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 the is 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?

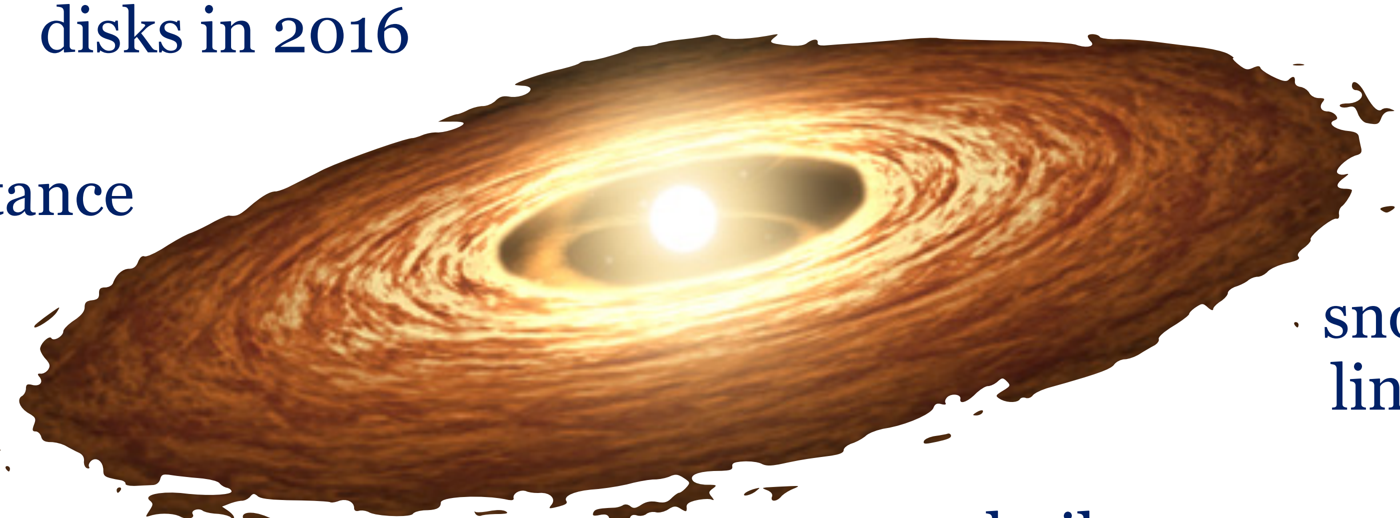
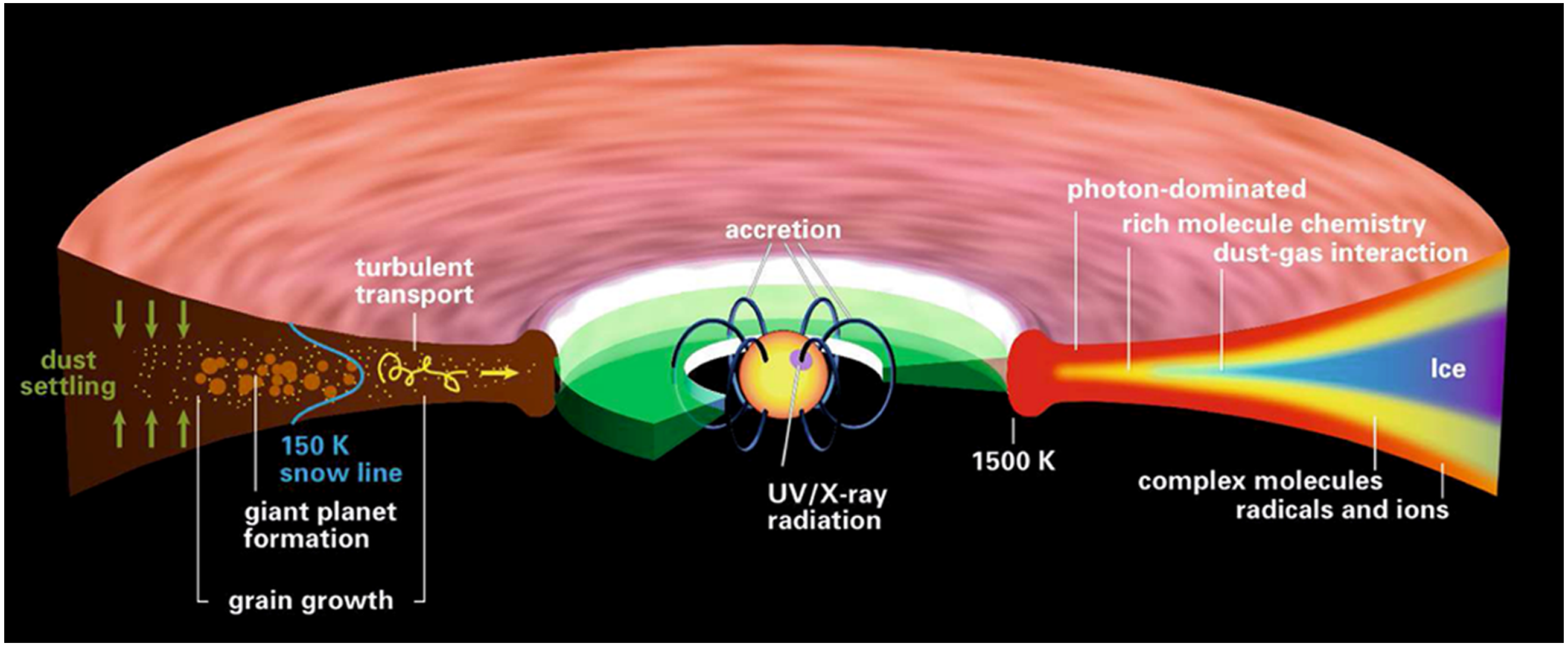


Image credit: NASA/JPL

Disk structure

- *Basic* structure of the disk
  - Radial surface density profile (gas, dust)
  - Vertical hydrostatic scale height
  - Irradiation by stellar spectrum
- Assumption: small (~μm) grains coupled (thermally, hydrodynamically) to gas
- ⇔ Spectral Energy Distribution fitting provides overall disk structure

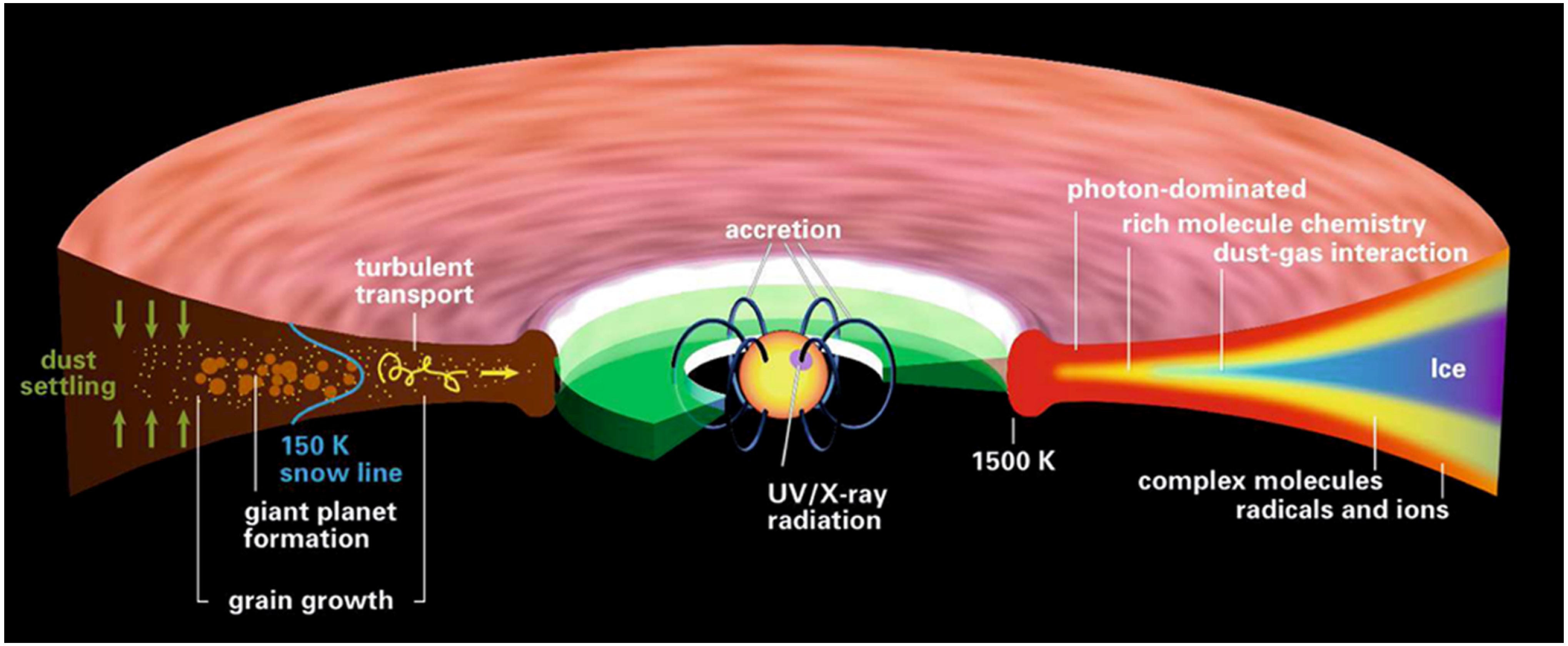


Henning & Semenov (2013)

$T(R,z)$, $G_O(R,z)$

- 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)

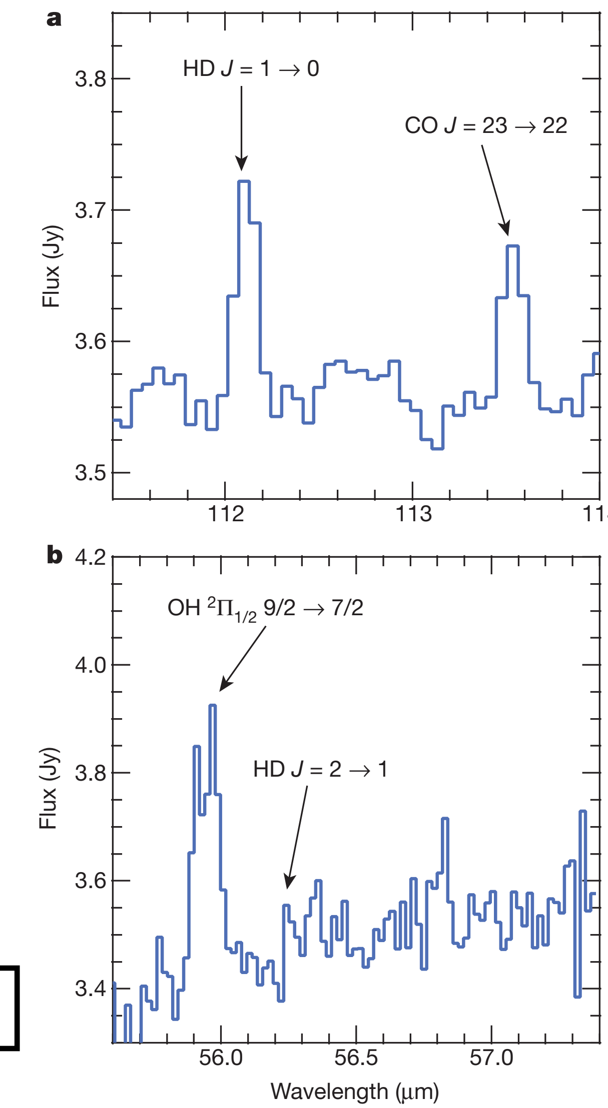


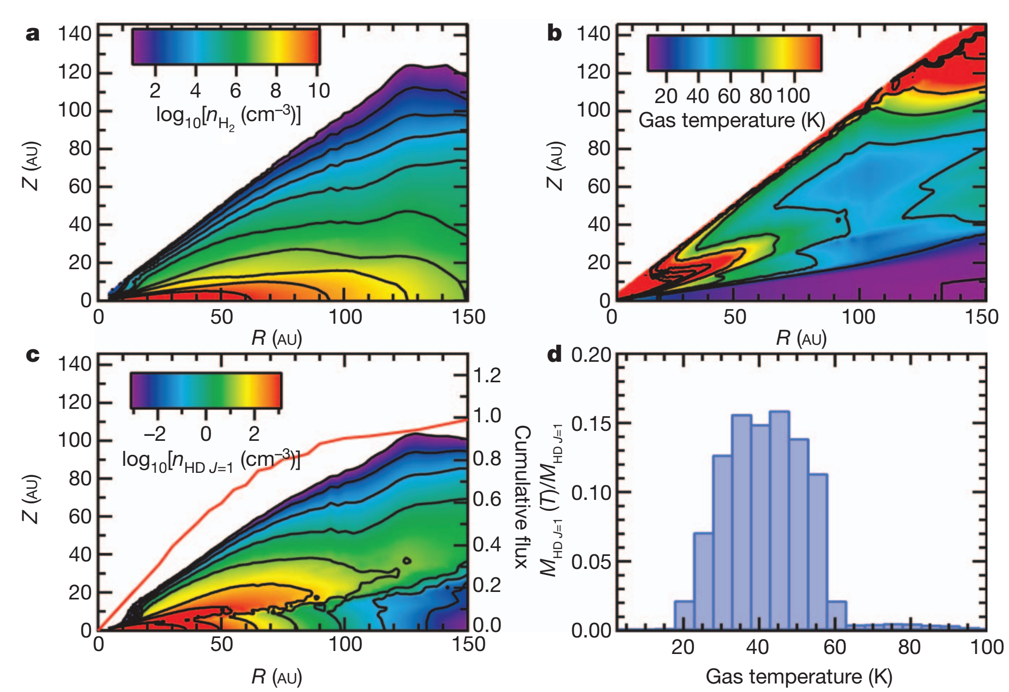
Henning & Semenov (2013)

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…)
    - H_2 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

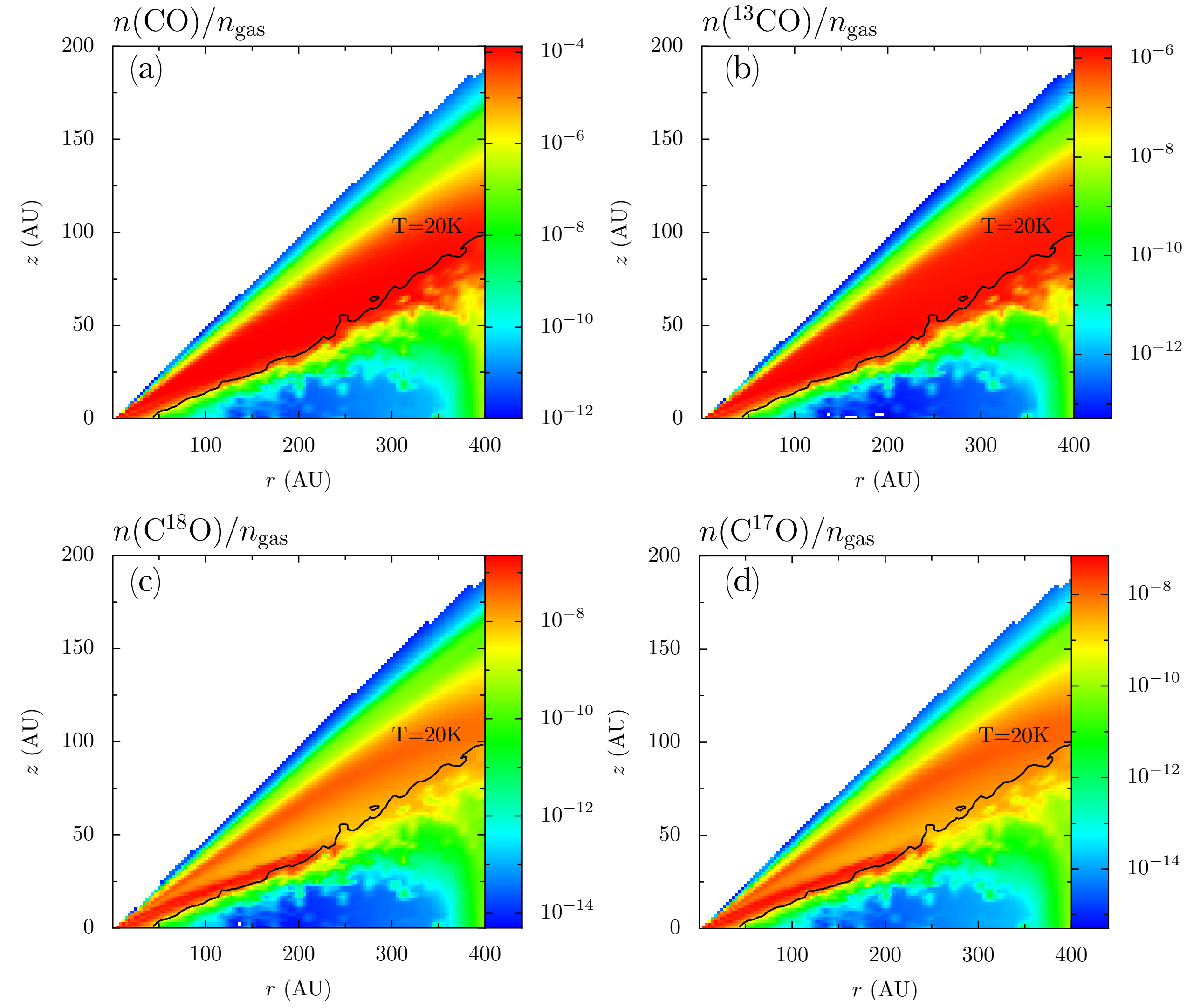




Bergin et al. (2013)

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)



Miotello et al. (2014)

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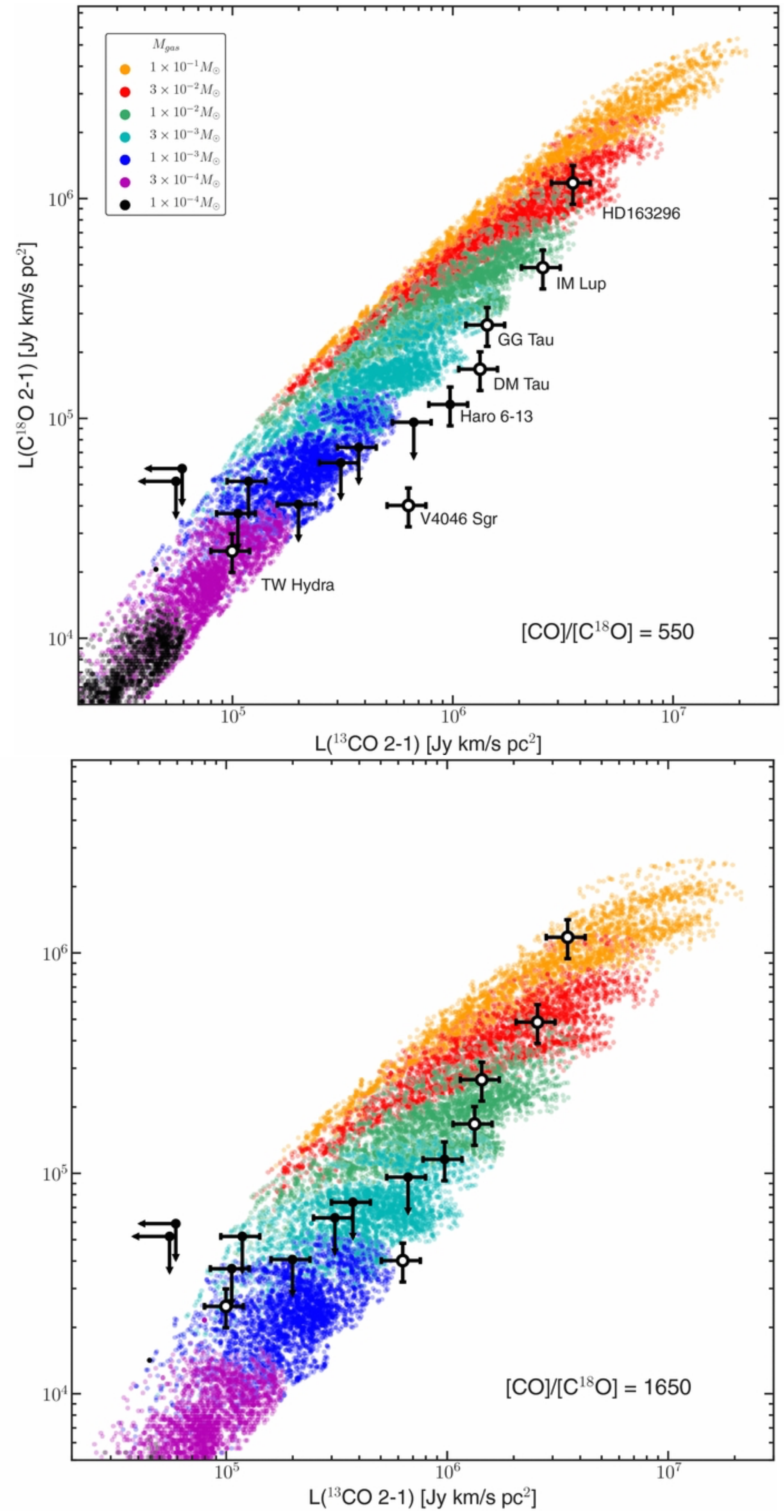


Williams & Best (2014)

Snow lines

- Radial temperature gradient → snow lines for major volatiles: H_2O, CO, N_2?

- Directly traced via CO isotopes

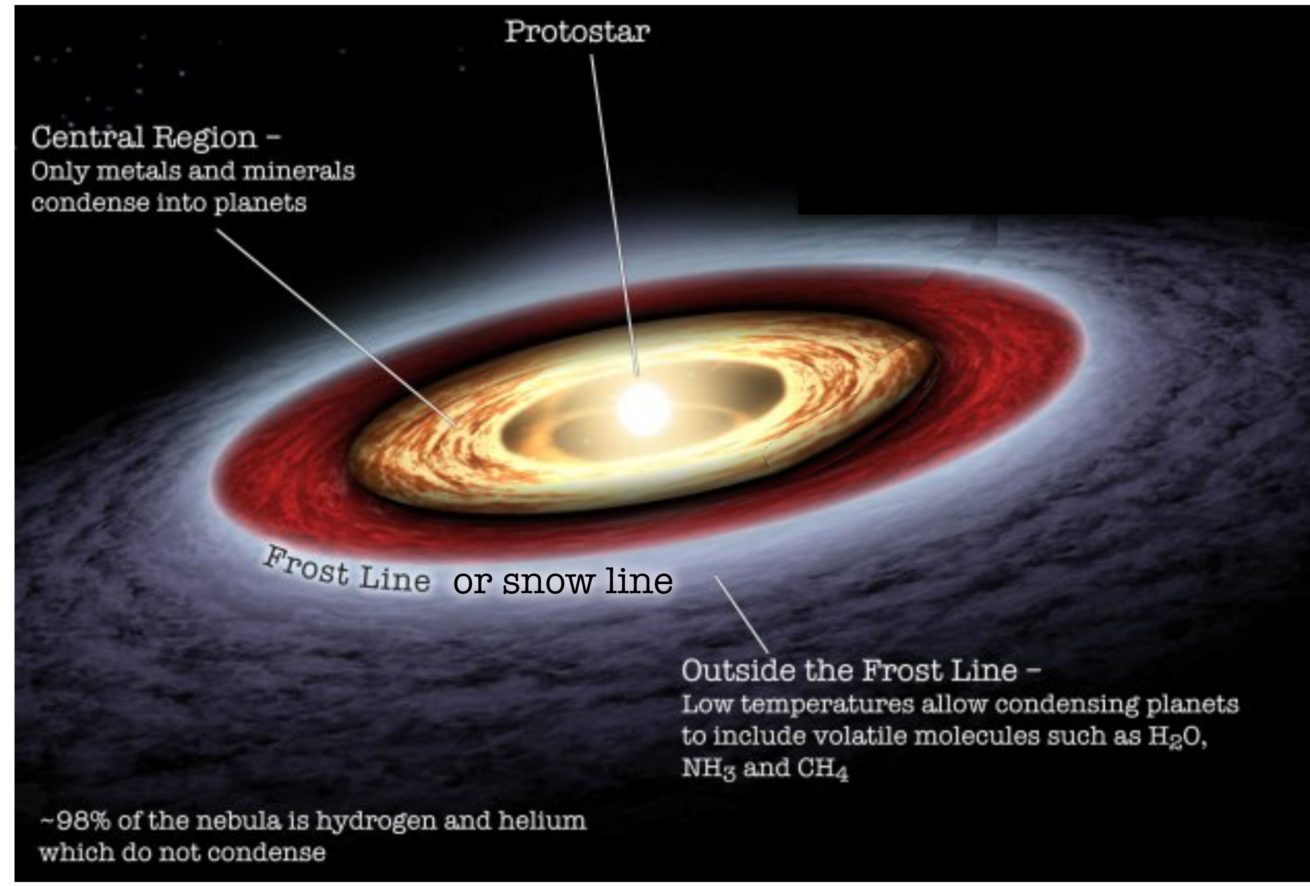
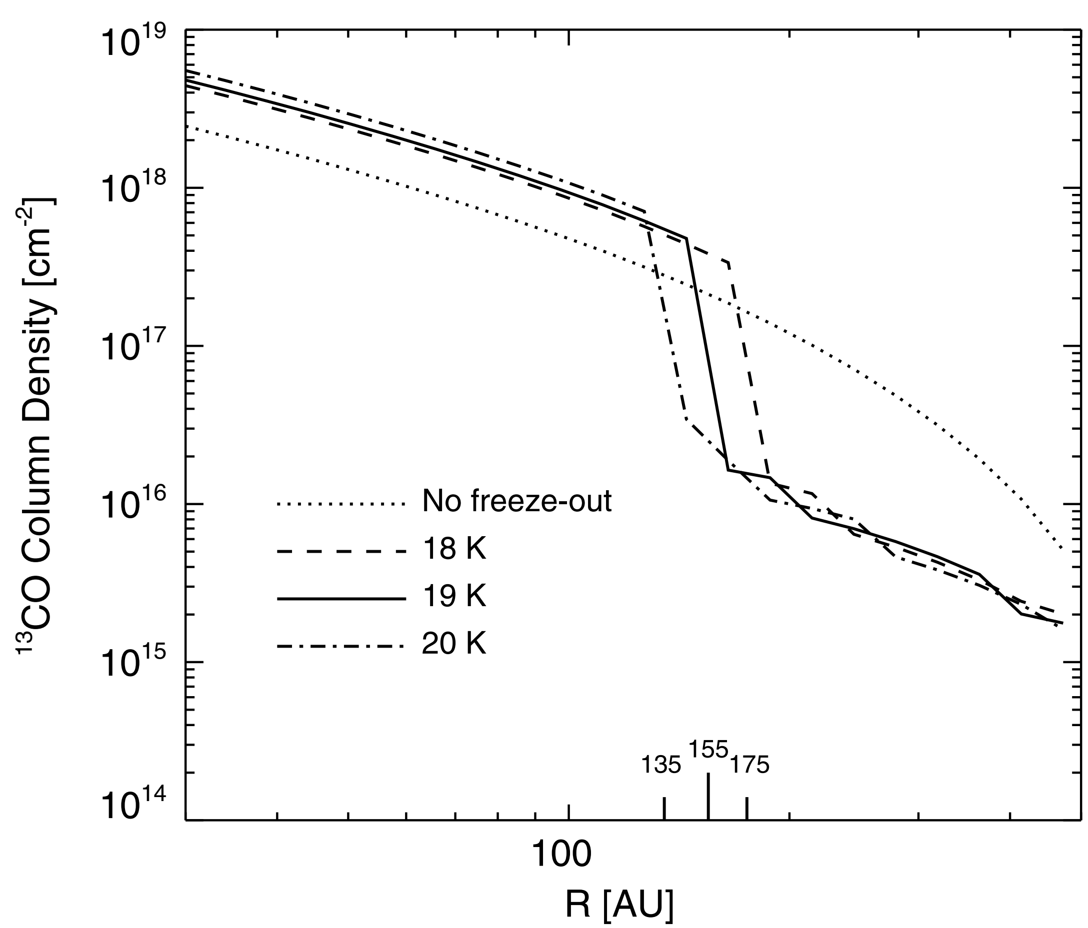
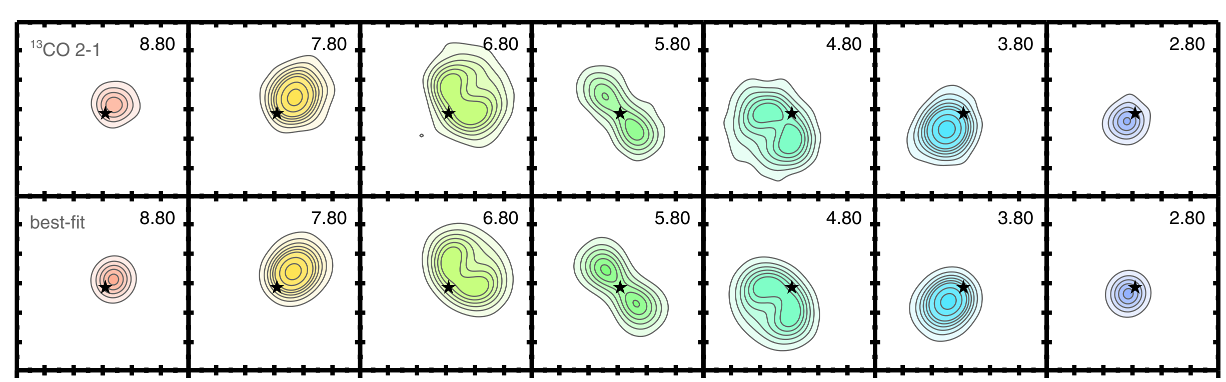


Image credit: NASA/JPL



HD163296



Qi et al. (2011)

Snow lines

- Radial temperature gradient → snow lines for major volatiles: H_2O, CO, N_2?

- …or indirectly via N_2H^+

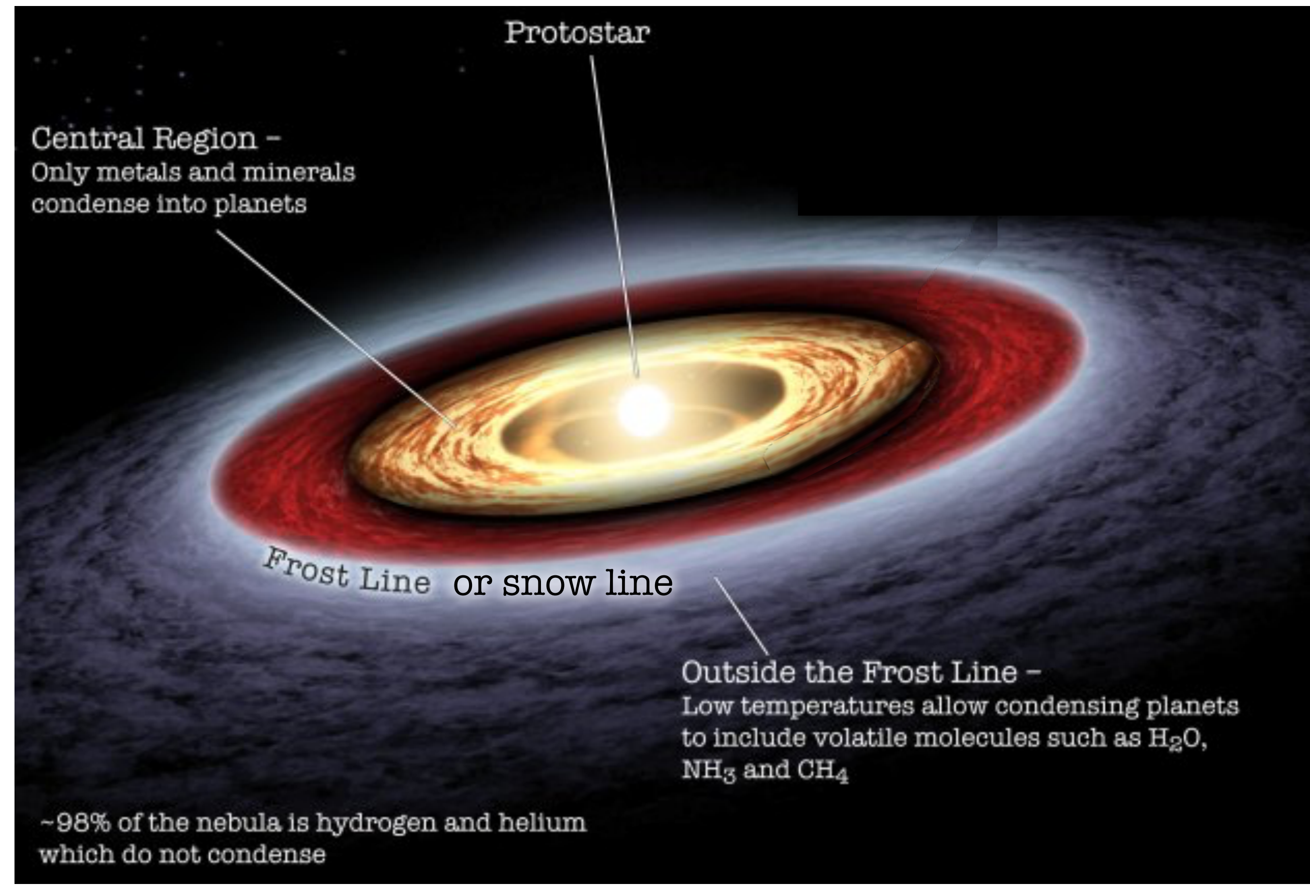
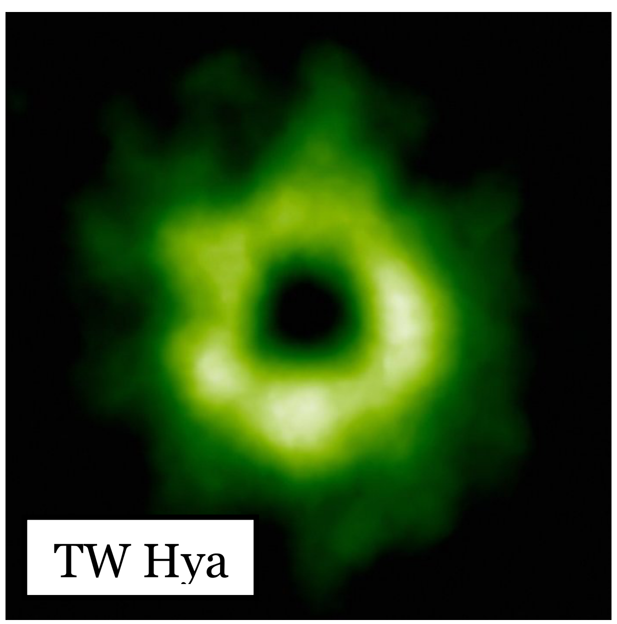
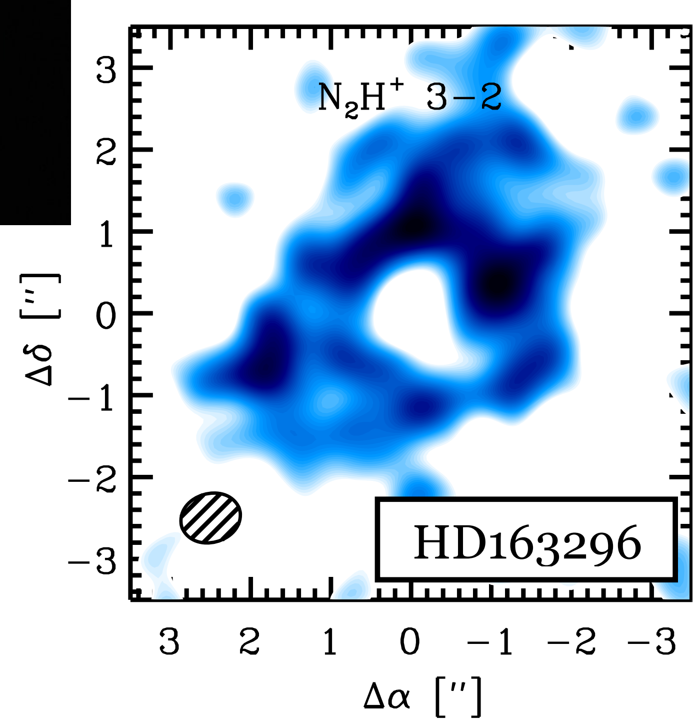


Image credit: NASA/JPL





production: $H_3^+ + N_2 \longrightarrow N_2H^+ + H_2$

$H_3^+ + CO \longrightarrow HCO^+ + H_2$

destruction: $N_2H^+ + CO \longrightarrow HCO^+ + H_2$

Qi et al. (2013, 2015)

Snow lines

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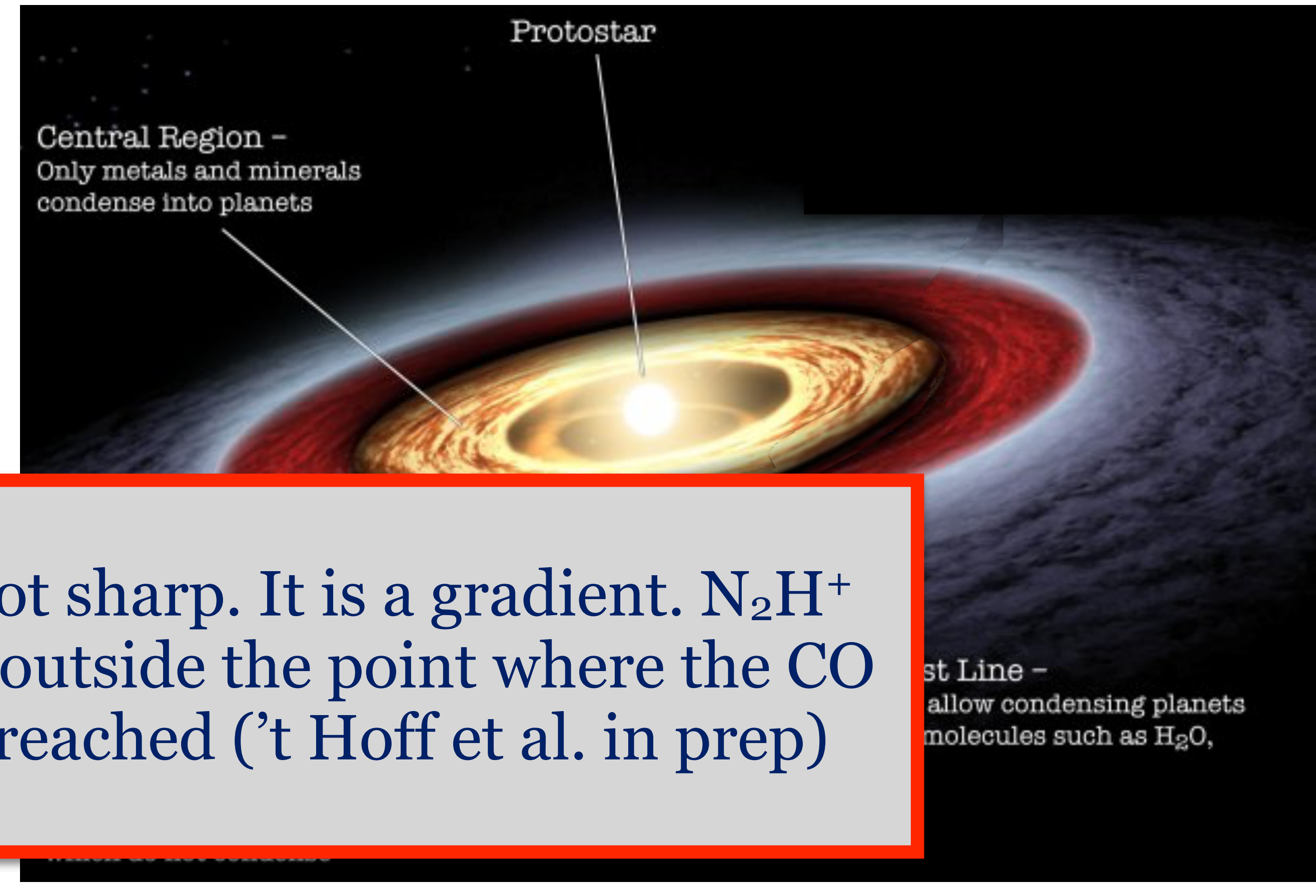
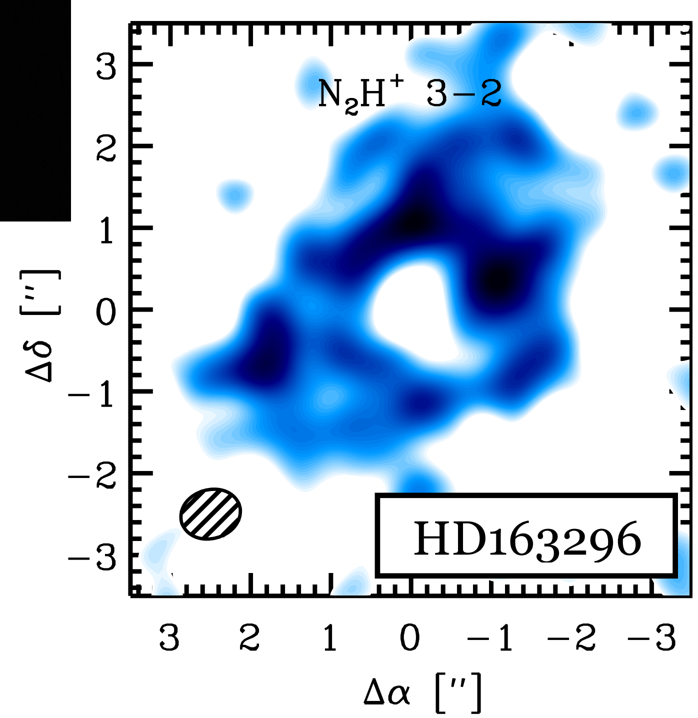


Caution: CO snow line is not sharp. It is a gradient. N_2H^+ may not show up until well outside the point where the CO freeze out temperature is reached ('t Hoff et al. in prep)

Image credit: NASA/JPL



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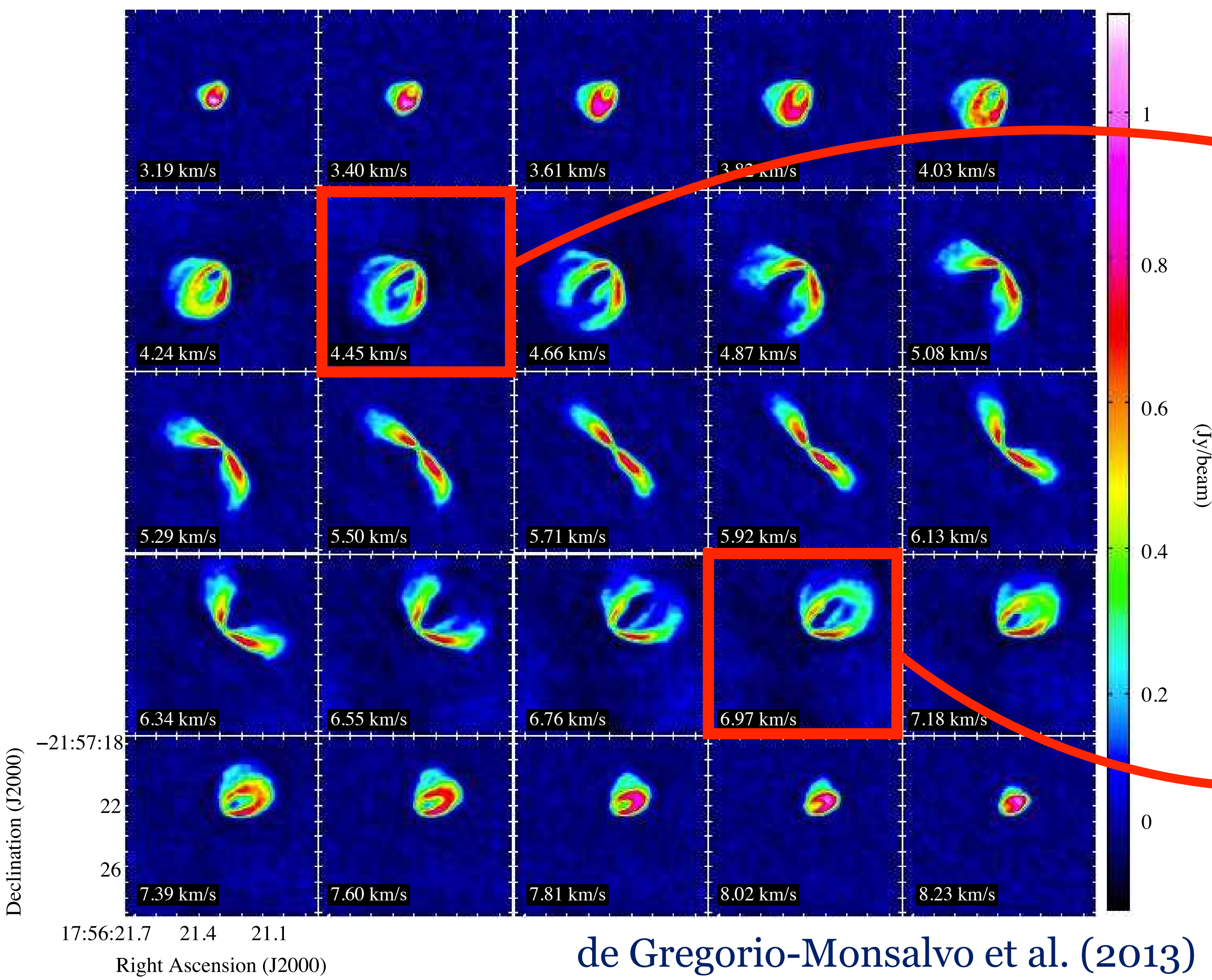
destruction: $N_2H^+ + CO \rightarrow HCO^+ + H_2$

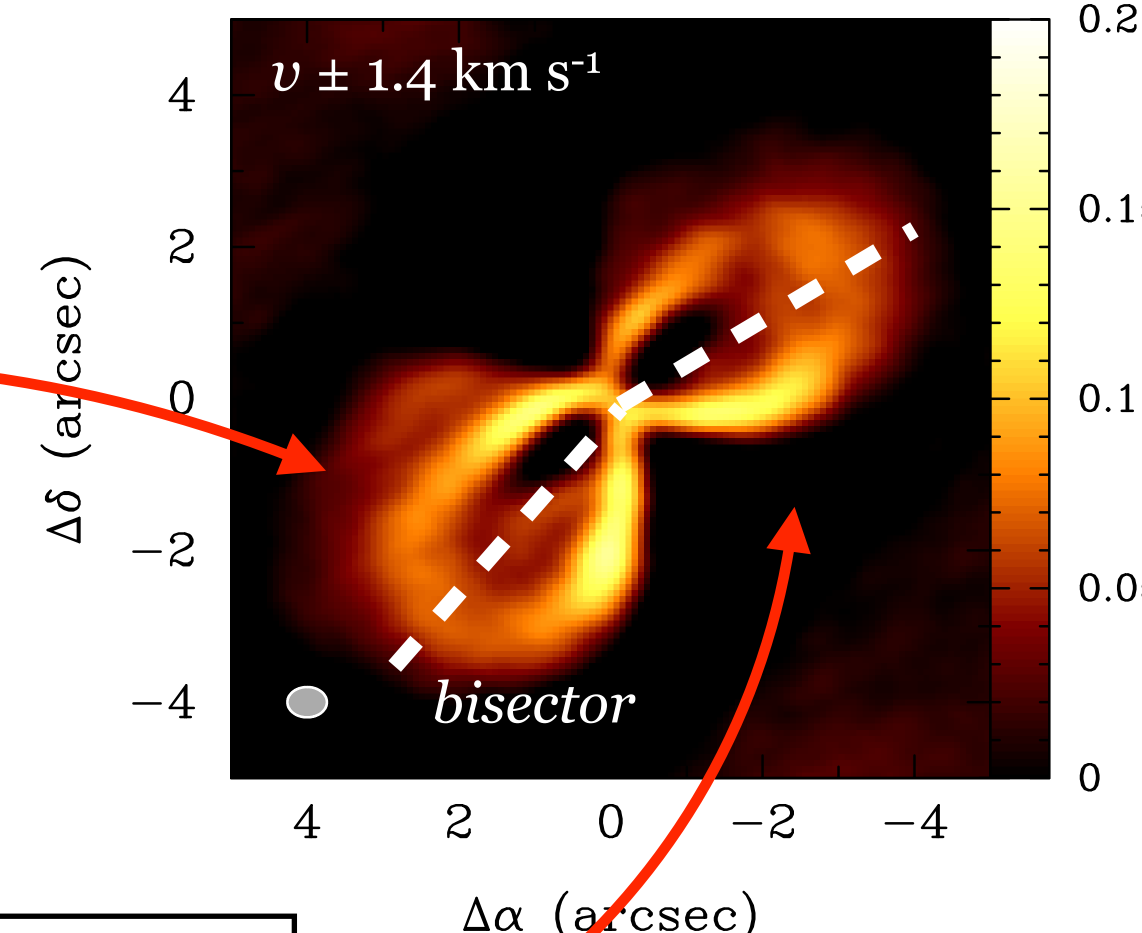
Qi et al. (2013, 2015)

Snow surface

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



de Gregorio-Monsalvo et al. (2013)

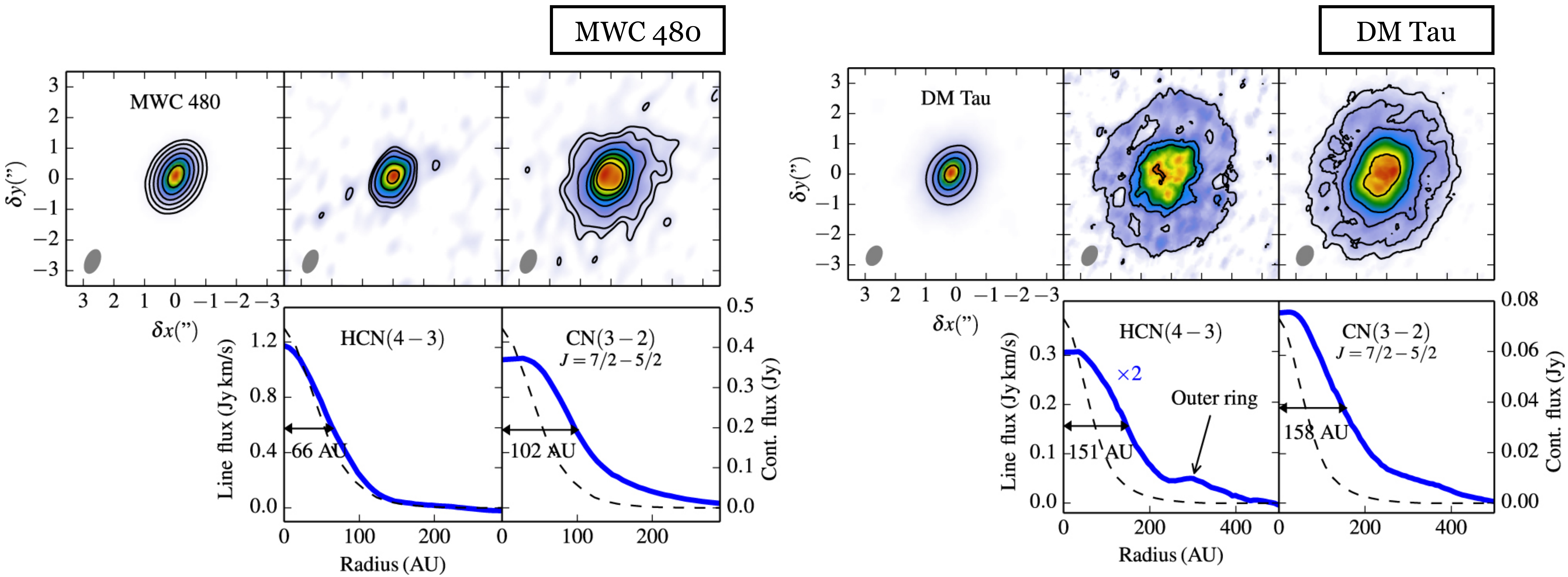


HD163296

BSc thesis van Houdt/
Rasappu (Leiden U., 2013)

UV irradiated outer regions

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

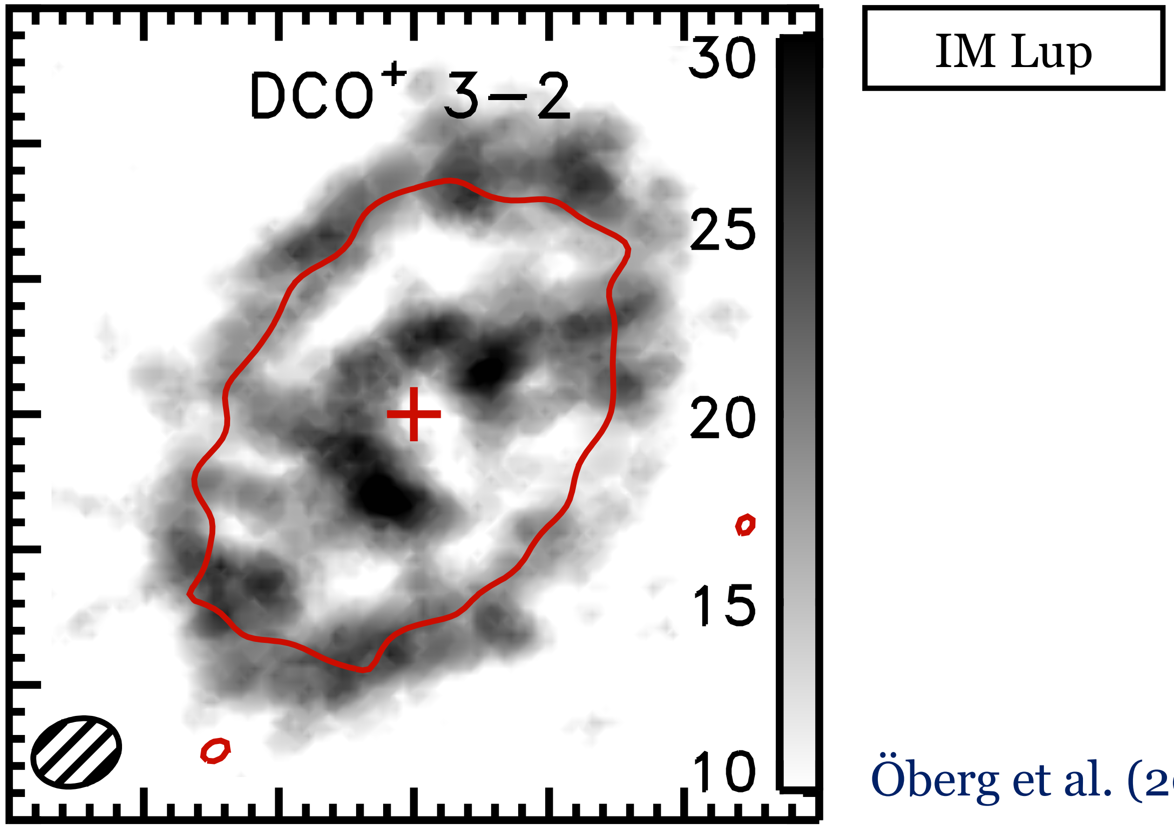


Guzmán et al. (2015)

See also Chapillon et al. (2012) for more results on HCN, CN, HC_3N

UV irradiated outer regions

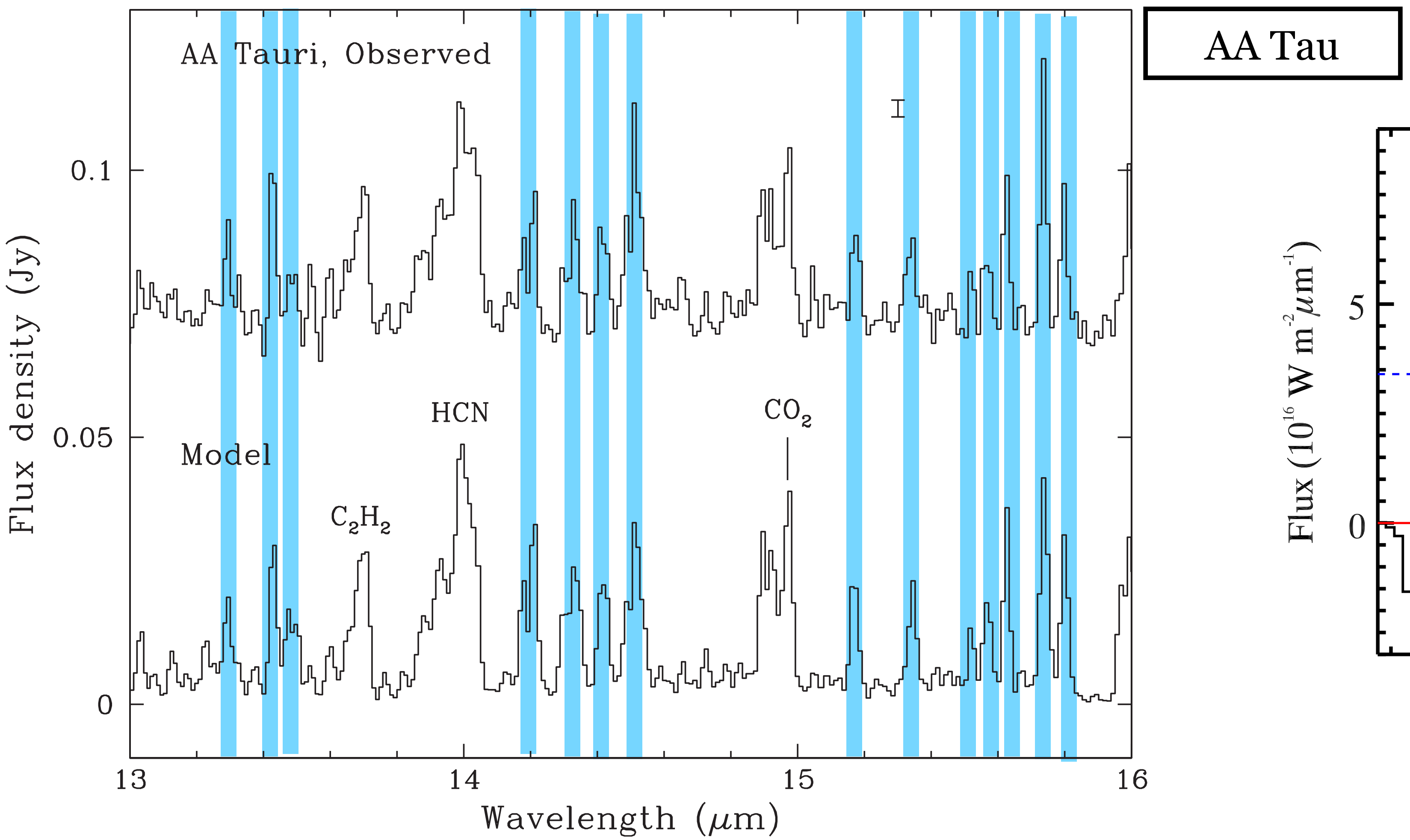
- Interstellar radiation field penetrates outer disk
- Extended CN emission compared to HCN
- Photodesorption (rather than thermal desorption) sets up a second, outer snow line

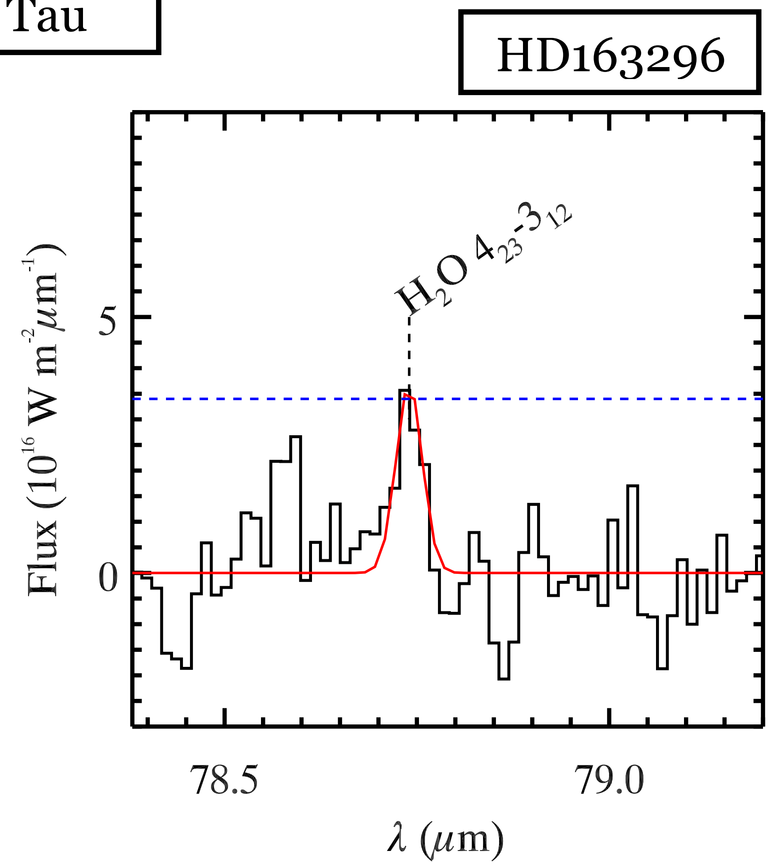


Öberg et al. (2015)

Volatiles

- Other detected volatiles
  - H_2O in several disks
  - gas-phase production / evaporation in inner disk

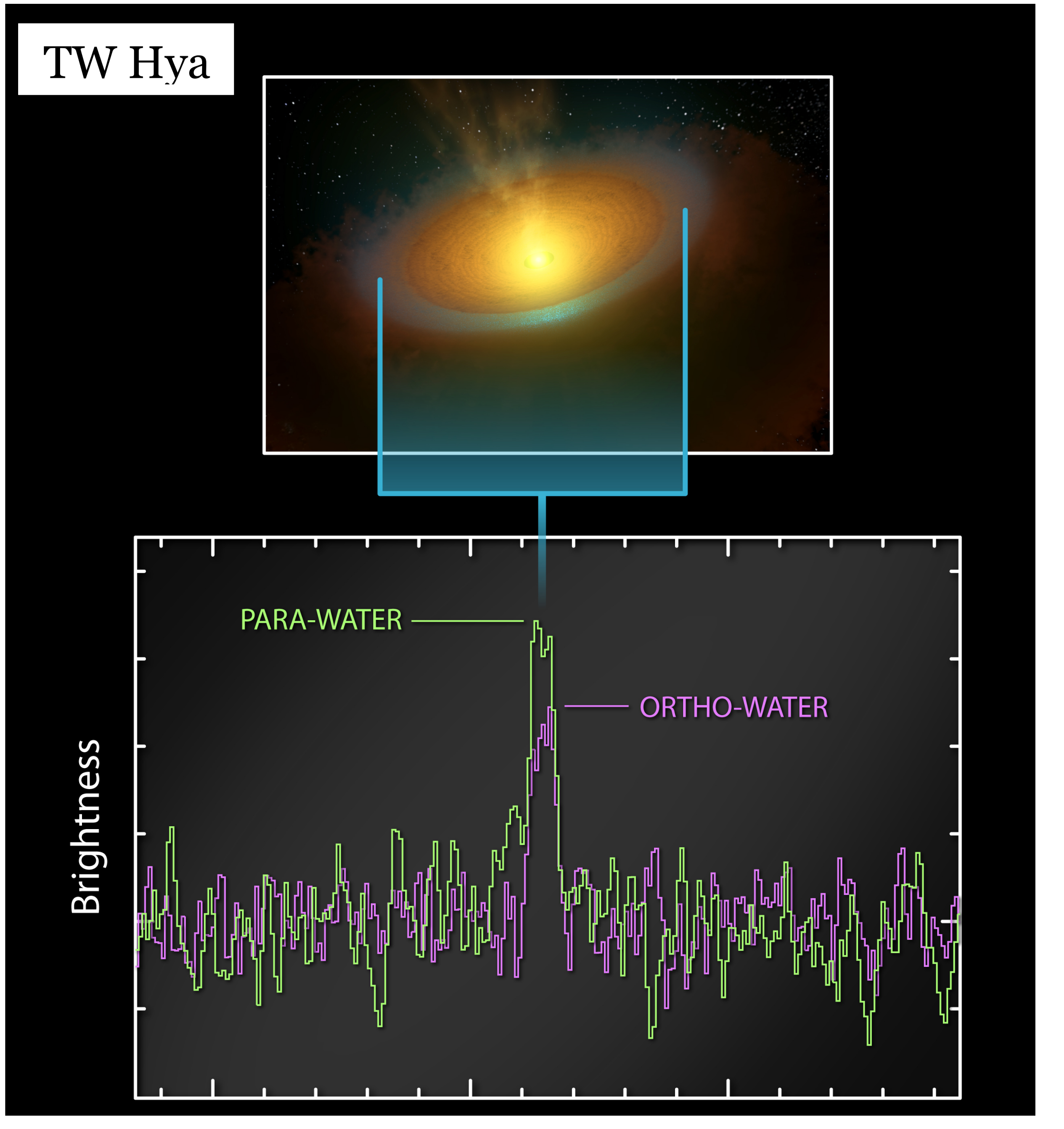


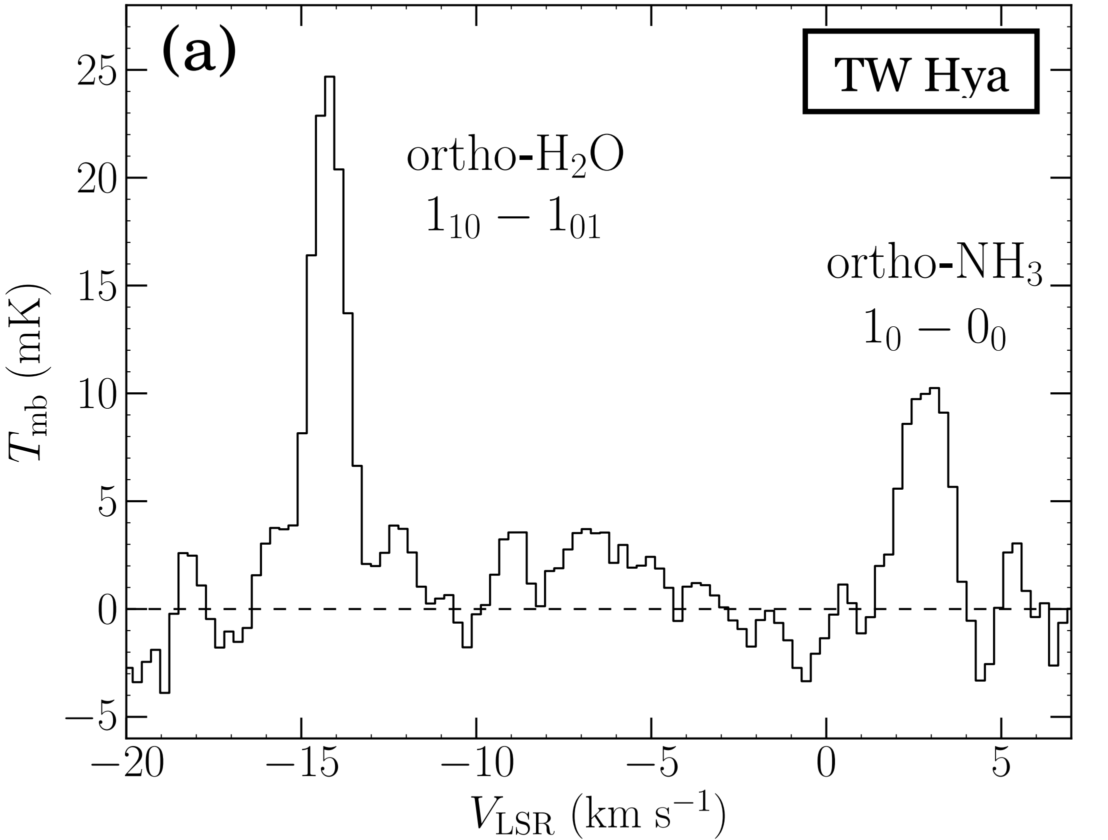


Carr & Najita (2008); Salyk et al. (2008, 2015); Pontoppidan et al. (2010); Meijerink et al. (2009); Zhang et al. (2013); Fedele et al. (2012); Riviere-Marichalar et al. (2012)

Volatiles

- Other detected volatiles
  - H_2O 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?
  - NH_3 in TW Hya

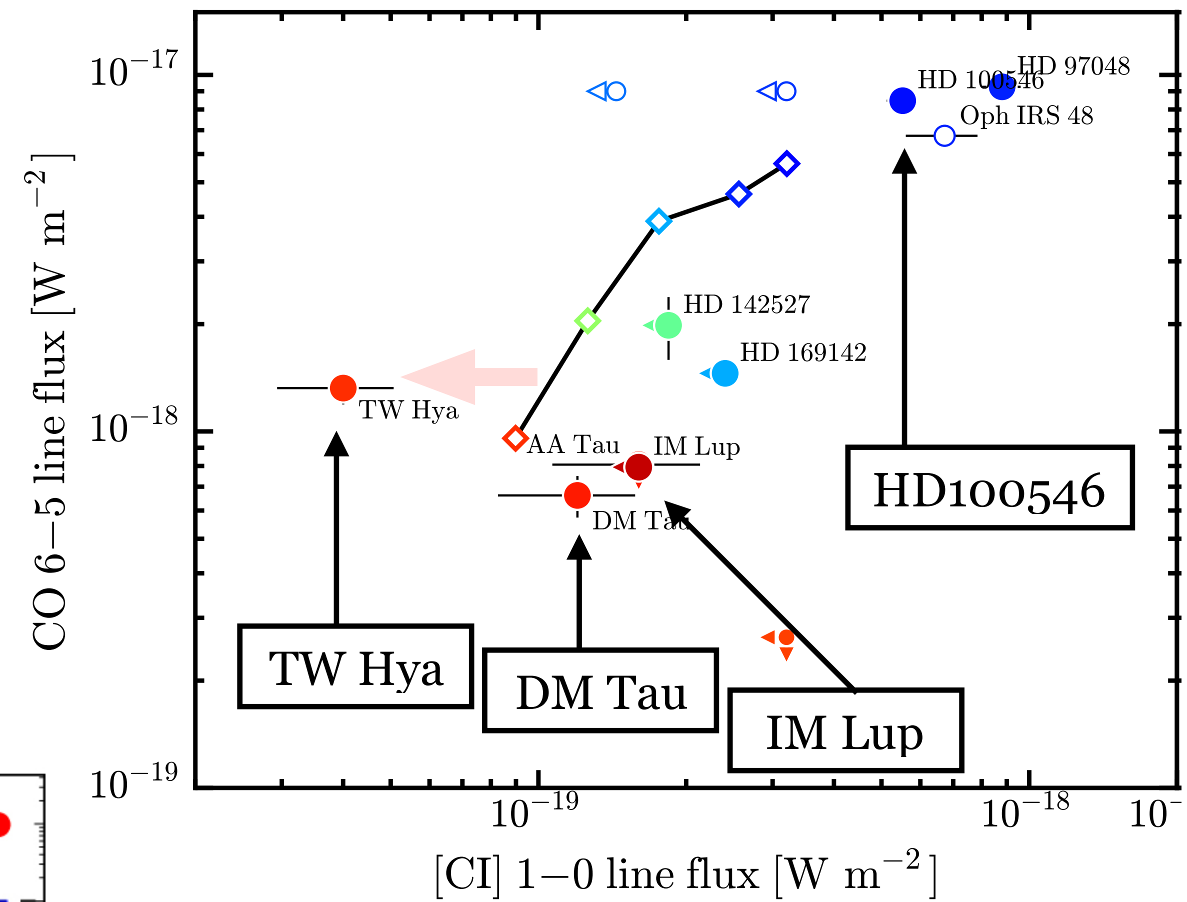


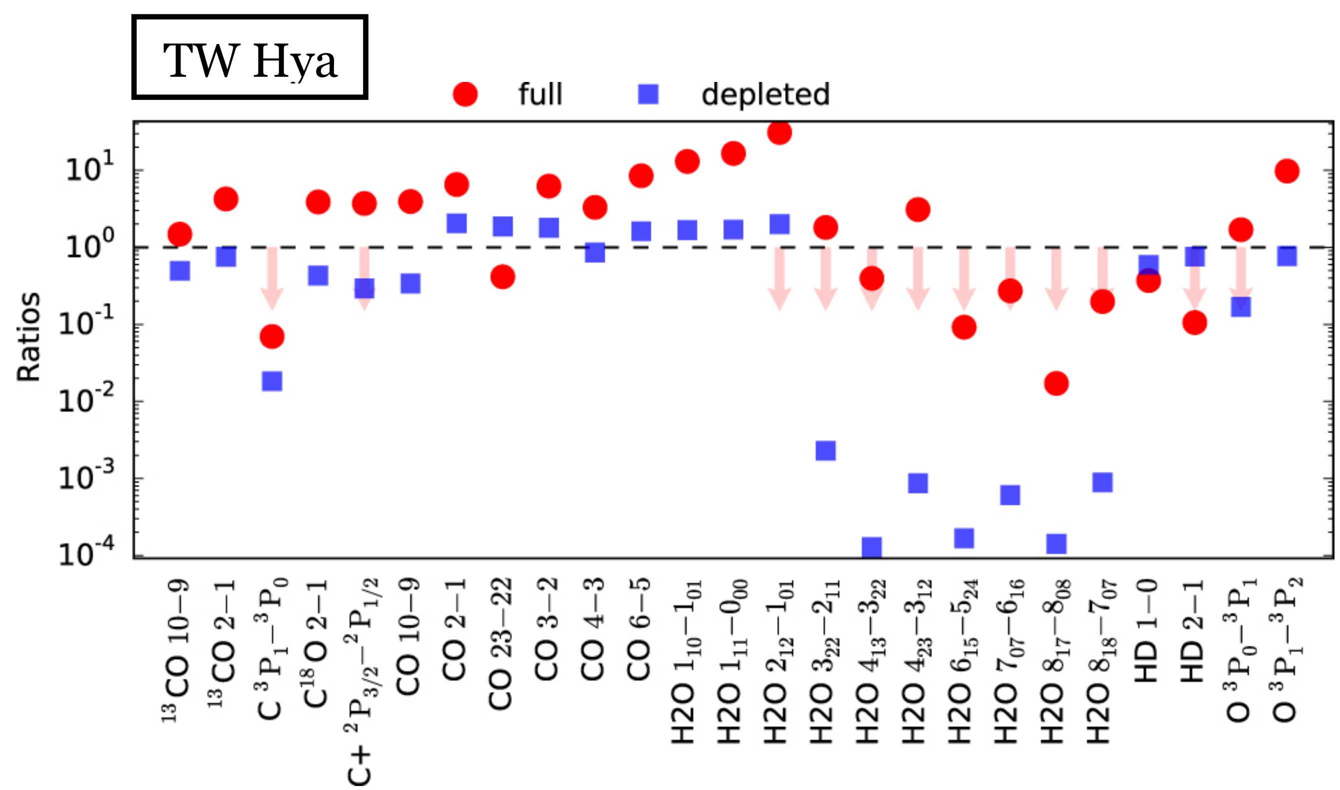


Hogerheijde et al. (2011), Salinas et al. (2016), Hogerheijde et al. (in prep), Du et al. (in prep)

Depletion of volatiles

- CO, C, and H_2O depleted in many disks
    - TW Hya in particular
- Locked up in the midplane



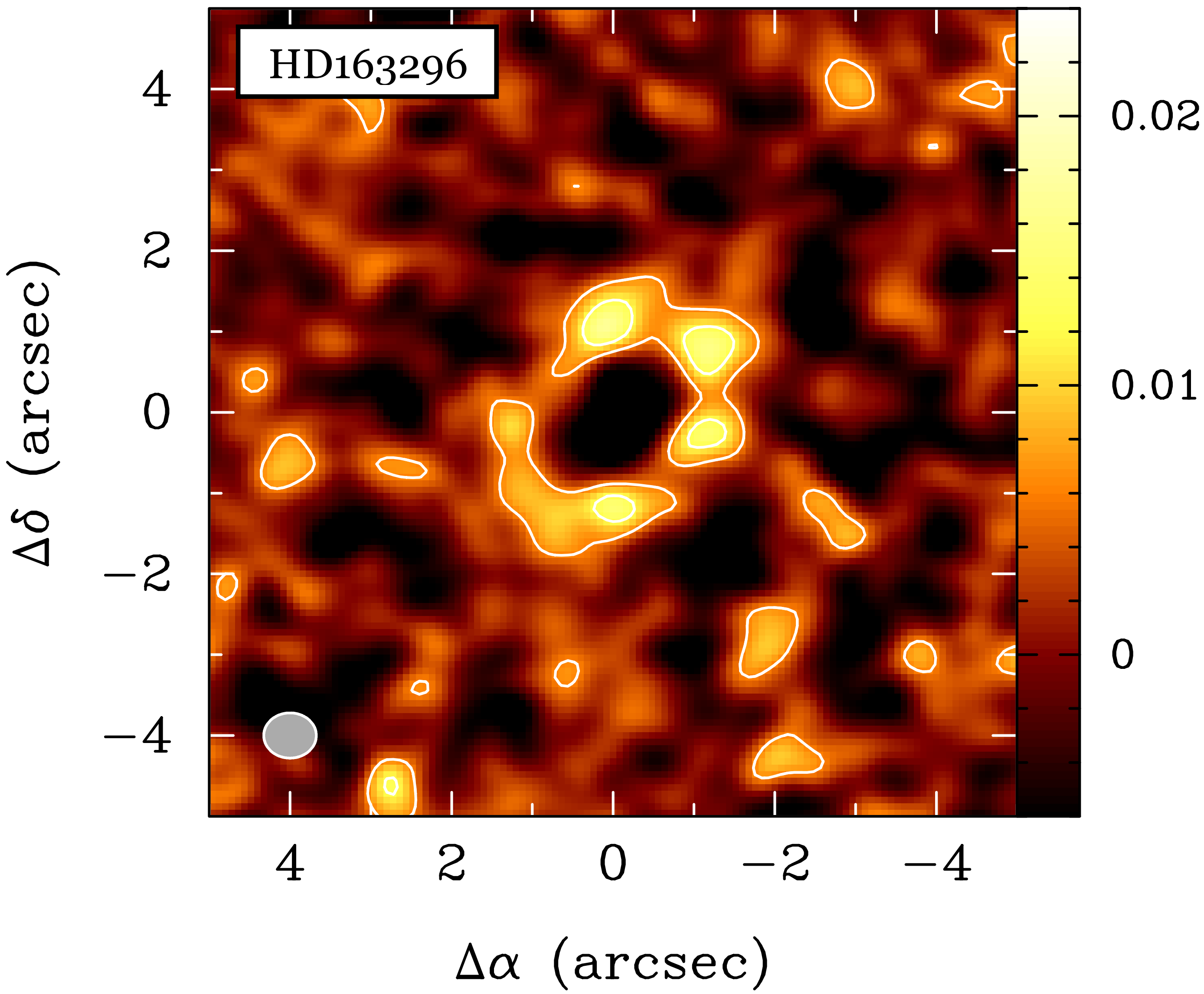


Kama et al. (2016), Du et al. (2015, in prep)

Deuteration

- Deuterated molecules are enriched in cold gas
  - $H_3^+ + HD <—> H_2D^+ + H_2$
  - $H_2D^+ + X —> XD^+ + H_2$

N_2D^+ in HD163296

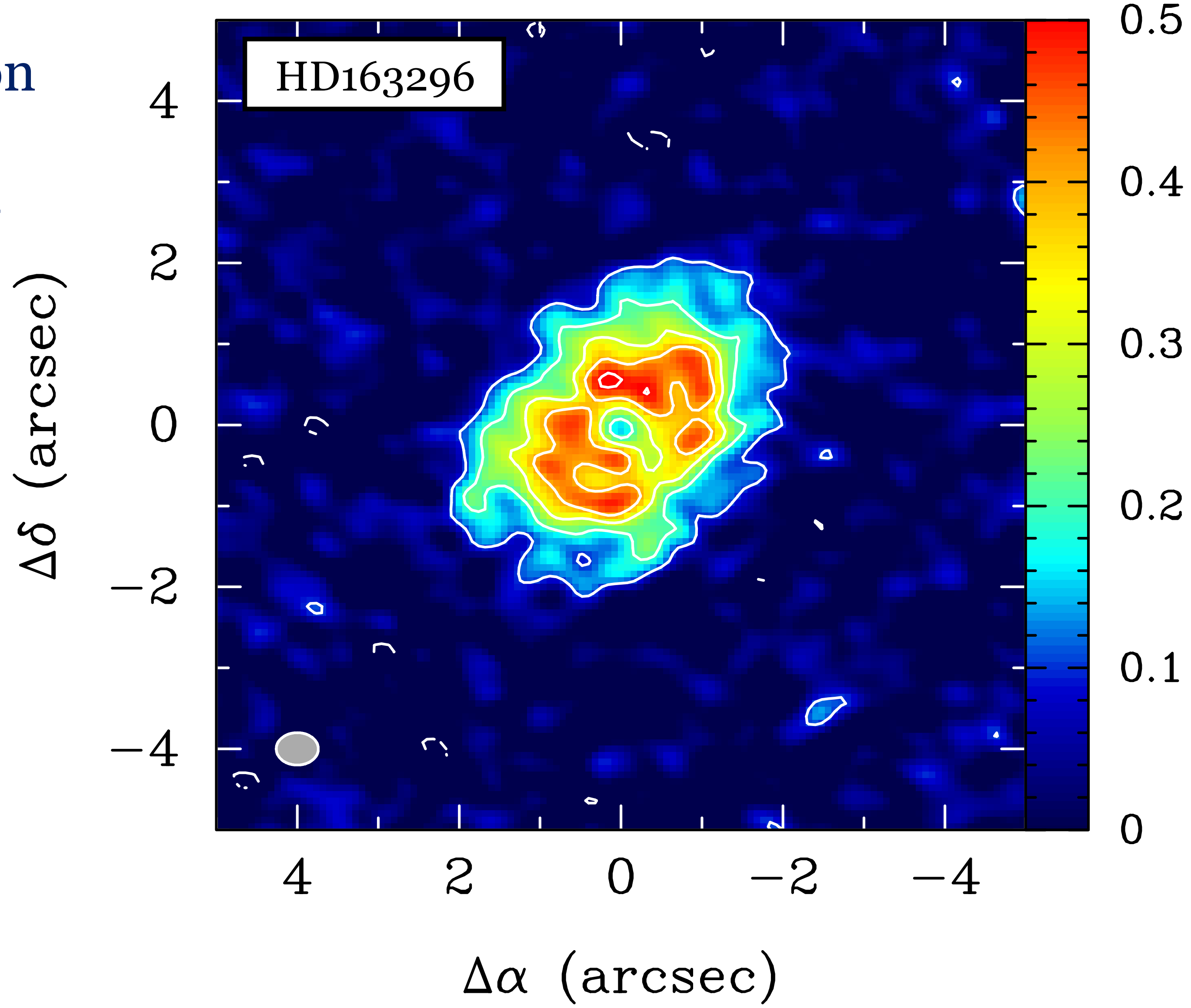


Salinas et al. (in prep)

Deuteration

- Deuterated molecules are enriched in cold gas
  - $H_3^+ + HD <\!\!-\!\!> H_2D^+ + H_2$
  - $H_2D^+ + X -\!\!> XD^+ + H_2$
- High(er) temperature deuteration
  - $CH_3^+ + HD <\!\!-\!\!> CH_2D^+ + H_2$
  - $... + O -\!\!> DCO^+ + ...$

DCO$^+$ in HD163296



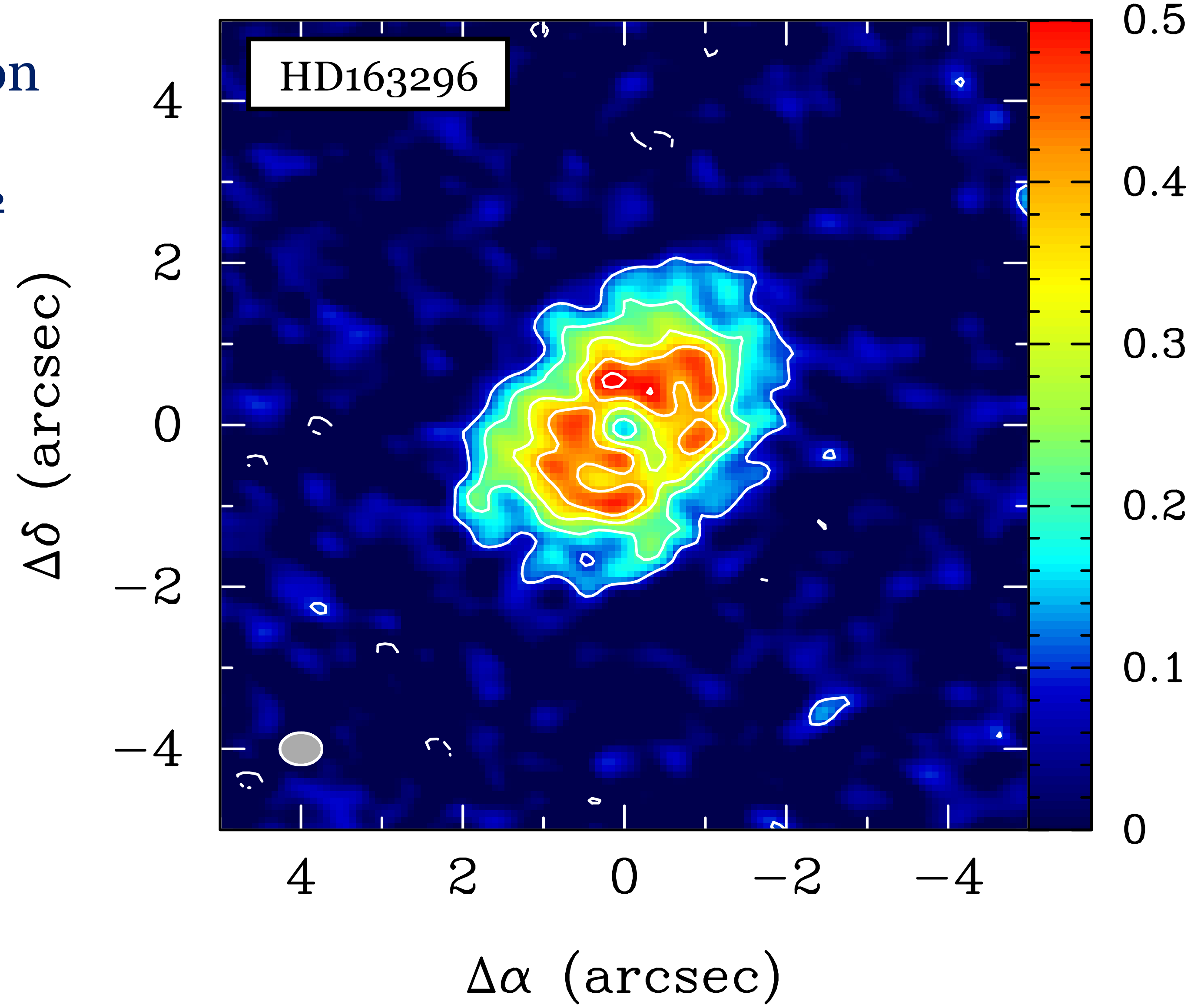
see also Favre et al. (2015)

Salinas et al. (in prep)

Deuteration

- Deuterated molecules are enriched in cold gas
  - $H_3^+ + HD <—> H_2D^+ + H_2$
  - $H_2D^+ + X —> XD^+ + H_2$
- High(er) temperature deuteration
  - $CH_3^+ + HD <—> CH_2D^+ + H_2$
  - ... + O —> DCO^+ + ...

DCO^+ in HD163296



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^+)

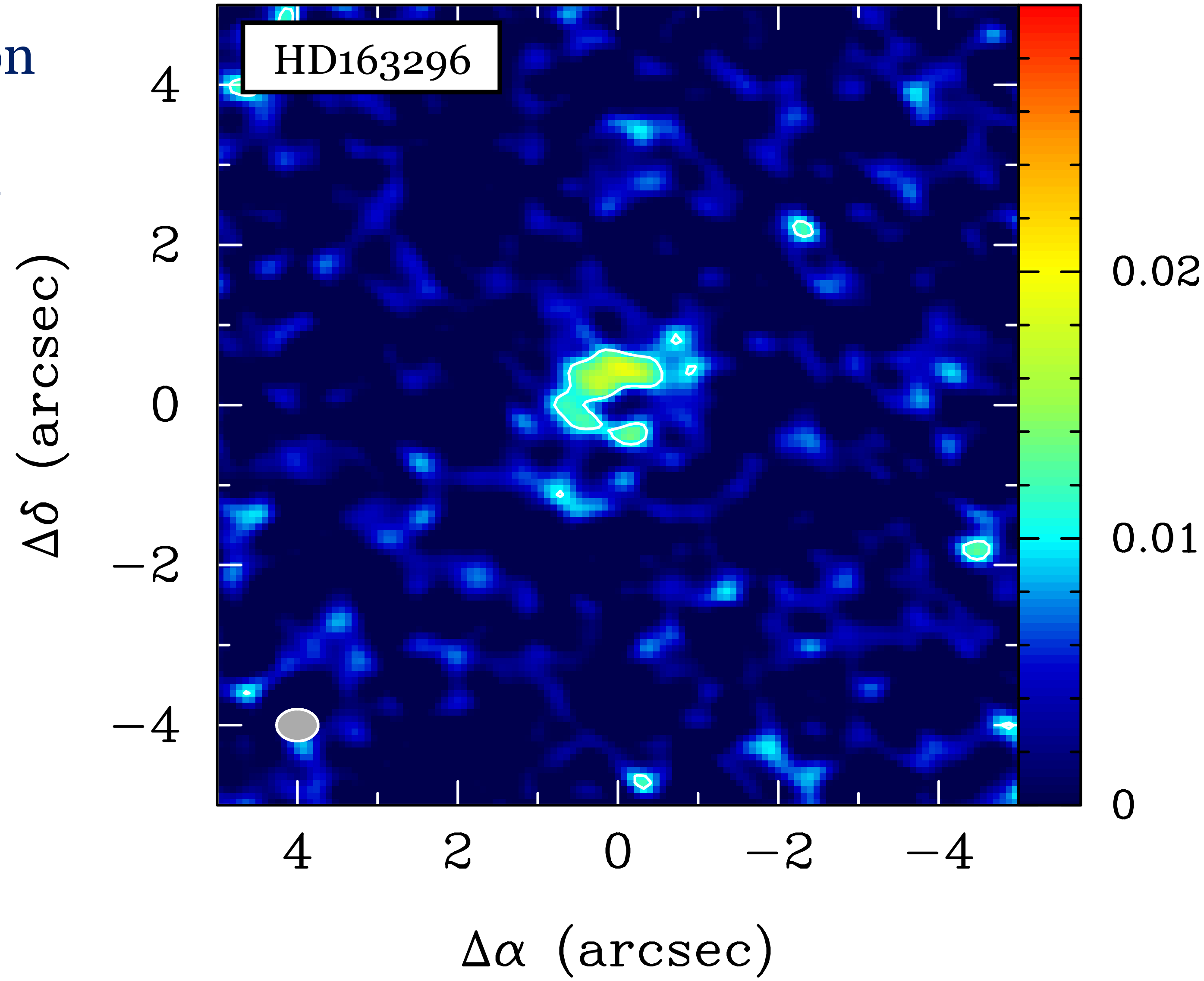
see also Favre et al. (2015)

Salinas et al. (in prep)

Deuteration

- Deuterated molecules are enriched in cold gas
  - $H_3^+ + HD <—> H_2D^+ + H_2$
  - $H_2D^+ + X —> XD^+ + H_2$
- High(er) temperature deuteration
  - $CH_3^+ + HD <—> CH_2D^+ + H_2$
  - ... + O —> DCO^+ + ...
  - ... + N —> DCN + ...

DCN in HD163296



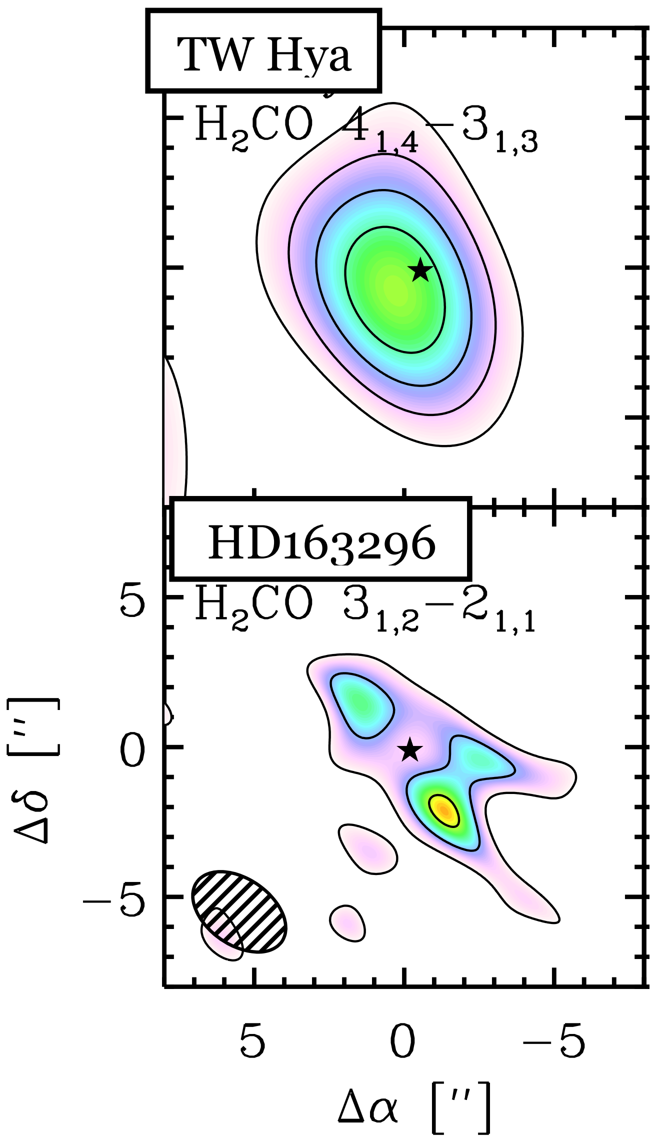
see also Öberg et al. (2012)

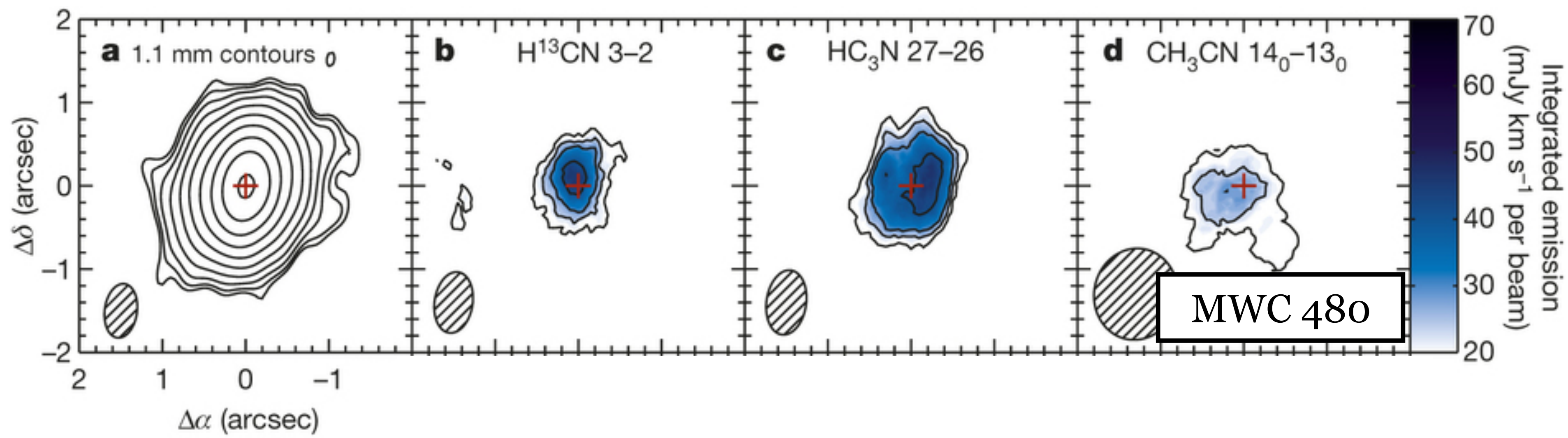
Salinas et al. (in prep)

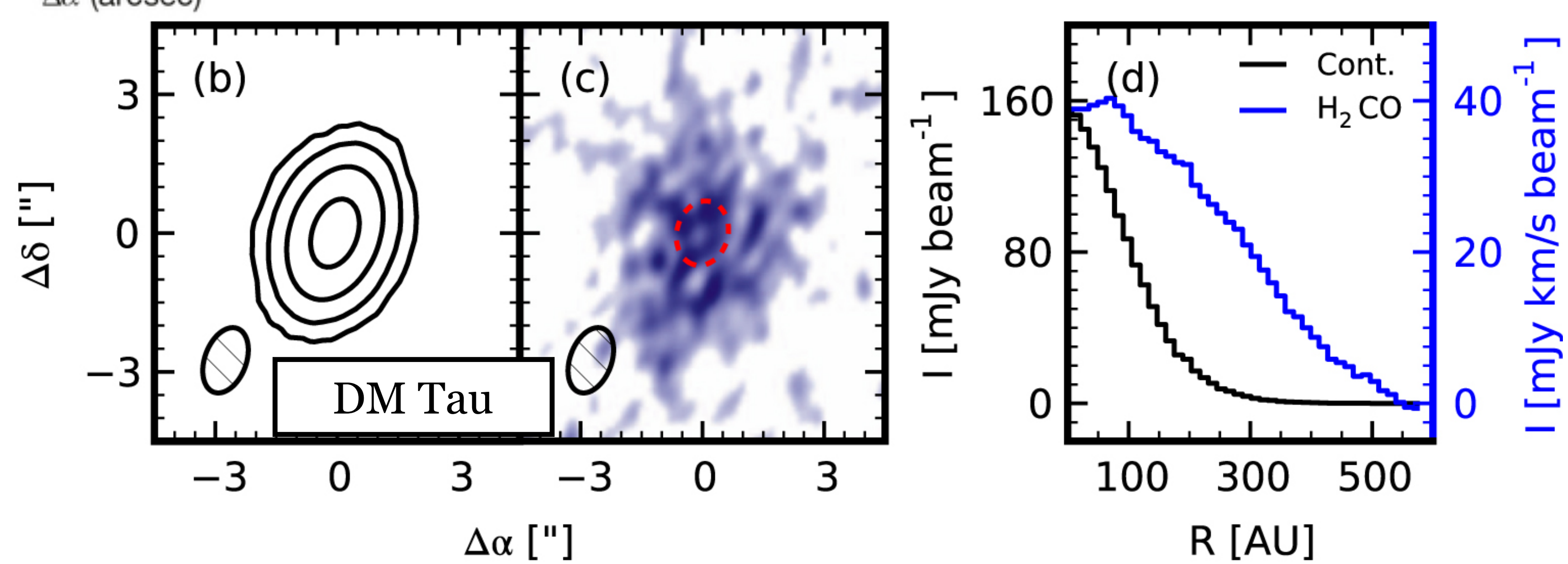
Organics

- 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)







Loomis et al. (2015)

Qi et al. (2013)

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

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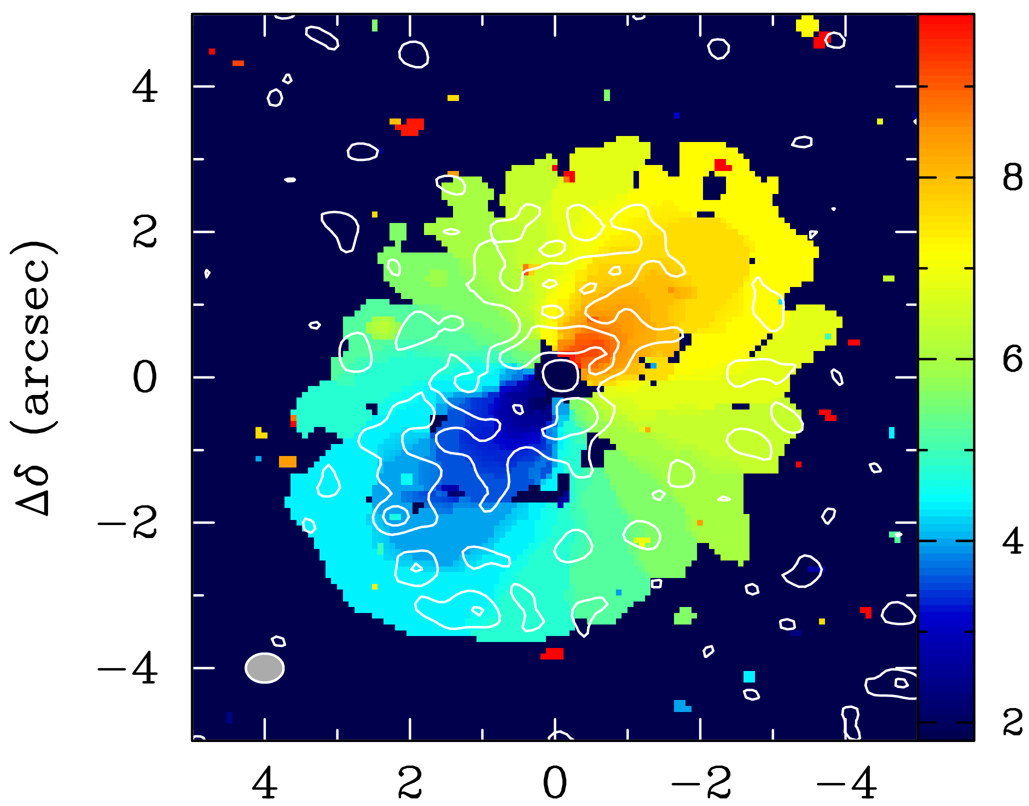
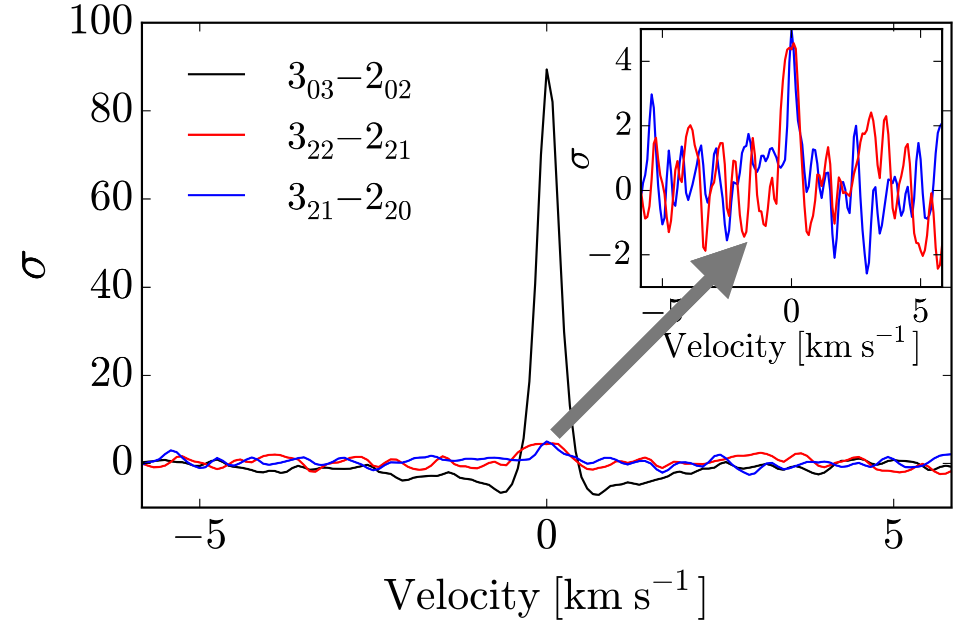
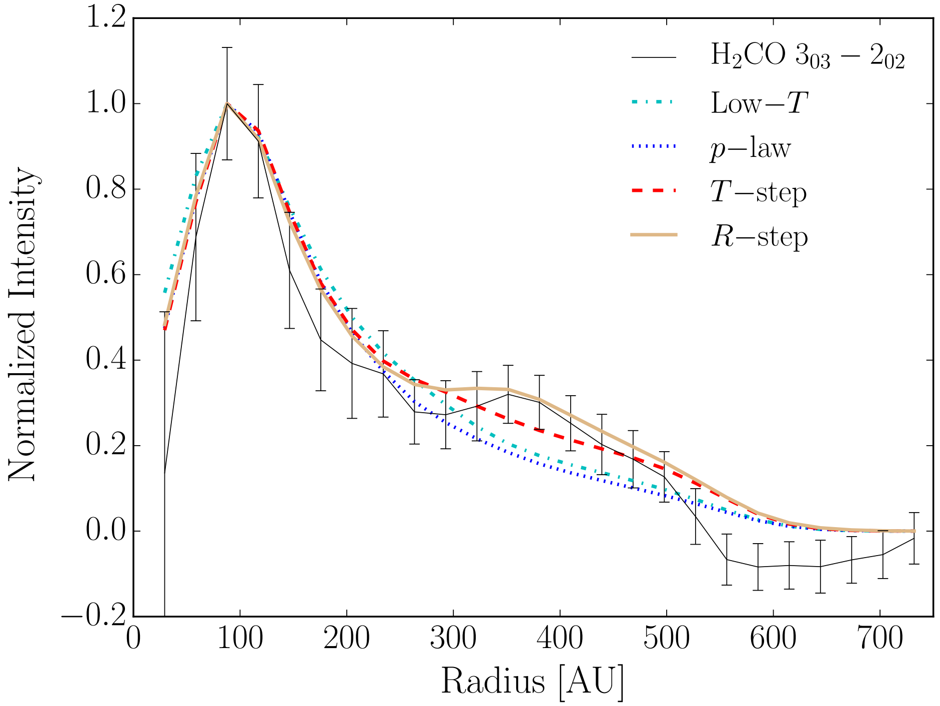




HD163296

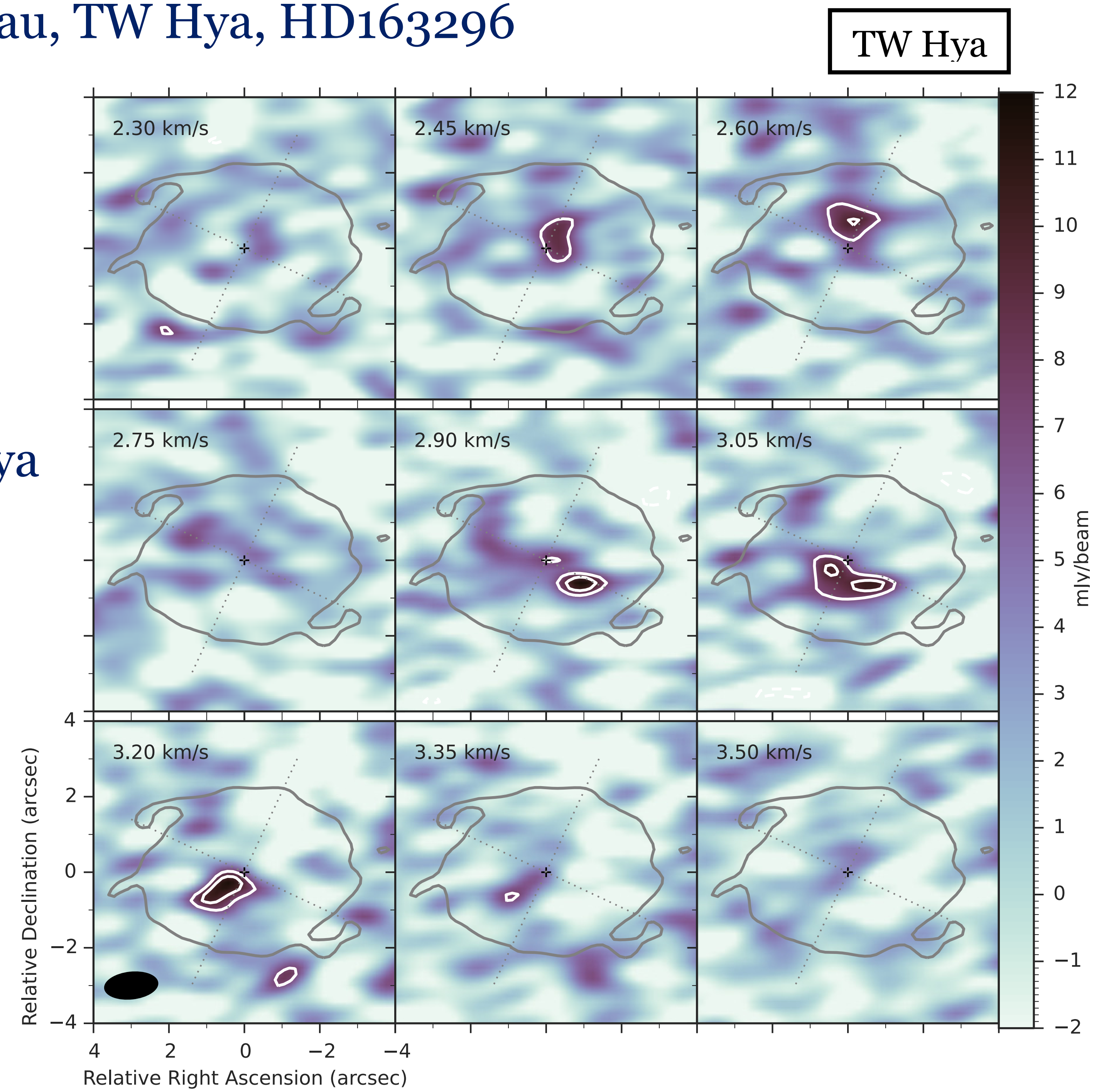


Carney et al. (in prep):
- H_2CO 3_2-2_2 detected via matched filtering (Loomis et al., in prep)
- additional reservoir of H_2CO outside ~300 au: UV photodesorption?

Organics

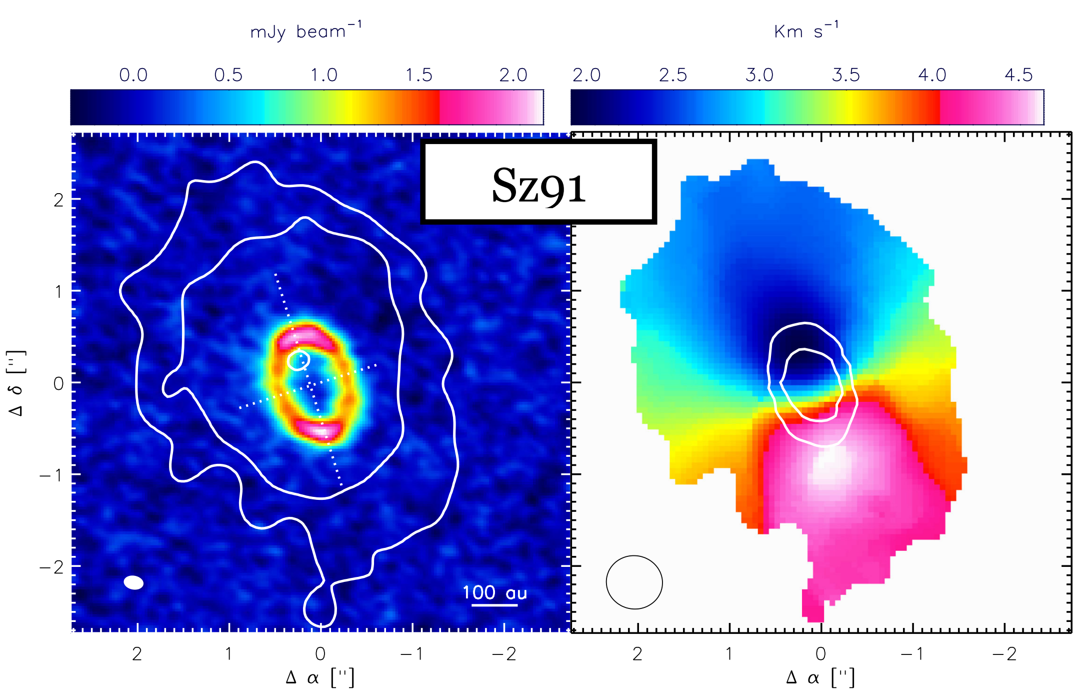
- Simple organics are being detected in disks
  - HC_3N and CH_3CN in MWC480
  - H_2CO across the disks of DM Tau, TW Hya, HD163296

Walsh et al. (in press)
- (stacked) CH_3OH detected in TW Hya
- see talk by Nomura



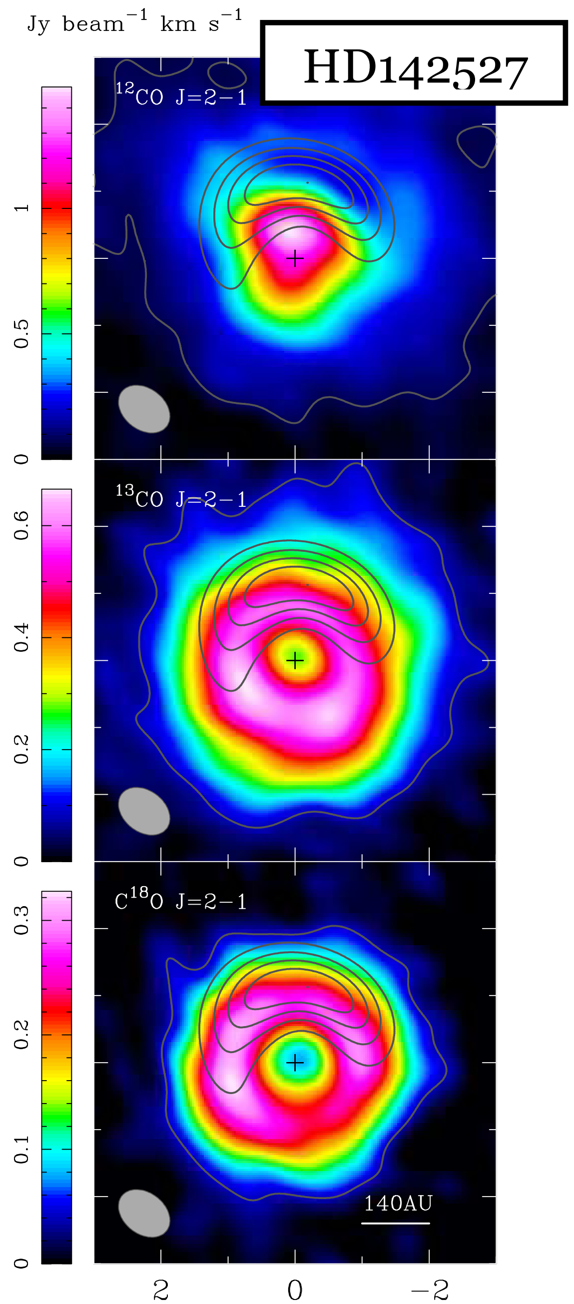
Gaps

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

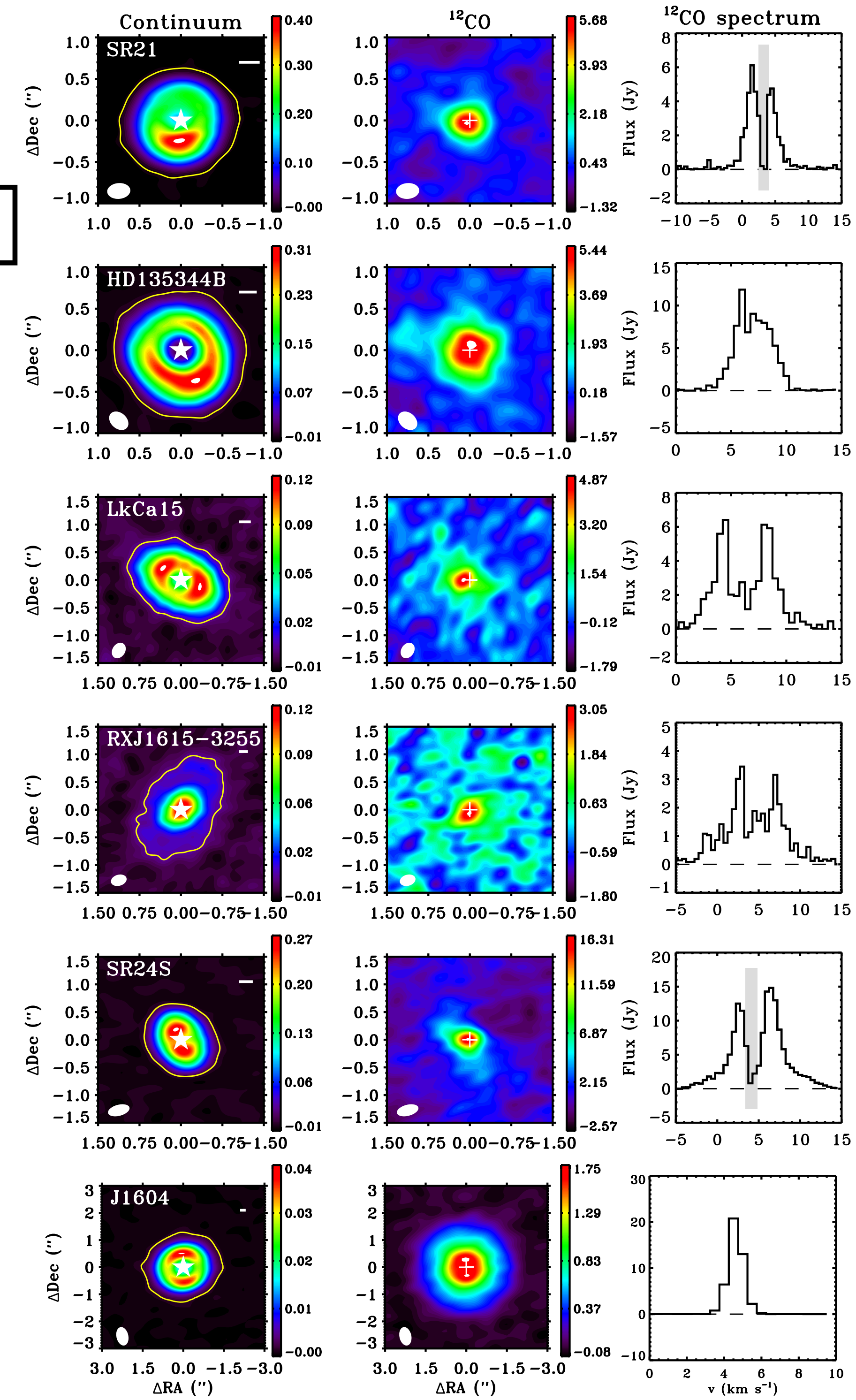


Canovas et al. (2016)

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



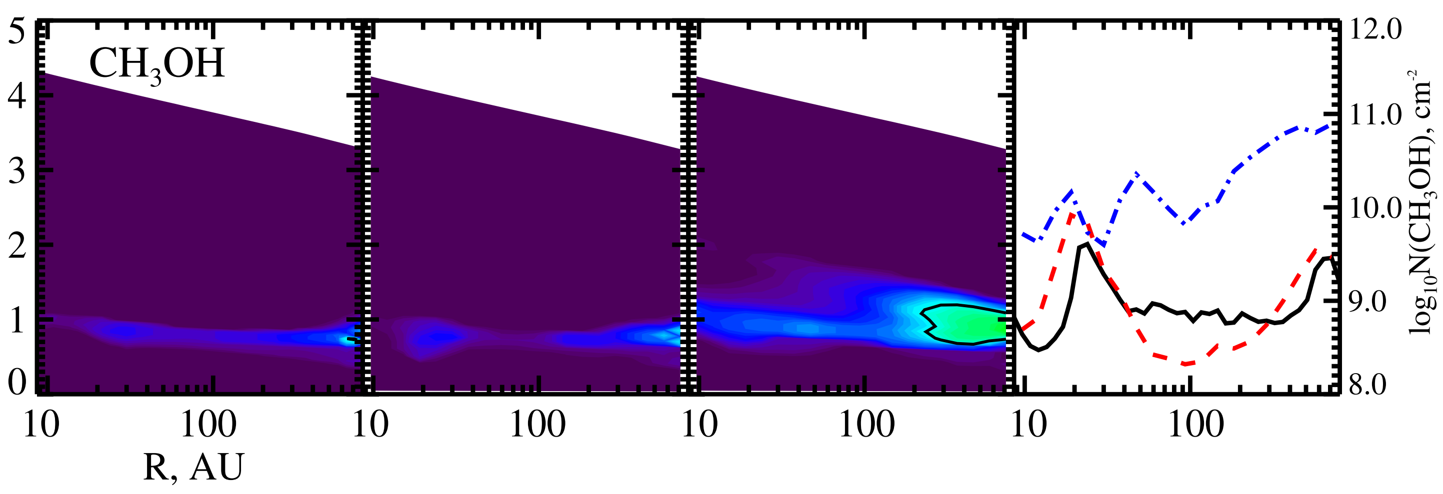
Perez et al. (2015)



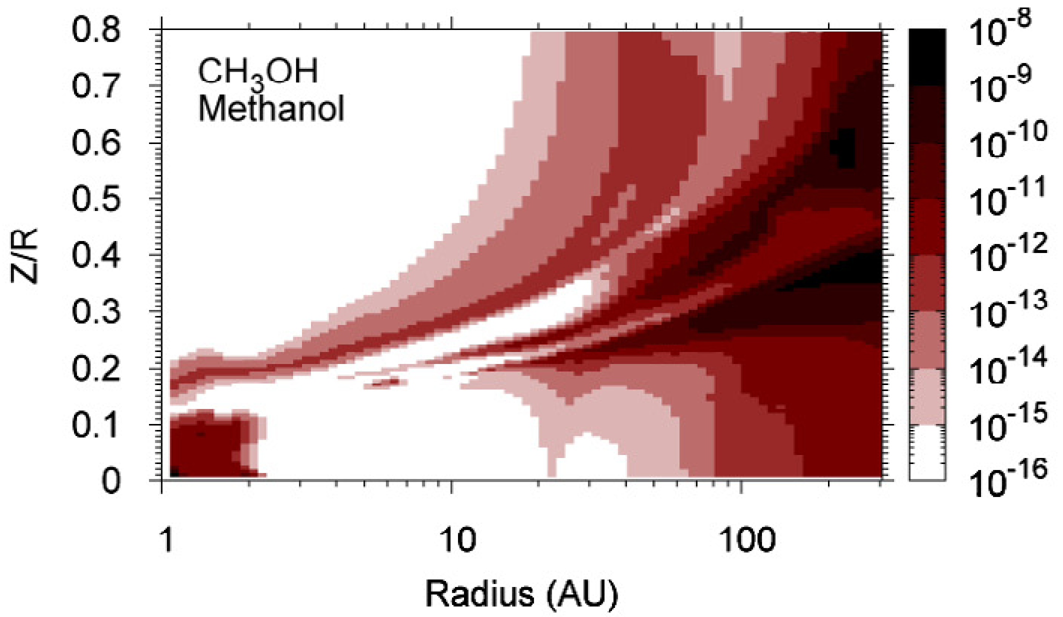
van der Marel et al. (2015)

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



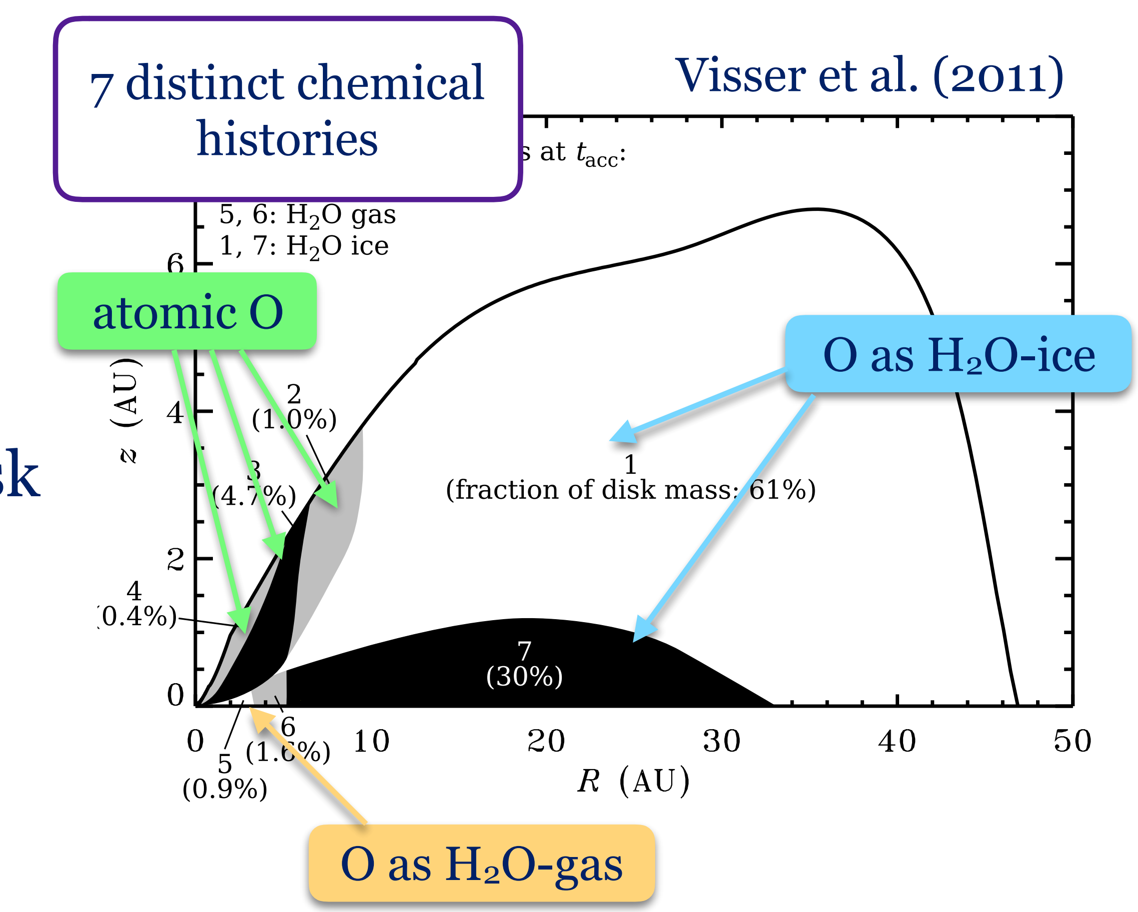
E.g., van Zadelhoff et al. 2003; Jonkheid et al. 2007; Aikawa et al. 2002, 2006, 2015; Fogel et al. 2011; Semenov et al. 2010, 2011; Woitke et al. 2010, 2016; Willacy et al. 2007, 2009; Walsh et al. 2010, 2012, 2013, 2014, 2015; …



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

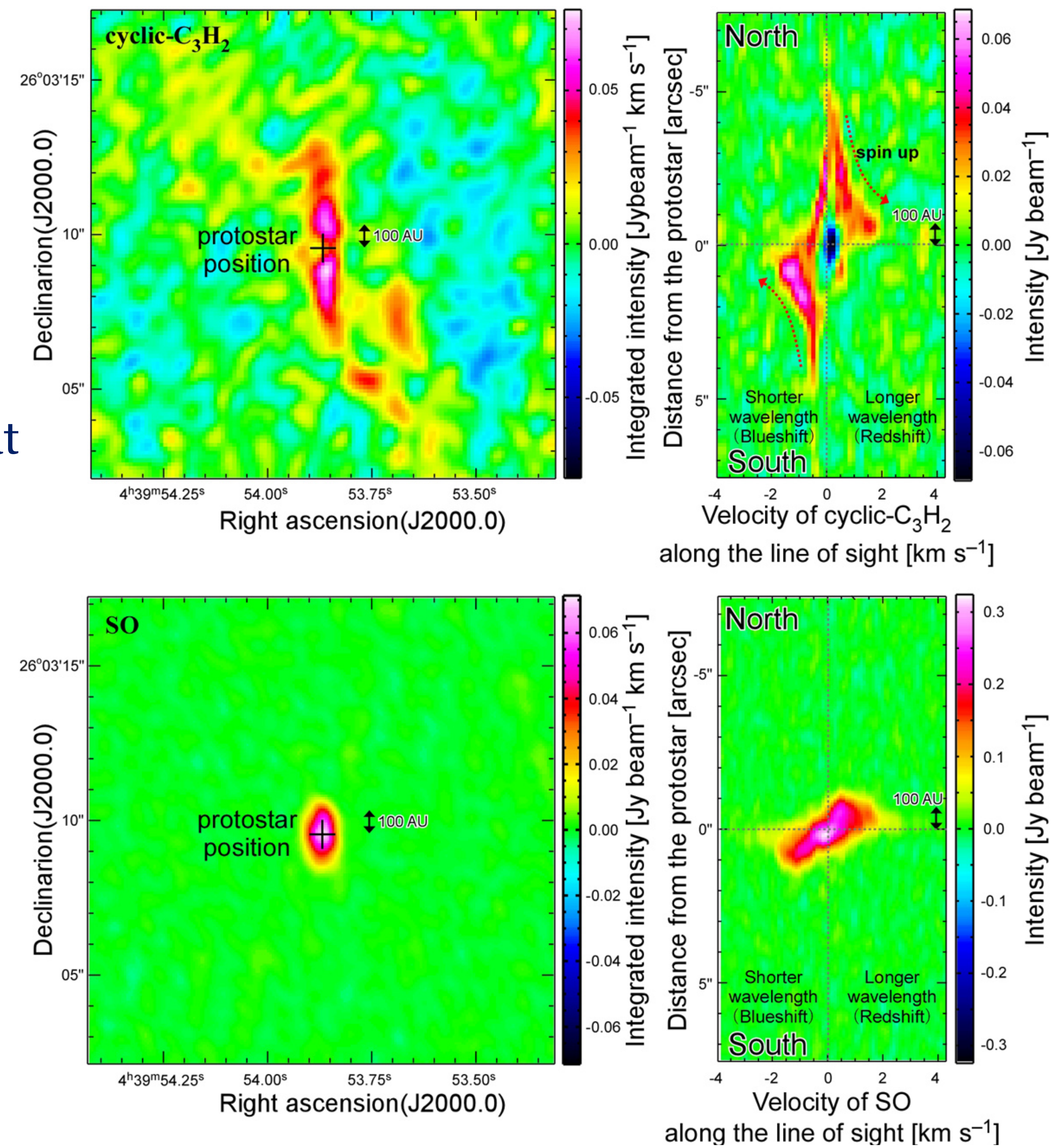
Inheritance

- 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
- **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?



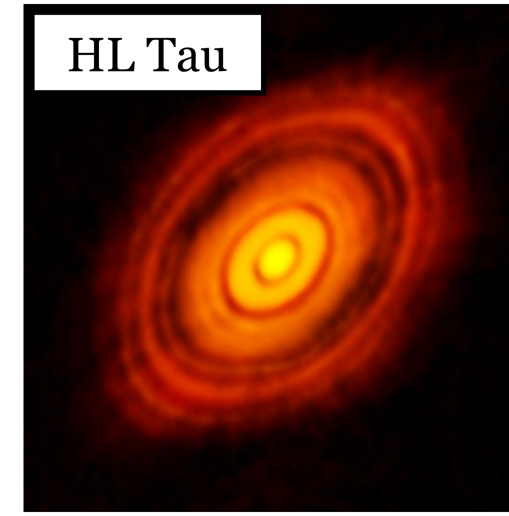
Inheritance

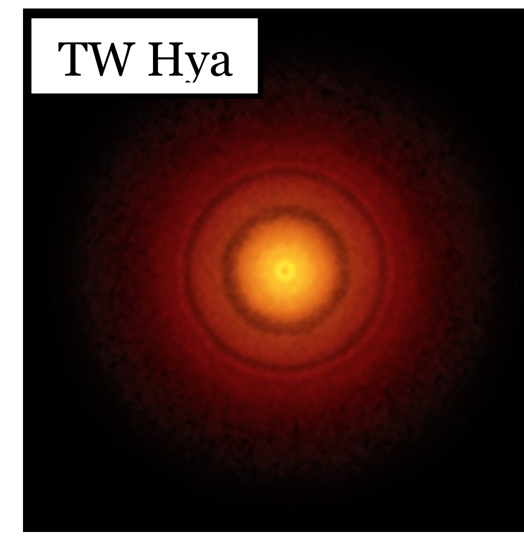
- Tracers of embedded disks
  - e.g., L1527
    - c-C_3H_2 shows rotation & infall: envelope
    - SO shows solid-body rotation: accretion shock at centrifugal barrier
- Alteration of ice/gas at point of entry into the disk



Sakai et al. (2014)

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 (⇔UV, ionization)?**

ALMA Partnership, Brogan et al. (2015); Andrews et al. (2016)

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

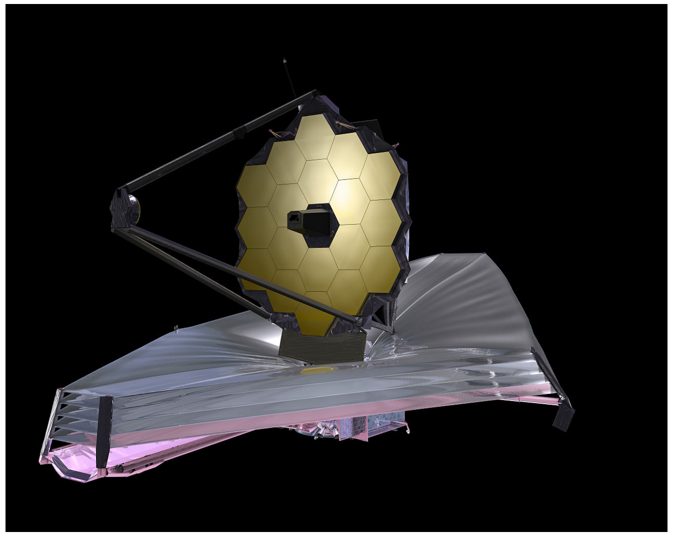


Image credit: ALMA (ESO/NAOJ/NRAO); NASA; ESO