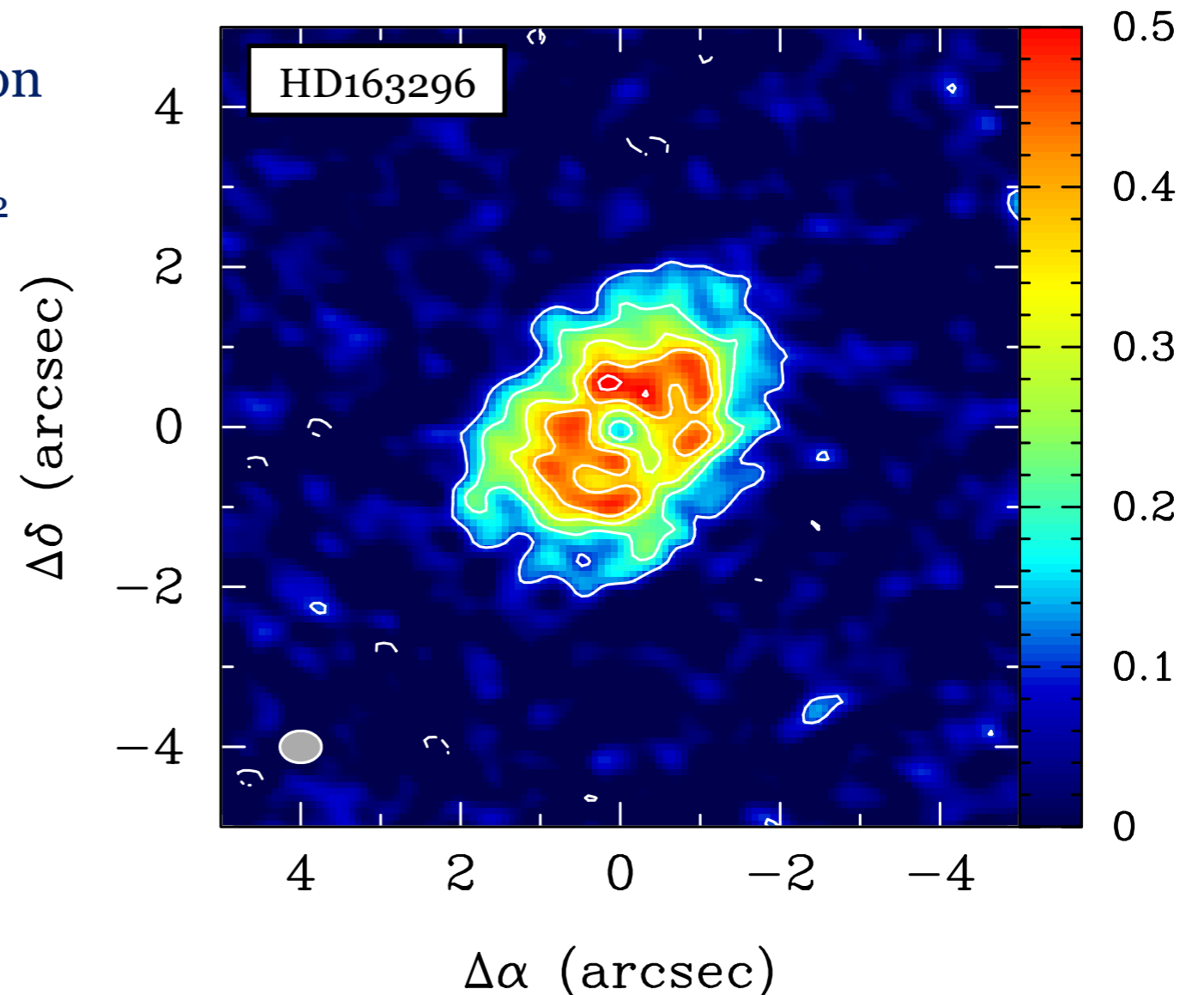


Deuteration

- Deuterated molecules are enriched in cold gas
 - $\text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2$
 - $\text{H}_2\text{D}^+ + \text{X} \rightarrow \text{XD}^+ + \text{H}_2$
- High(er) temperature deuteration
 - $\text{CH}_3^+ + \text{HD} \rightleftharpoons \text{CH}_2\text{D}^+ + \text{H}_2$
 - $\dots + \text{O} \rightarrow \text{DCO}^+ + \dots$

DCO⁺ is not as much a CO snow line tracer as it is an ionization tracer (cf. Teague et al. 2015; Guilloteau et al. 2016 for HCO⁺, DCO⁺)

DCO⁺ in HD163296



Deuteration

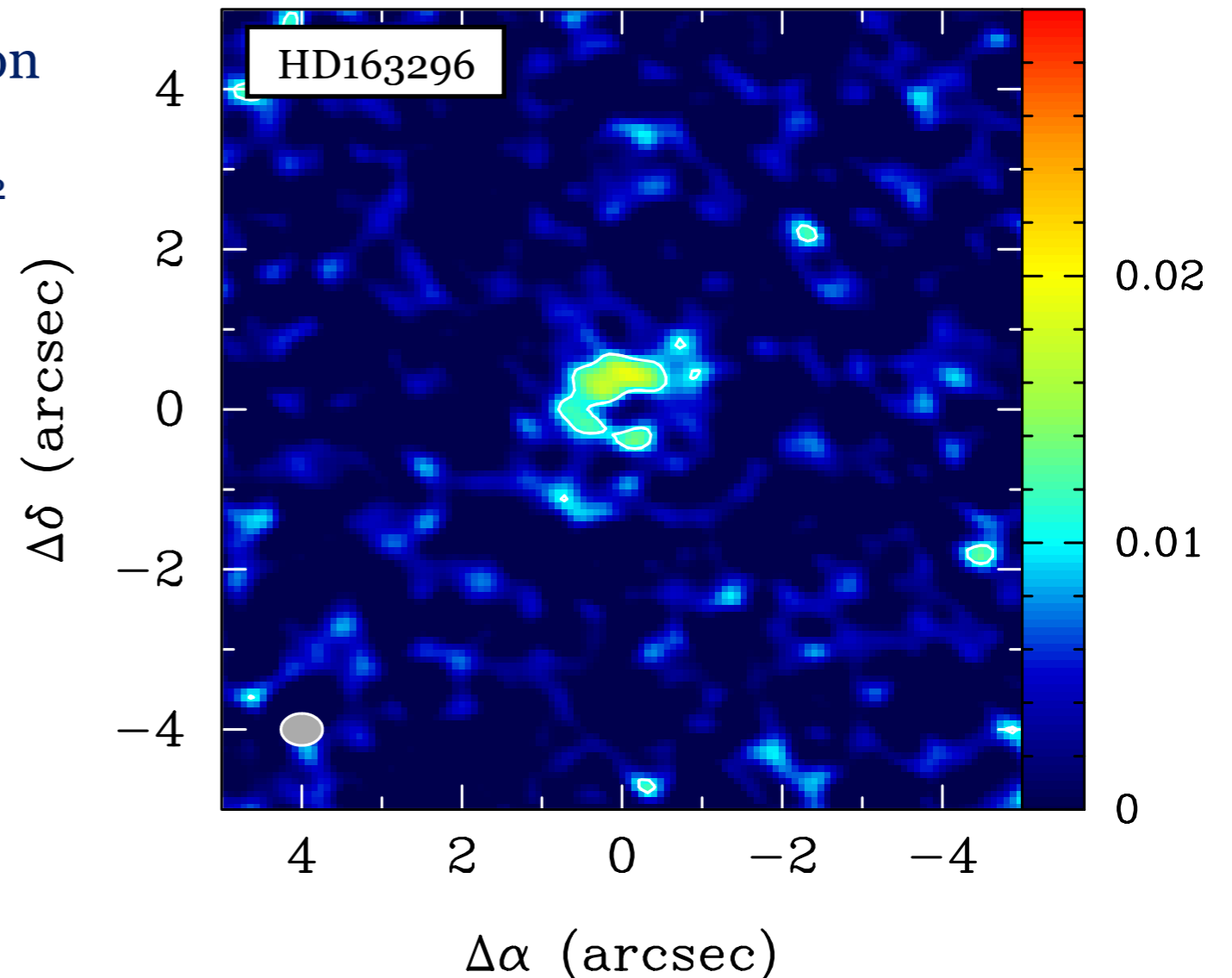
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- High(er) temperature deuteration



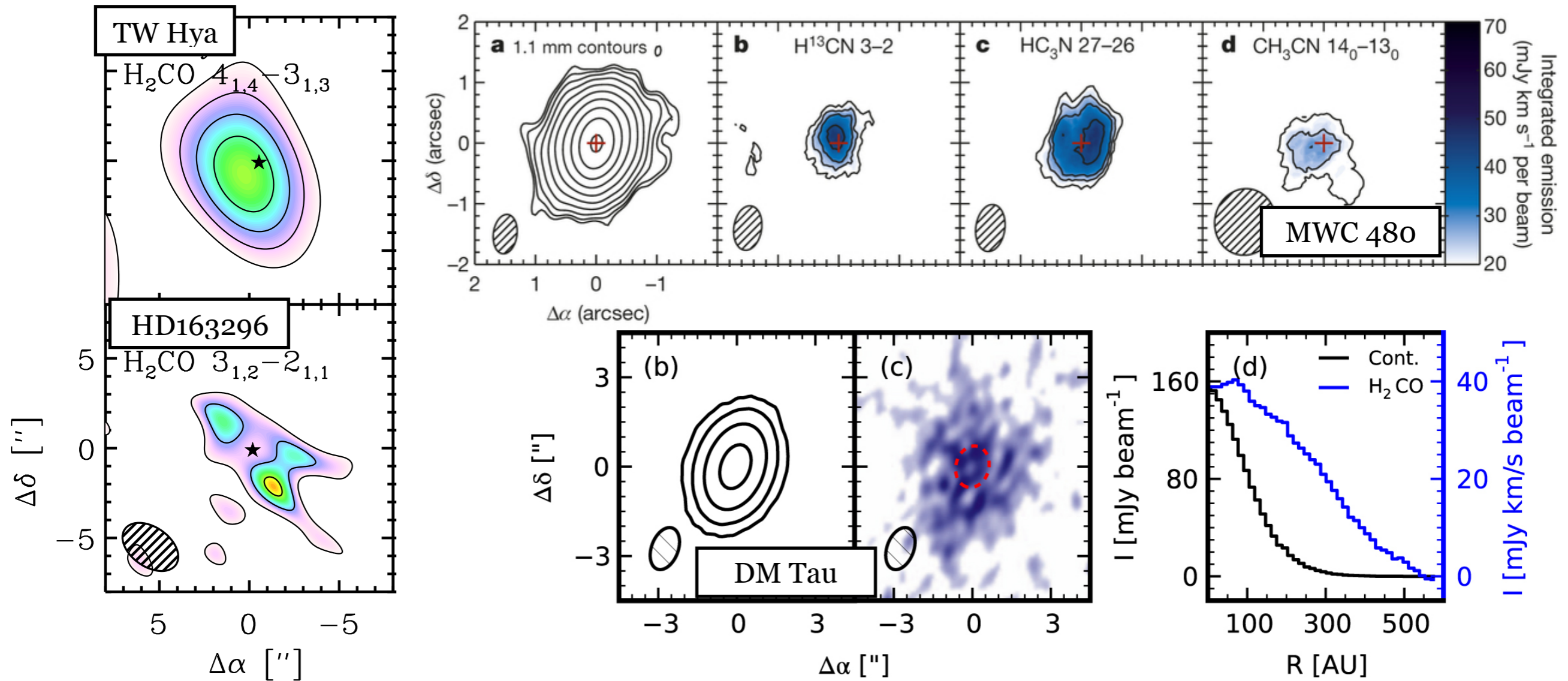
DCN in HD163296



Organics

- Simple organics are being detected in disks
 - HC_3N and CH_3CN in MWC480
 - H_2CO across the disks of DM Tau, TW Hya, HD163296

Öberg et al. (2015)



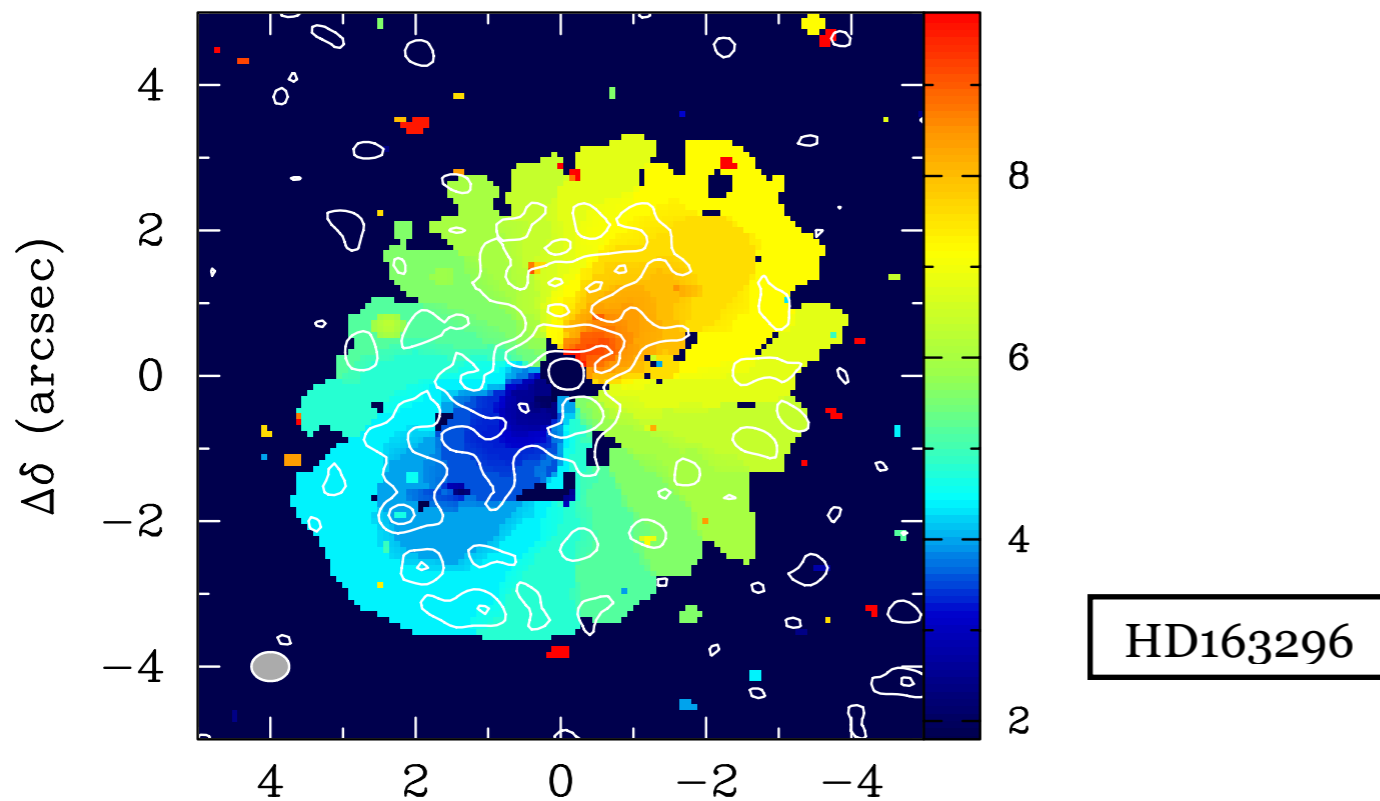
Qi et al. (2013)

Loomis et al. (2015)

See also: HC_3N , Chapillon et al. (2012)

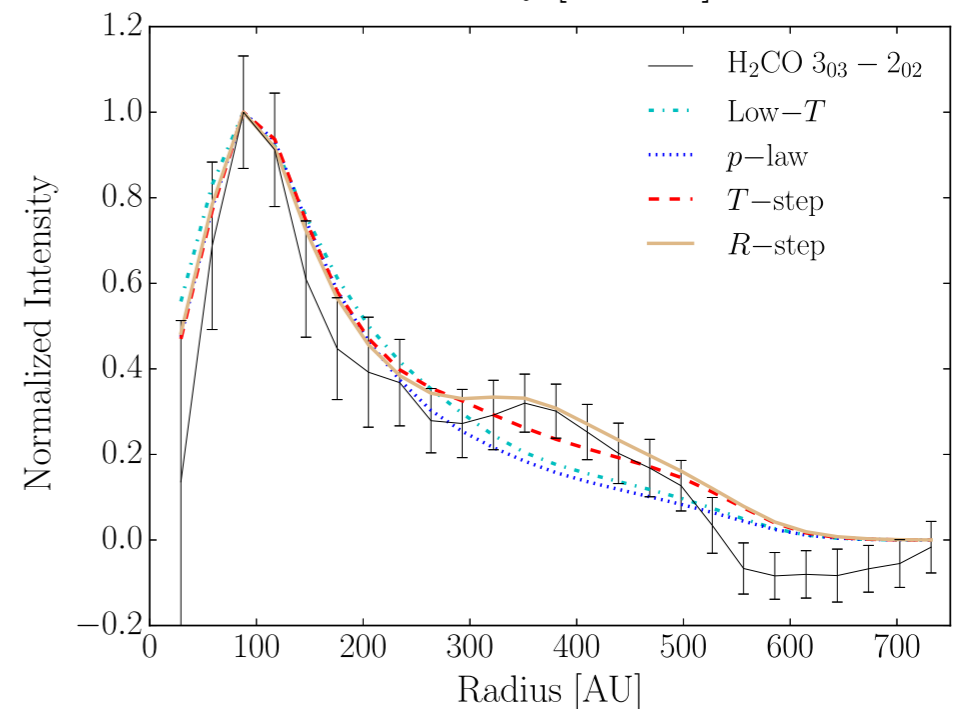
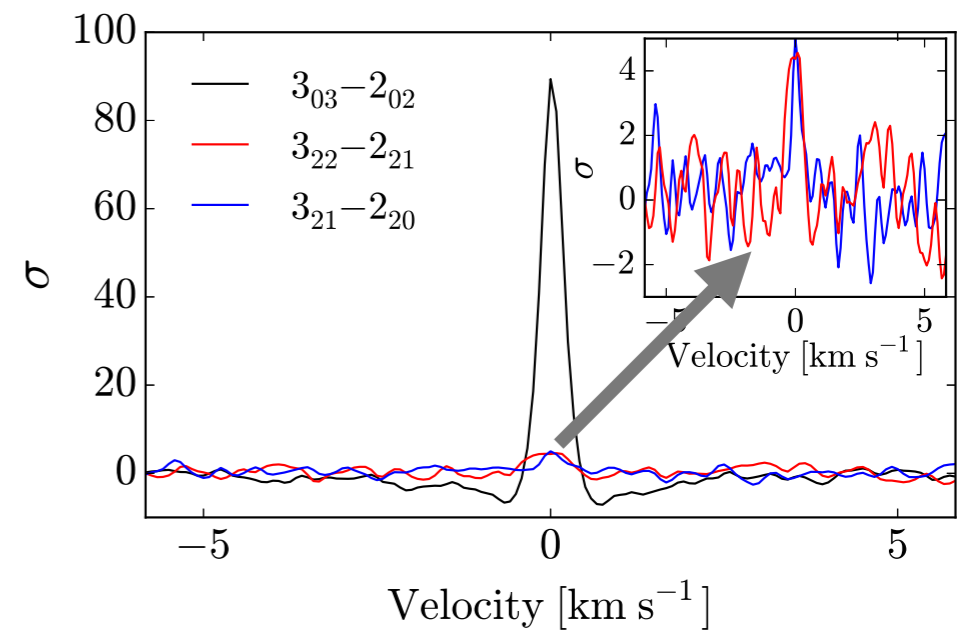
Organics

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 - HC₃N and CH₃CN in MWC480
 - H₂CO across the disks of DM Tau, TW Hya, HD163296



Carney et al. (in prep):

- H₂CO 3₂-2₂ detected via matched filtering (Loomis et al., in prep)
- additional reservoir of H₂CO outside ~300 au: UV photodesorption?

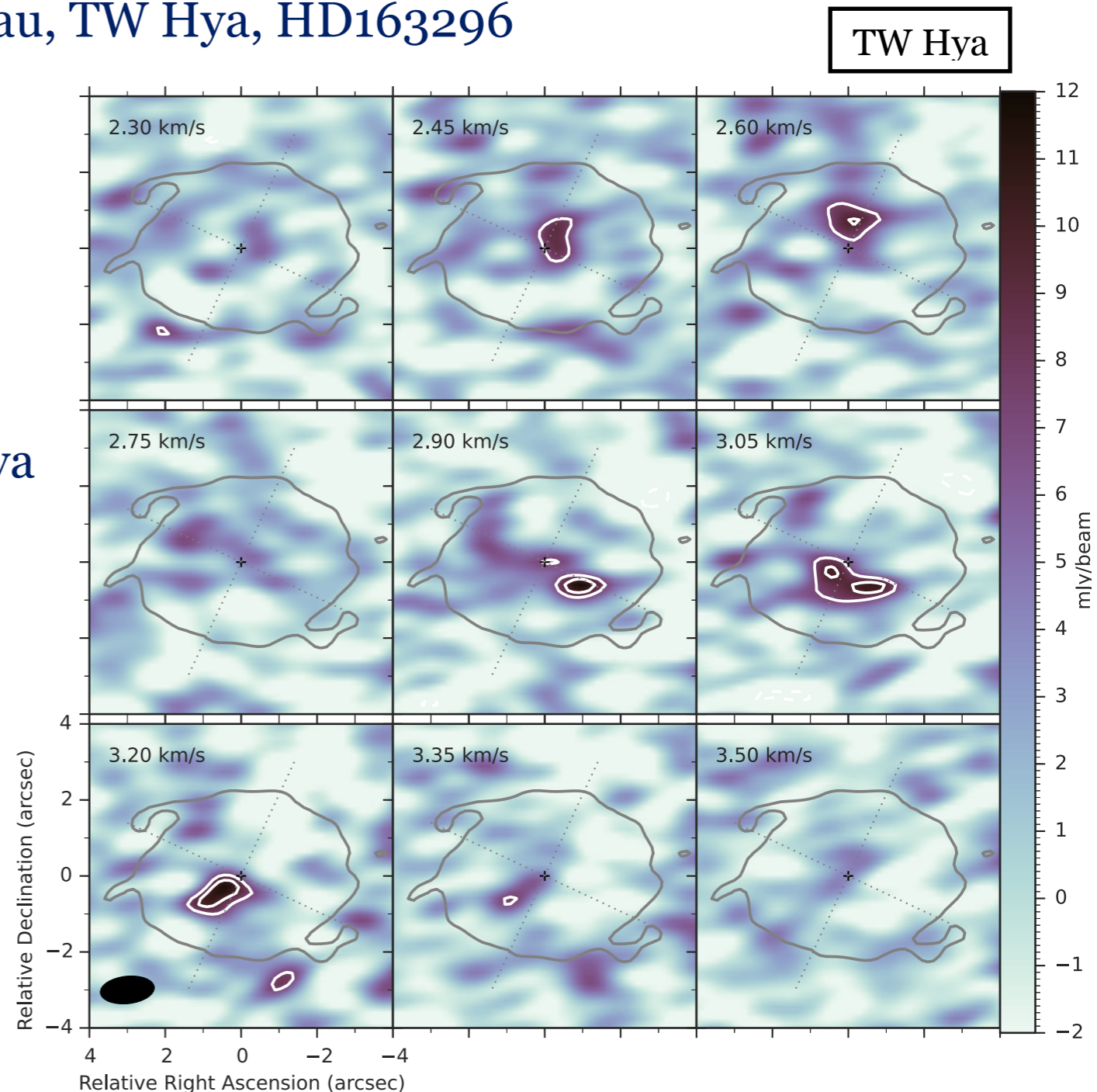


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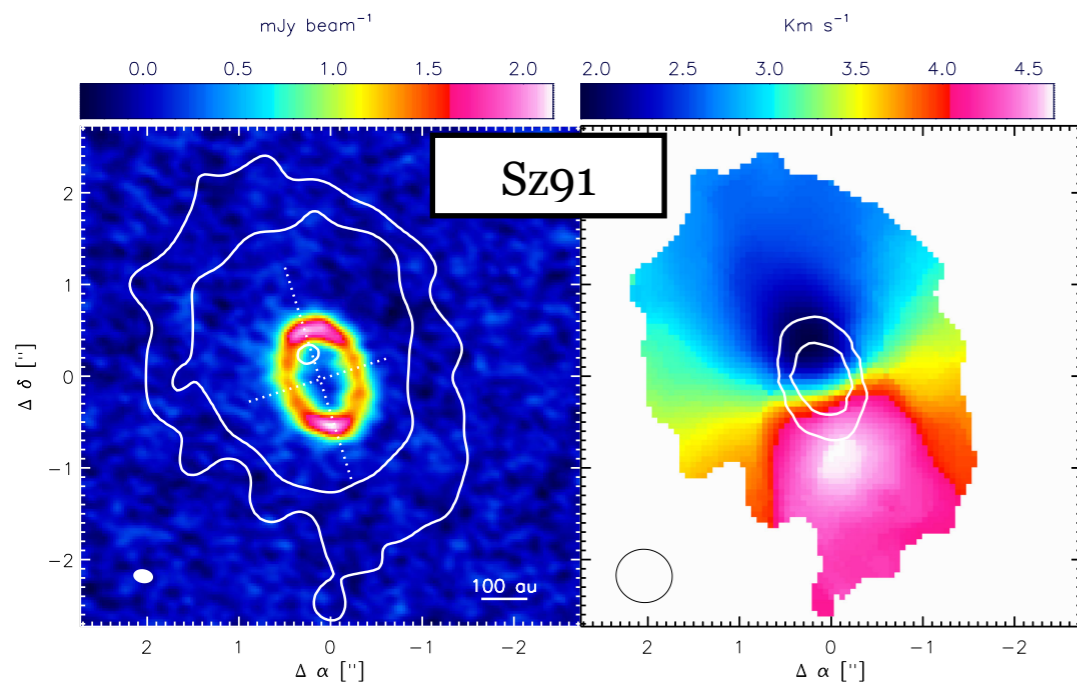
Walsh et al. (in press)

- (stacked) CH_3OH detected in TW Hya
- see talk by Nomura



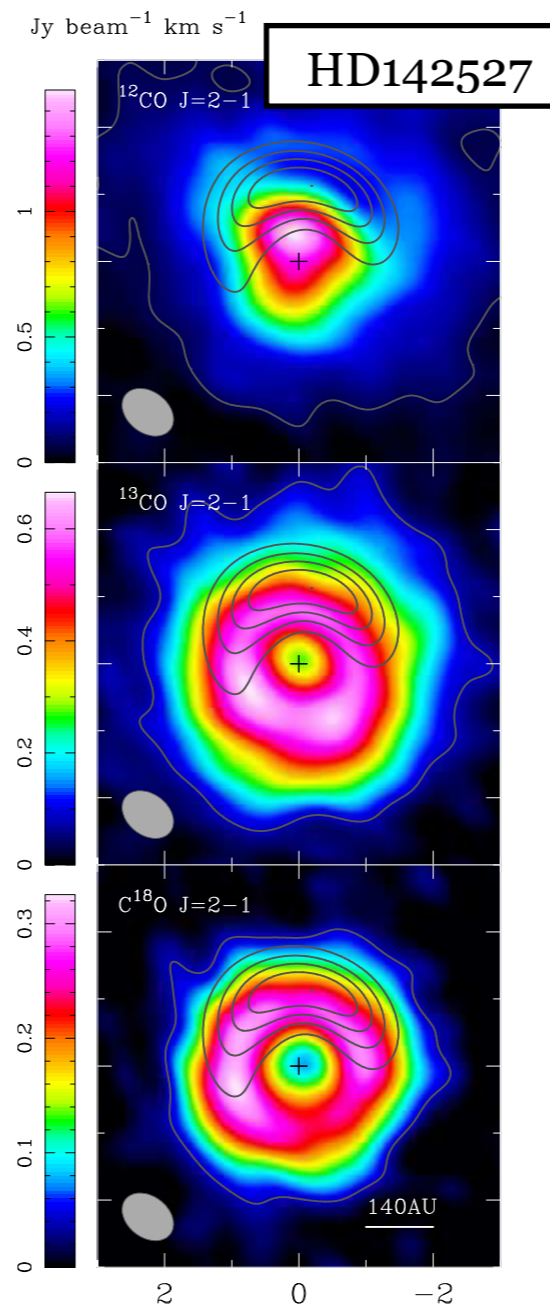
Gaps

- Fair fraction of disks are transitional: large (dust) gaps
- (Reduced amount of) gas fills the gaps
- Photodissociation effects?

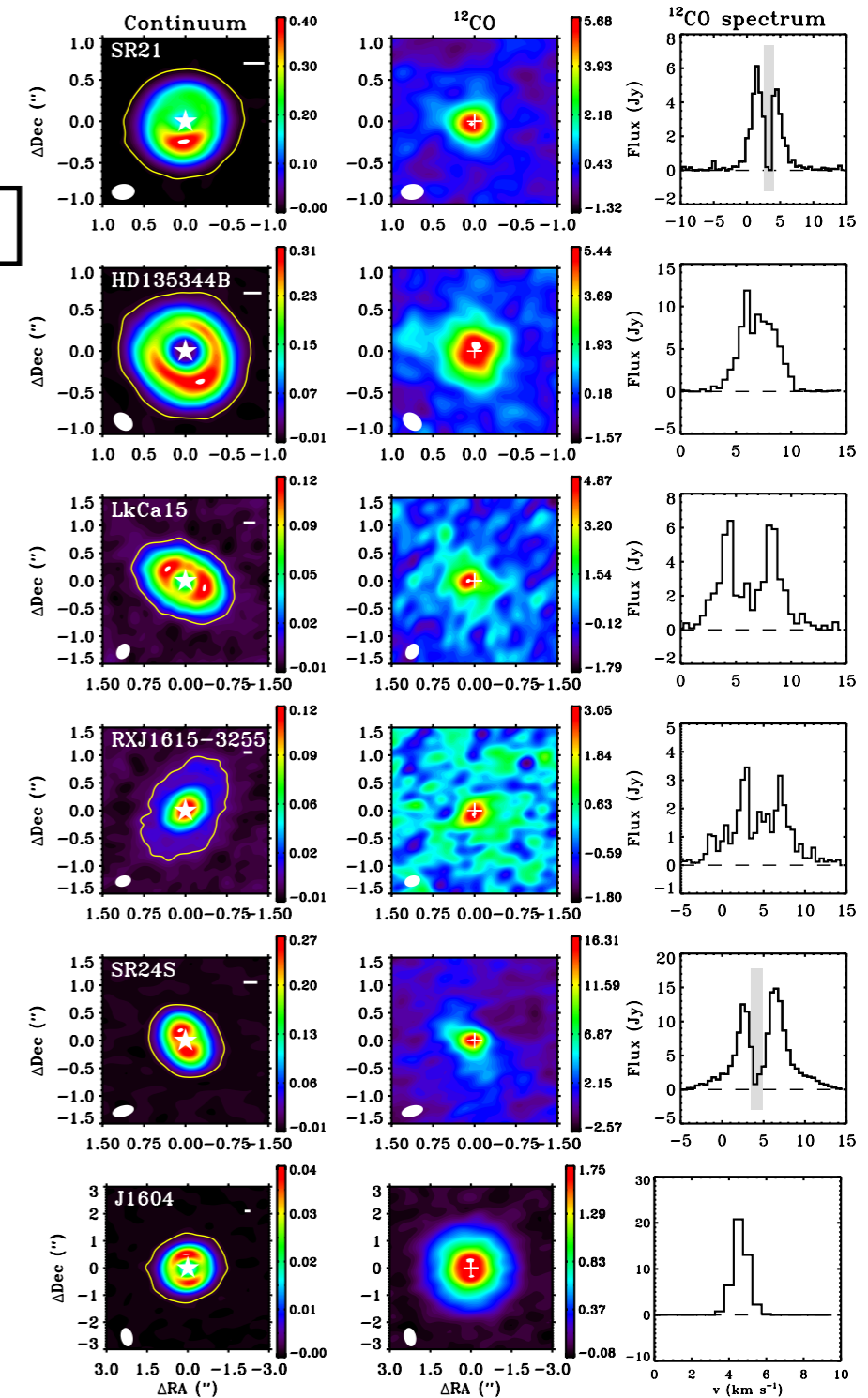


Canovas et al. (2016)

see also Carmona et al. (2014),
Bruderer et al. (2014), ...



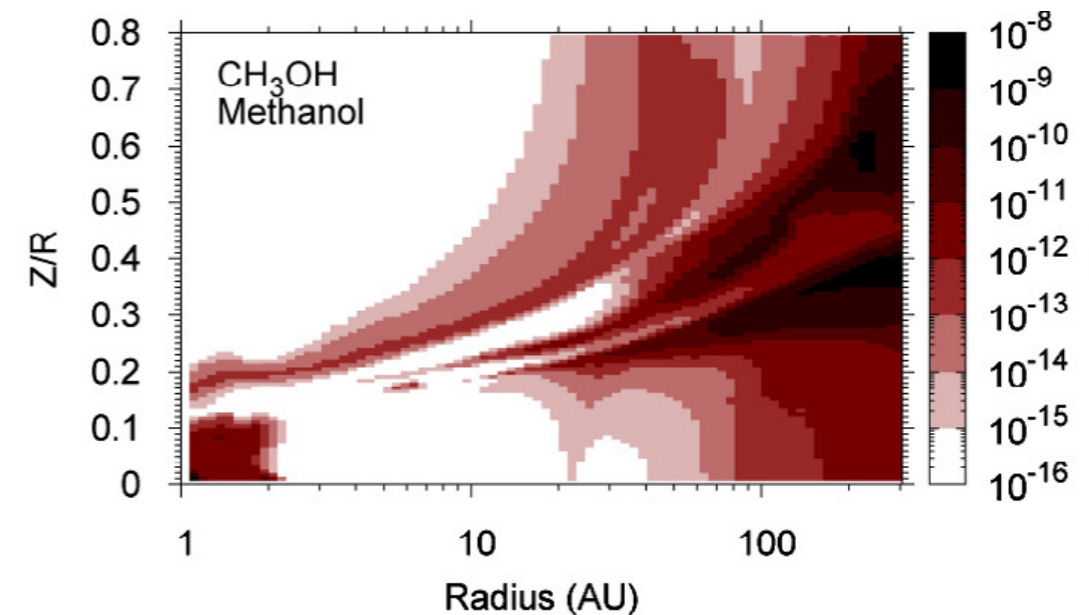
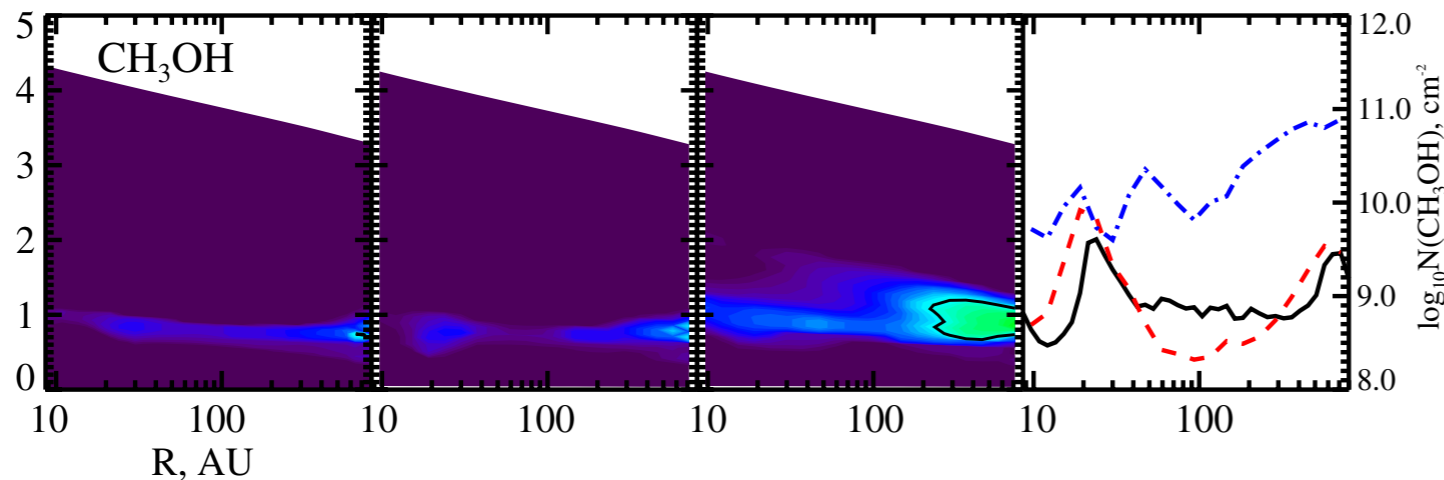
Perez et al. (2015)



van der Marel et al. (2015)

Inheritance

- Models of disk chemistry:
 - gas-phase & grain-surface formation; full or reduced networks
 - freeze out & evaporation
 - photodesorption by UV
 - ionization by UV, CR, X-rays, short-lived radionuclides
 - steady state, time dependent, or fully coupled with hydrodynamic solution and/or grain evolution



E.g., van Zadelhoff et al. 2003; Jonkheid et al. 2007; Aikawa et al. 2002, 2006, 2015; Fogel et al. 2011; Semenov et al. 2010, 2011; Woitke et al. 2010, 2016; Willacy et al. 2007, 2009; Walsh et al. 2010, 2012, 2013, 2014, 2015; ...

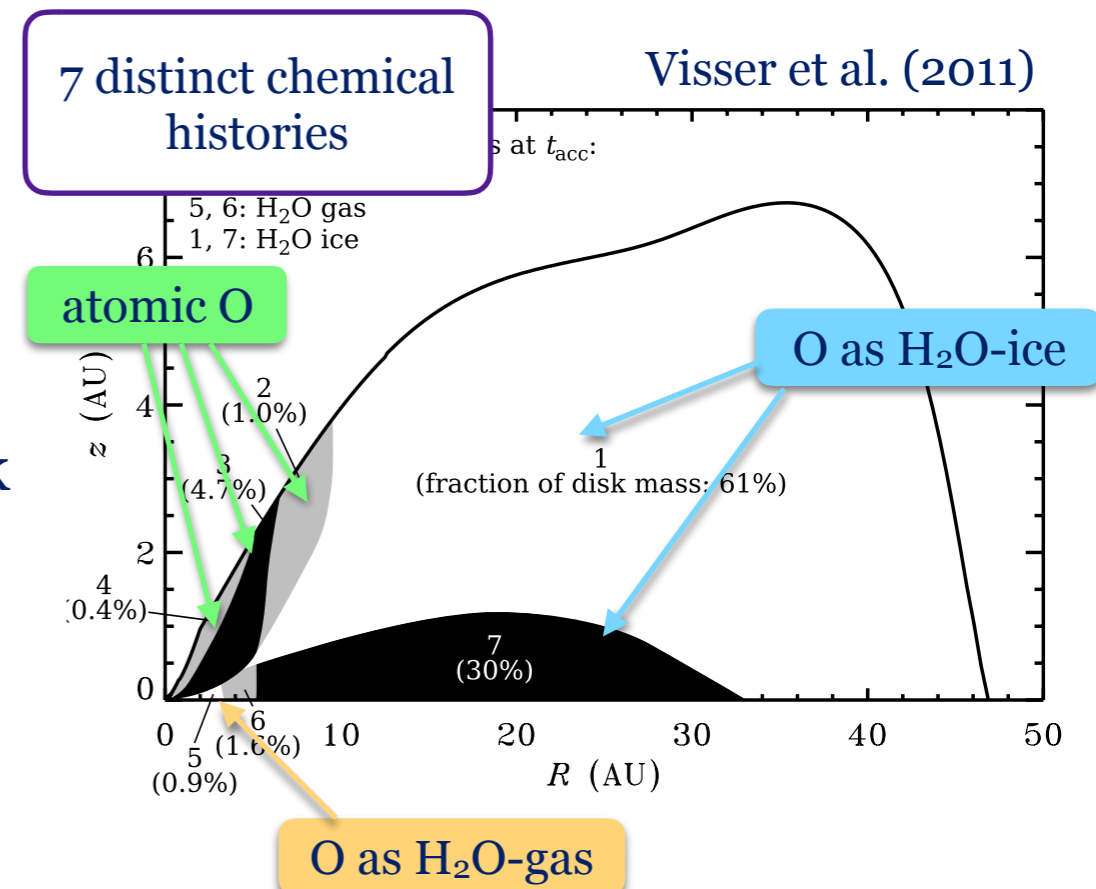
Semenov & Wiebe (2011); Walsh et al. (2014)

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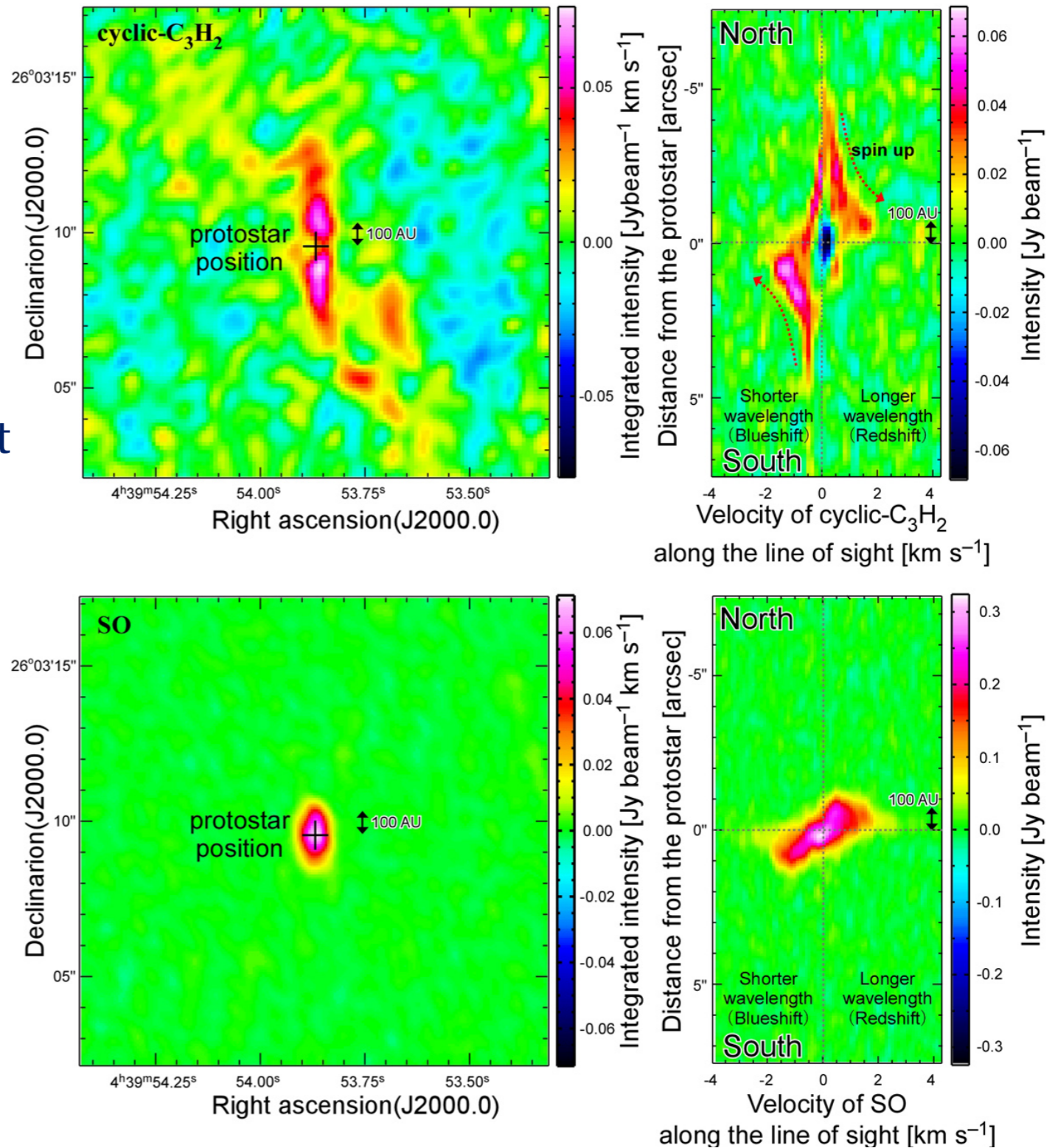
- **How about initial conditions?**

- How much of the chemistry is inherited from the ISM, protostellar phase?
- How much is reprocessed during star /disk formation, esp. ices/volatiles
- Influence of episodic heating?



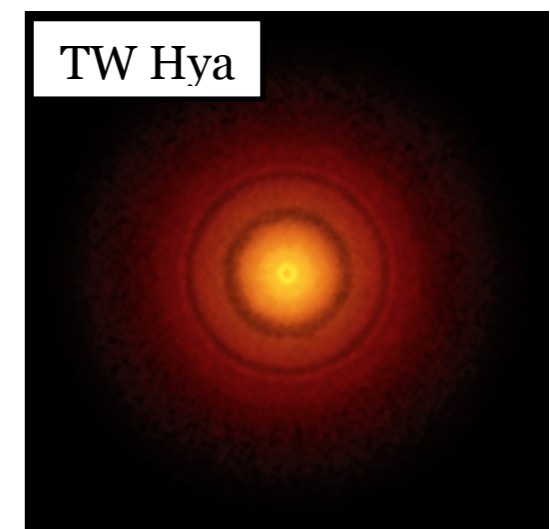
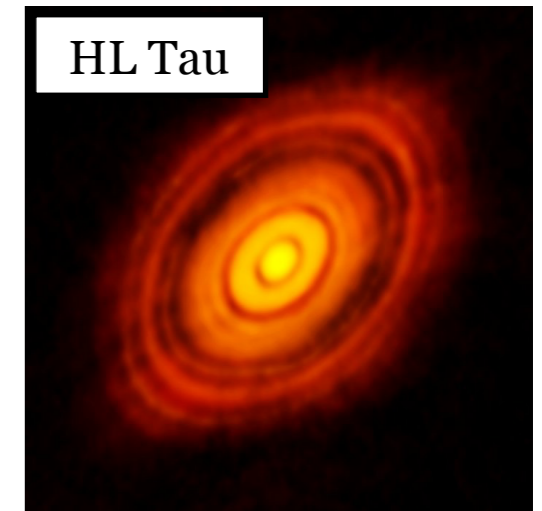
Inheritance

- Tracers of embedded disks
 - e.g., L1527
 - c-C₃H₂ shows rotation & infall: envelope
 - SO shows solid-body rotation: accretion shock at centrifugal barrier
- Alteration of ice/gas at point of entry into the disk



Disks in 2016

- So far, disk structure taken from SED modeling
 - Radial, vertical gradients in density and temperature
 - Freeze out & snow lines, deuteration, photodesorption...
 - (Large) gaps in transitional disks
 - Often seen to be filled with (reduced amounts of) gas
 - Accretion shocks at centrifugal barrier of forming disks
- HL Tau, TW Hya (how general?)
 - Disks are series of rings, gaps, wiggles
 - Traced in millimeter-sized grains
 - **Underlying gas surface density distribution?**
 - **Associated distribution of μm -sized grains (\Leftrightarrow UV, ionization)?**



ALMA

- **This talk has been ALMA-centric**

- Great progress in the last few years, and many exciting results to come

- **Fundamental limitation**

- Sensitivity to small-scale structure in thermal continuum will *always* be larger than to small-scale structure in gas emission lines
- Weak lines require very good bandpass calibration and very accurate continuum subtraction
- Inner, densest regions become optically thick in dust continuum at all/many ALMA wavelengths

- **Other ways to probe gas in (inner) disks**

- Long-slit spectroscopy
- MATISSE
- JWST

