Herschel Constraints on Ice Formation and Destruction in Protoplanetary Disks

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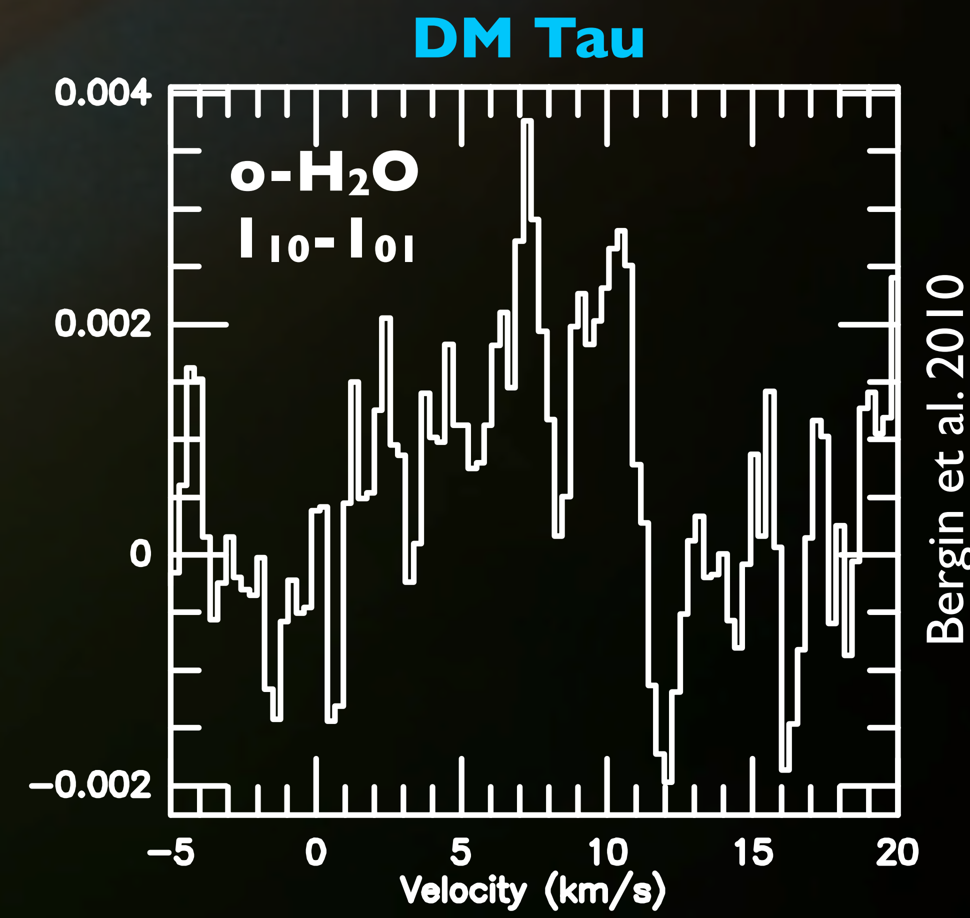
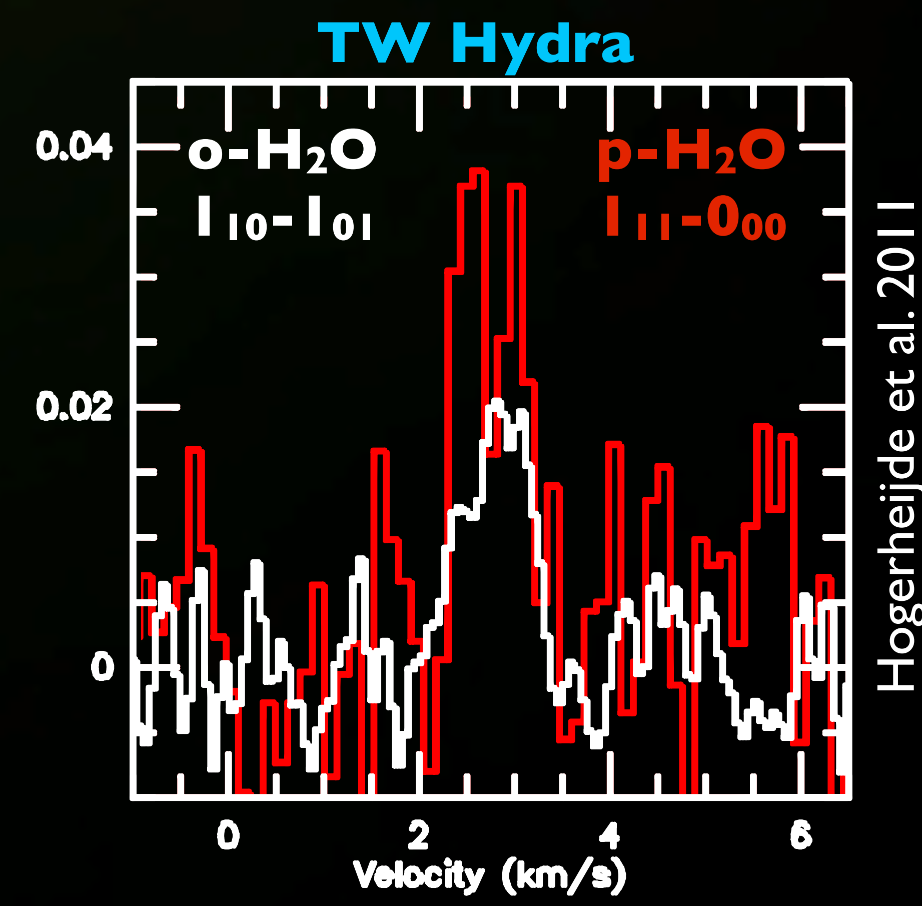
Astronomy

Images Courtesy of: Herschel, ESA;,TW Hydra, NASA/JPL; SMA: Cleeves

Introduction

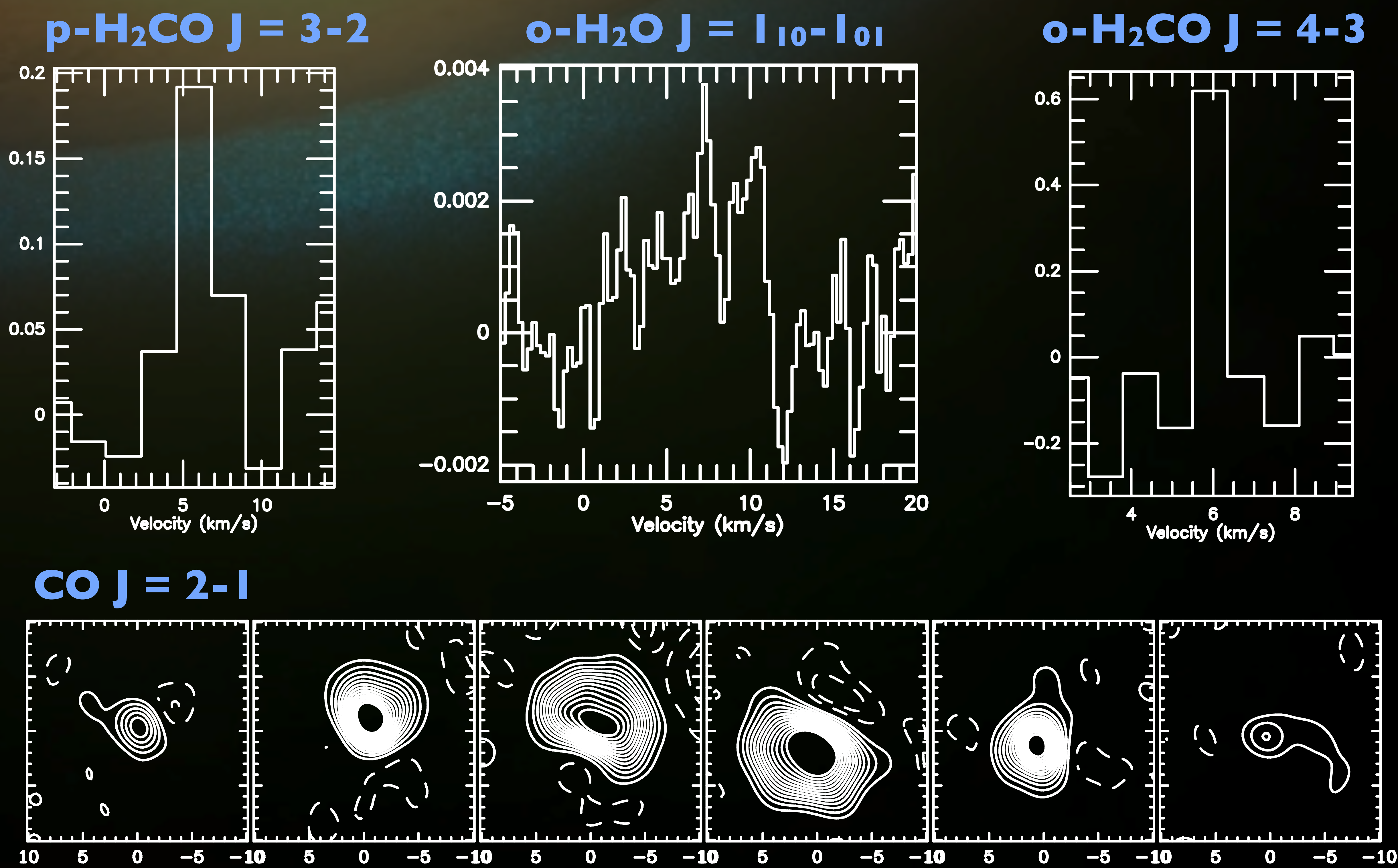
- Cold H_2O detected by Herschel in the outer regions of protoplanetary disks! (Hogerheijde et al. 2011, Bergin et al. 2010).
- The detection was significantly weaker than the models predicted:
  - Postulated dry surface grains → icy grains settled to midplane? Not without problems. (Vasyunin et al. 2011)
- We explore alternative scenarios to attempt to explain the cold H_2O puzzle in DM Tau with:
  - The Herschel o-H_2O limit (Bergin et al. 2010).
  - SMA H_2CO data from DISCS (Öberg et al. 2010) for additional potential grain surf. product constraints.





Constraints

DM Tau



Bergin et al. 2010, Öberg et al. 2010

What happened to the water?
Alternative Mechanisms

I) X-ray Desorption of H_2O Precursors

- X-rays can deposit energy/heat into the grain lattice (Dwek & Smith 1996, Hasegawa & Herbst 1993, Leger et al. 1985).
- More E deposited into larger grains, however, shared over a larger volume ➡ ΔT_{grain} is less.
  - For E_{XR} > 0.3 keV: 50 Å grains heated to > 120K; 300 Å grains heated to > 30K (Najita et al. 2001).
- Grains are thought to be coagulative.
  - Small 'spherical' subunits have small contact points, impede the transfer of E.
    - Maintain hotter grains!

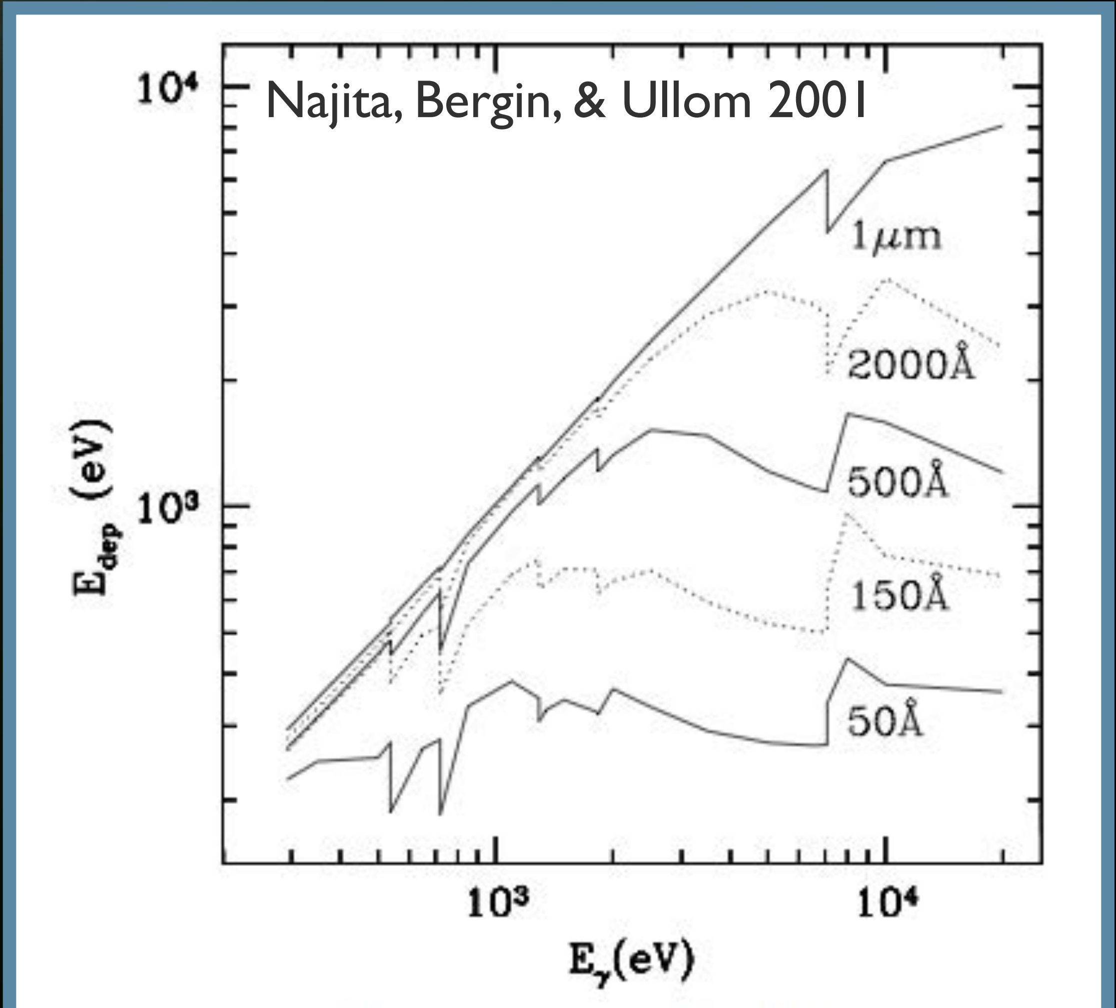
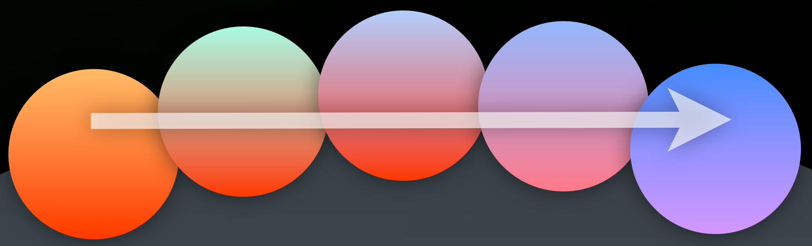


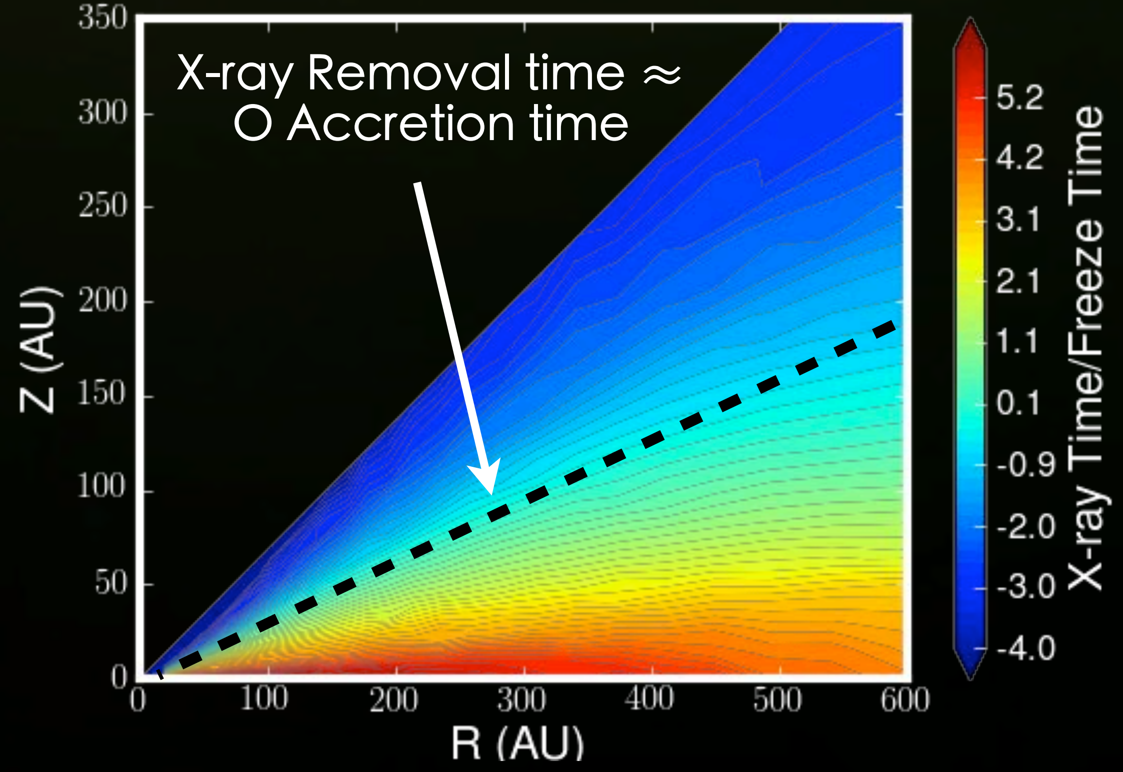
FIG. 1.—Deposited energy as a function of incident X-ray energy

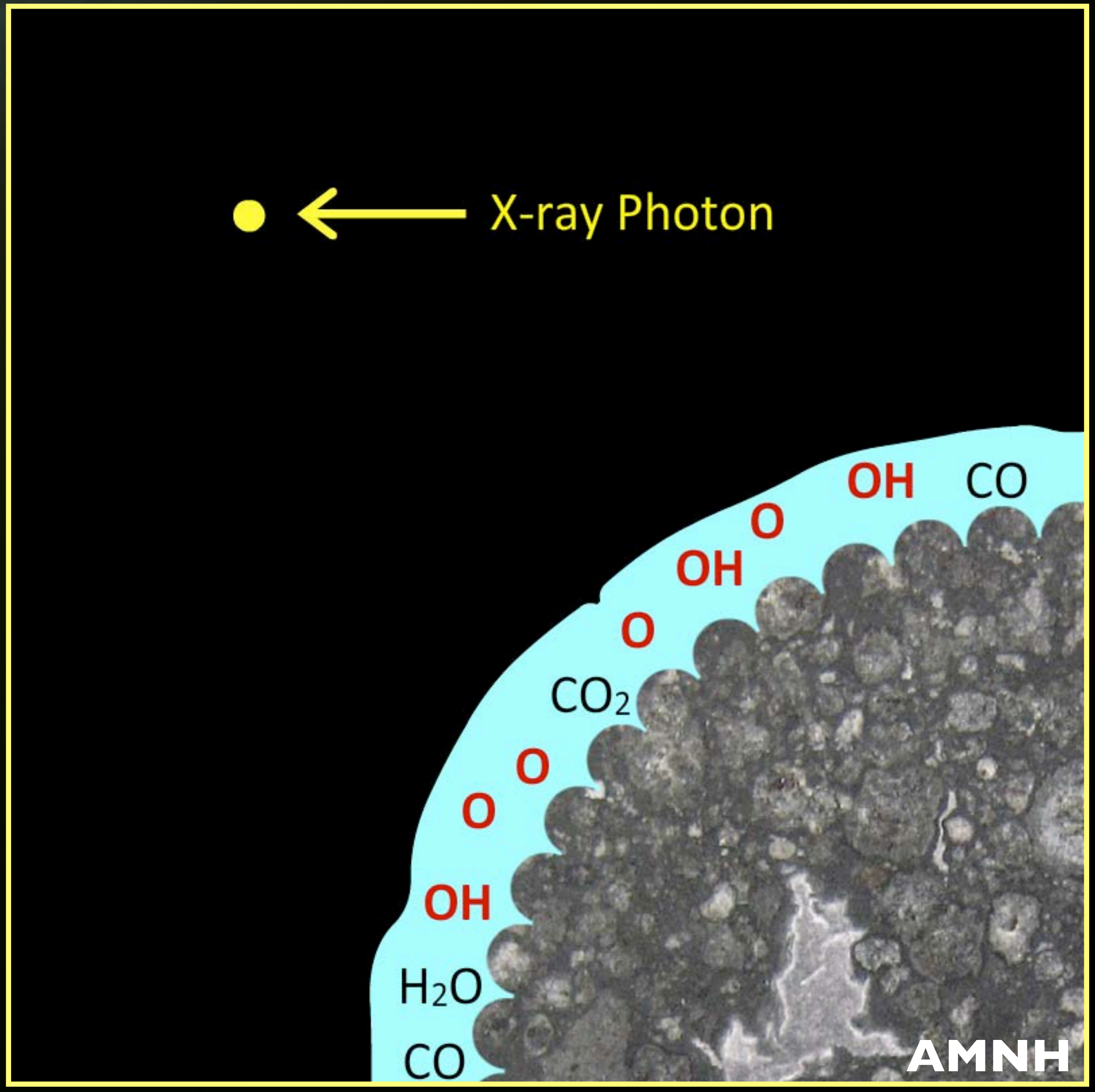


I) X-ray Desorption of H_2O Precursors

- X-ray heated grain cools via:
  - Ice evaporation (O, C, CO, NH_3).
  - Transfer between neighboring subunits.
  - Transfer to the bulk grain mass.
  - Radiative cooling.

$$\kappa_{\rm xr} \sim \kappa_{\rm th}(70\ {\rm K}) \times \frac{\rm t_{cool}}{\rm t_{xr}}$$





If the O, OH can be kept-off the grains - can decrease H_2O formation efficiency!

2) 'Carbon-goo' Coating on Grains

- Goo: (noun) \'gü\

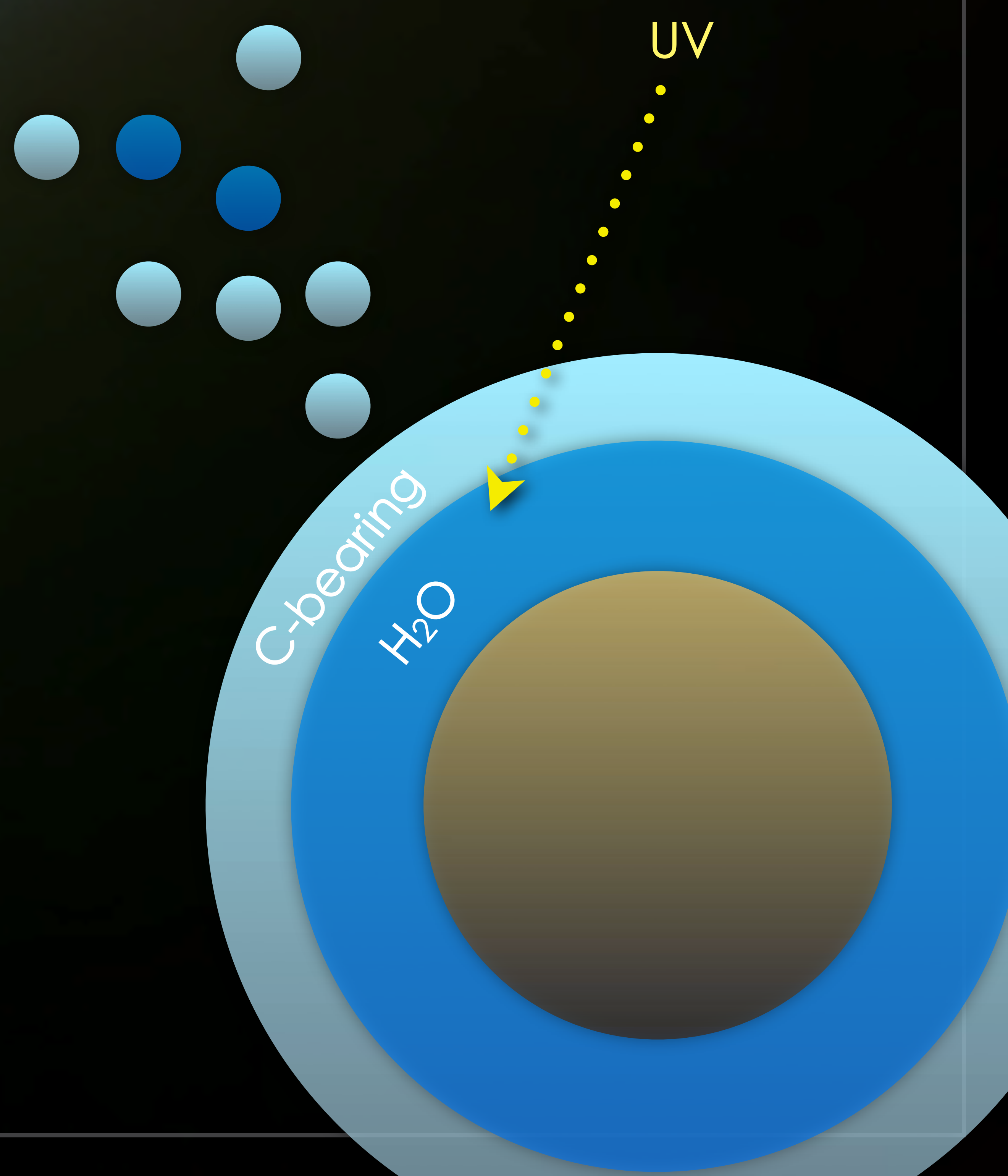
  1 : a viscid or sticky substance

  2 : sentimental tripe

  Merriam-Webster

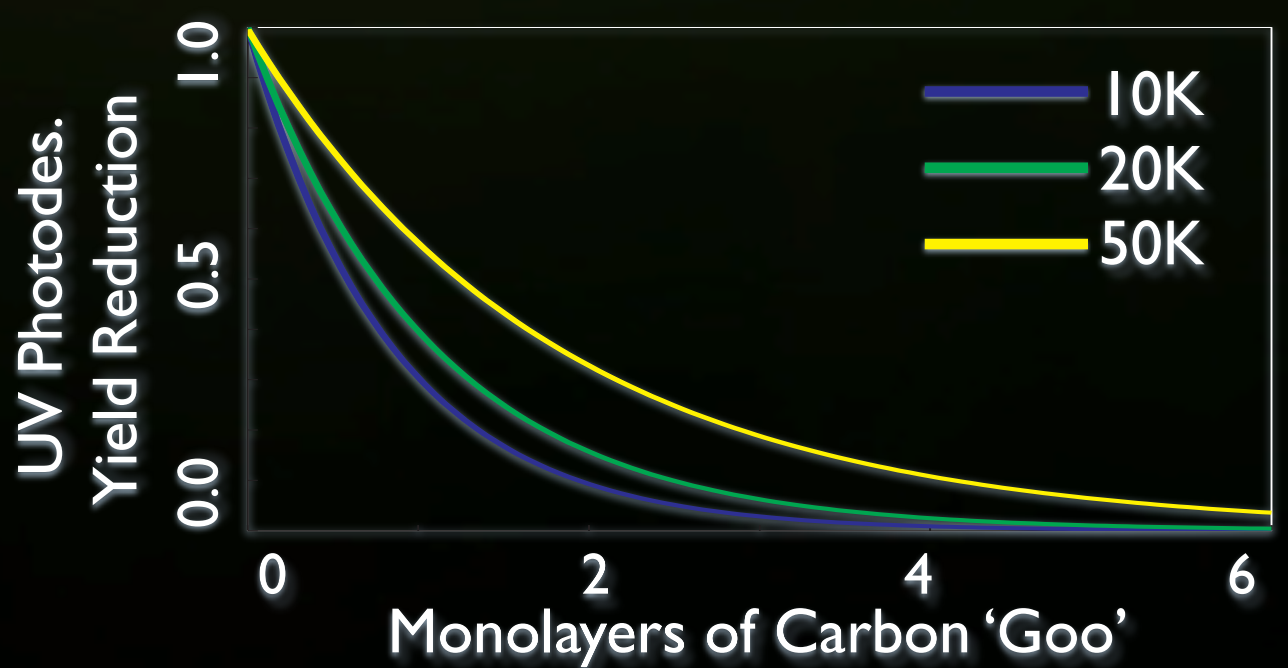
- Ice-structure potentially layered (Hasegawa & Herbst 1993, Garrod et al. 2011).

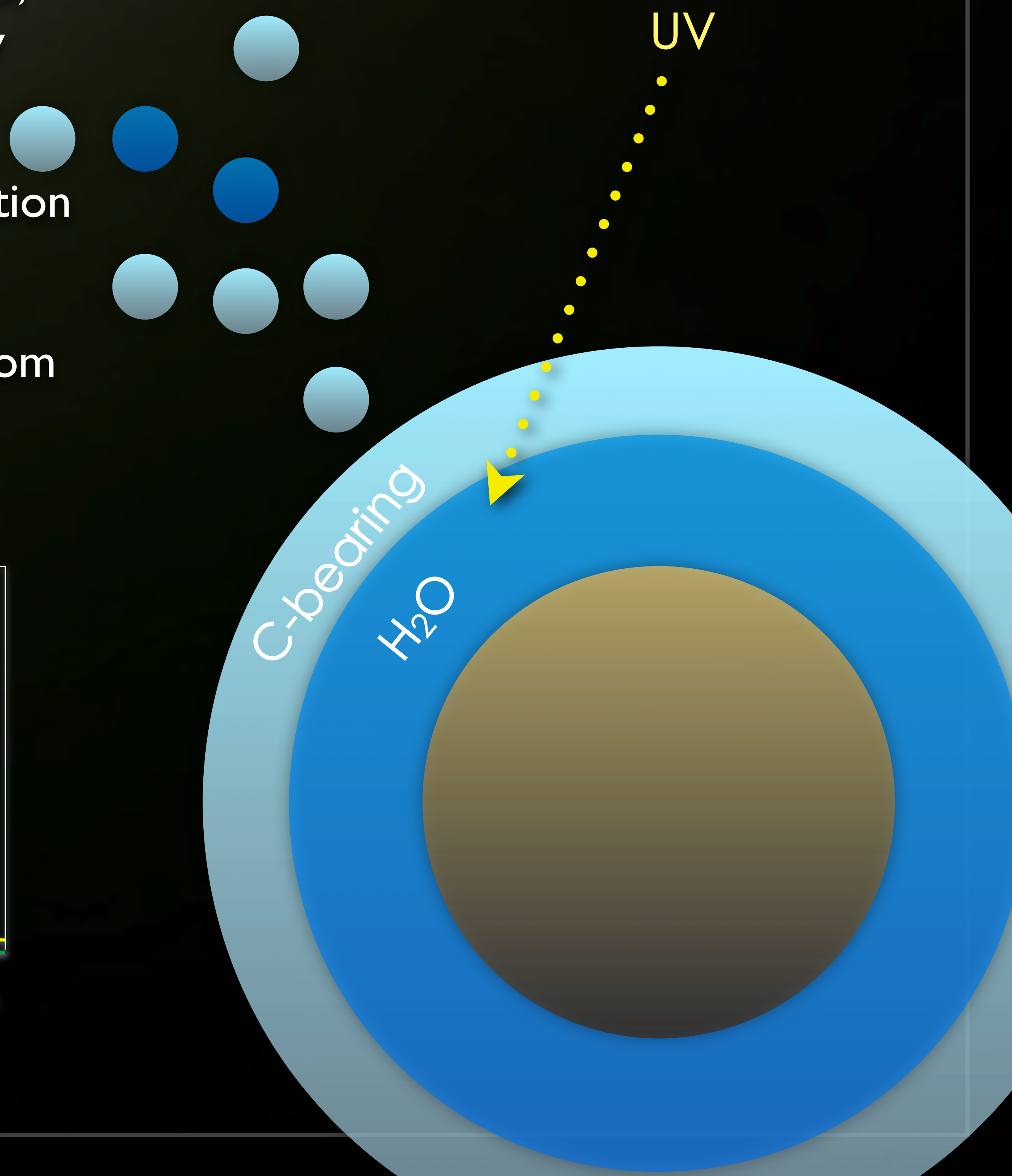
- High organic fraction (>70%) seen in meteorites, carbon species comprised of largely aromatic, CH_X, $CH_X(O,N)$ and CO-derived (e.g. Cody & Alexander 2005. Large, carbon-bearing molecules.



2) 'Carbon-goo' Coating on Grains

- If the H2O-ice rich mantle is buried below >2ML of carbon-rich ices (CO, CO_2, H_2CO, CH_4, CH_3OH) ➡ UV desorption efficiency significantly reduced.
- Competition between carbon-ice reformation and UV photo-erosion.
- Yields per monolayer of coverage taken from H_2O ice studies (Öberg et al. 2009).



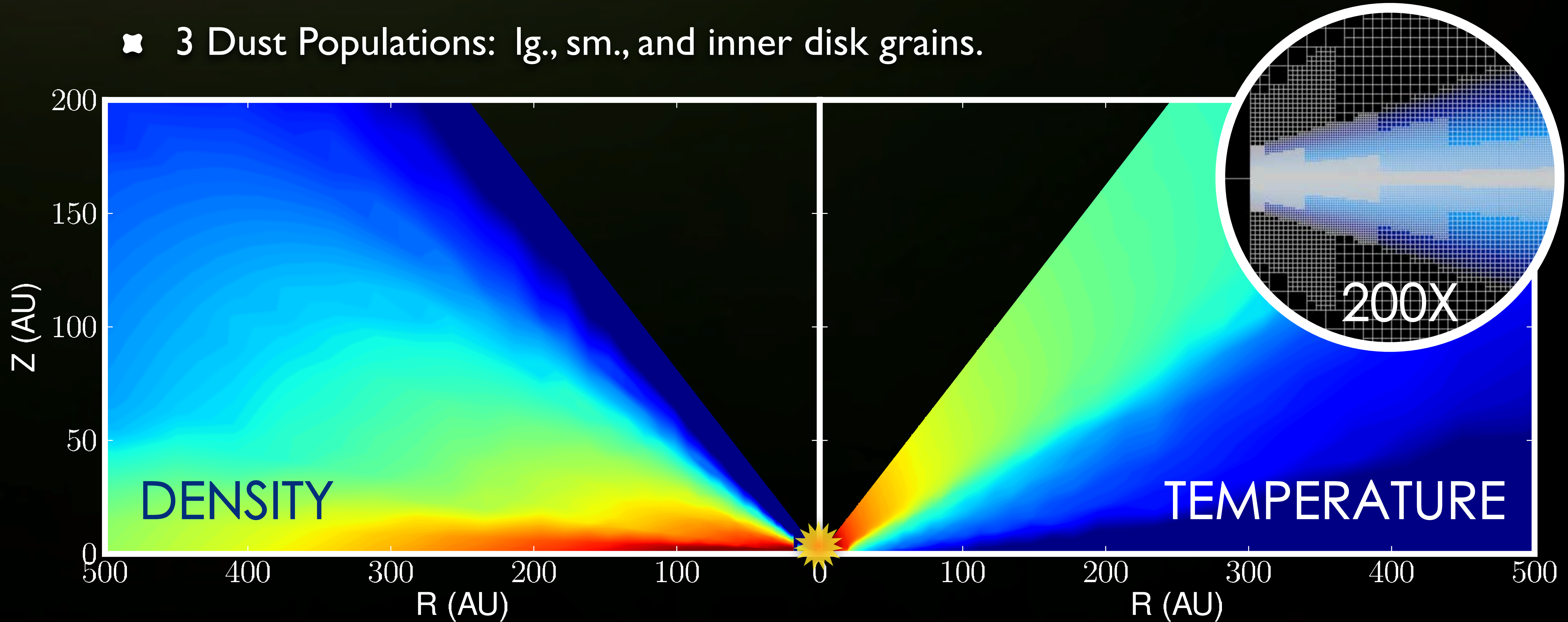


DM Tau: The Model

- AMR code *Torus* (Tim Harries, U. Exeter) for the dust disk physical structure.
  - Disk-model formalism from Andrews et al. 2011 for SED fit.
  - Gas mass derived from $C^{18}O$, ^{13}CO fluxes (Dutrey et al. 1997); $f_g \sim 25$.
  - 3 Dust Populations: lg., sm., and inner disk grains.

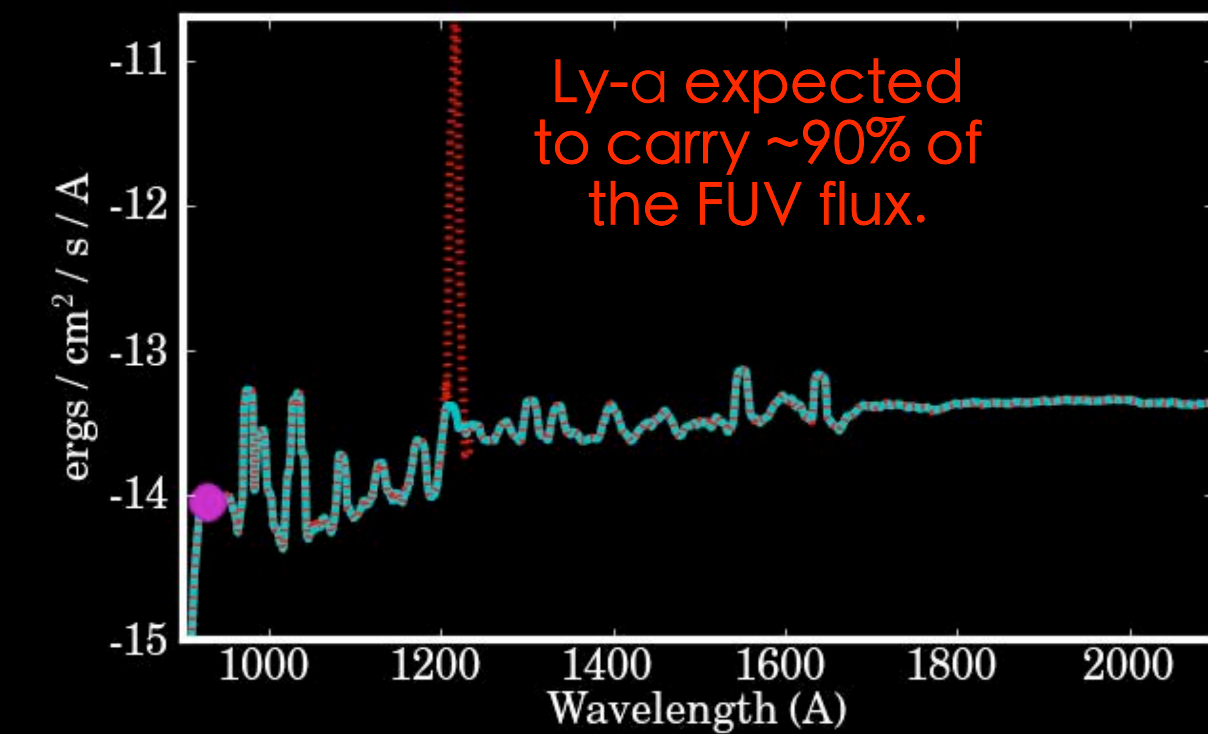
Star:
- Spec. Type: M1
- $M = 0.53\ M_\odot$; $L = 0.3\ L_\odot$

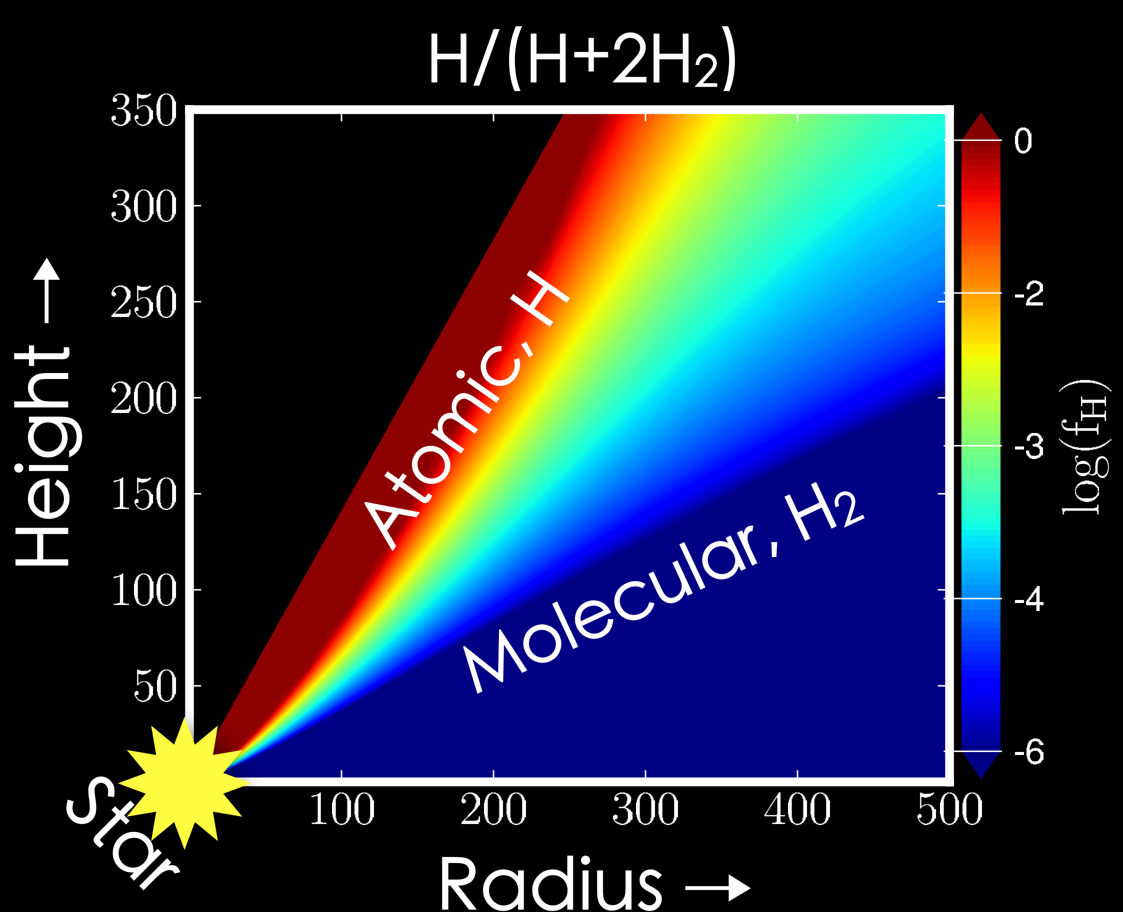
Model Results:
- $M_{disk,dust} = 1.1e\text{-}4\ M_\odot$
- $M_{disk,gas} = 2.8e\text{-}3\ M_\odot$
- R_{inner} = 1-15 AU
- R_{outer} = 19 - 800 AU

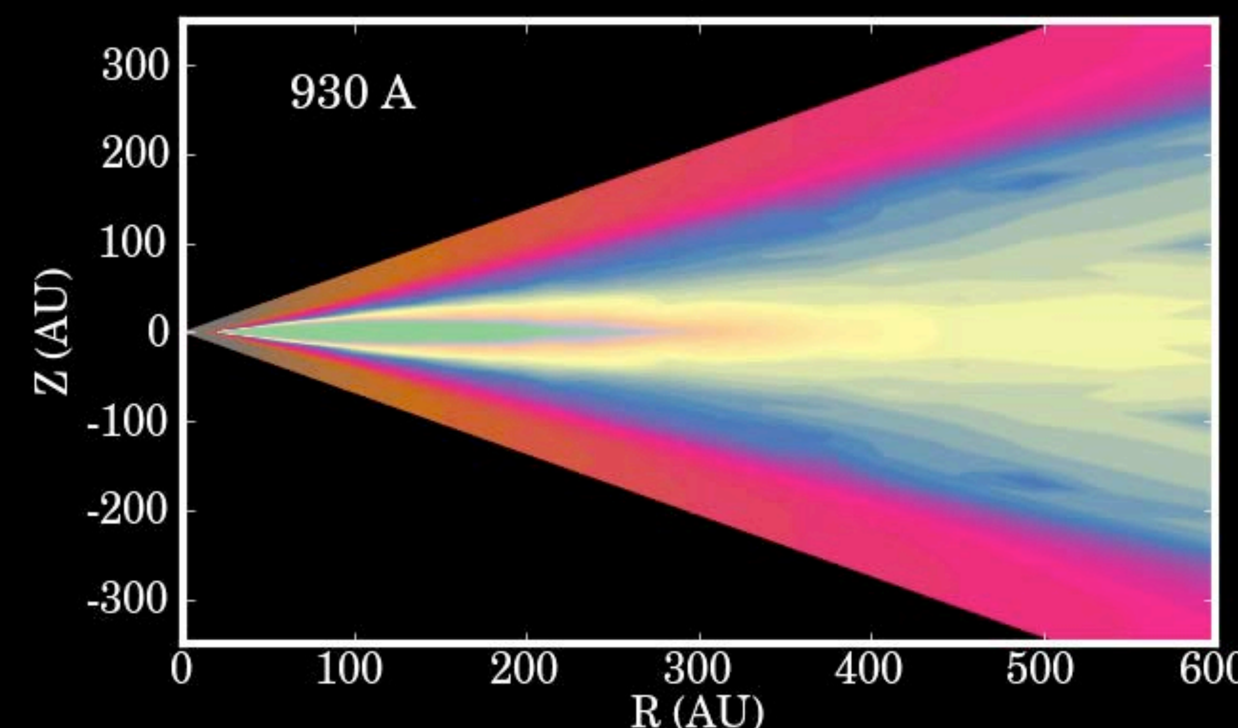


Model Radiative Transfer: Stellar UV

- Calculated via Monte Carlo radiative transfer (Bethell & Bergin 2011a):
    - Continuum opacity → dust extinction.
    - Line RT → Ly-α H-scattering + dust.
        - H vs. H2 surface calculated using the prescription detailed in Spaans & Neufeld 1997.



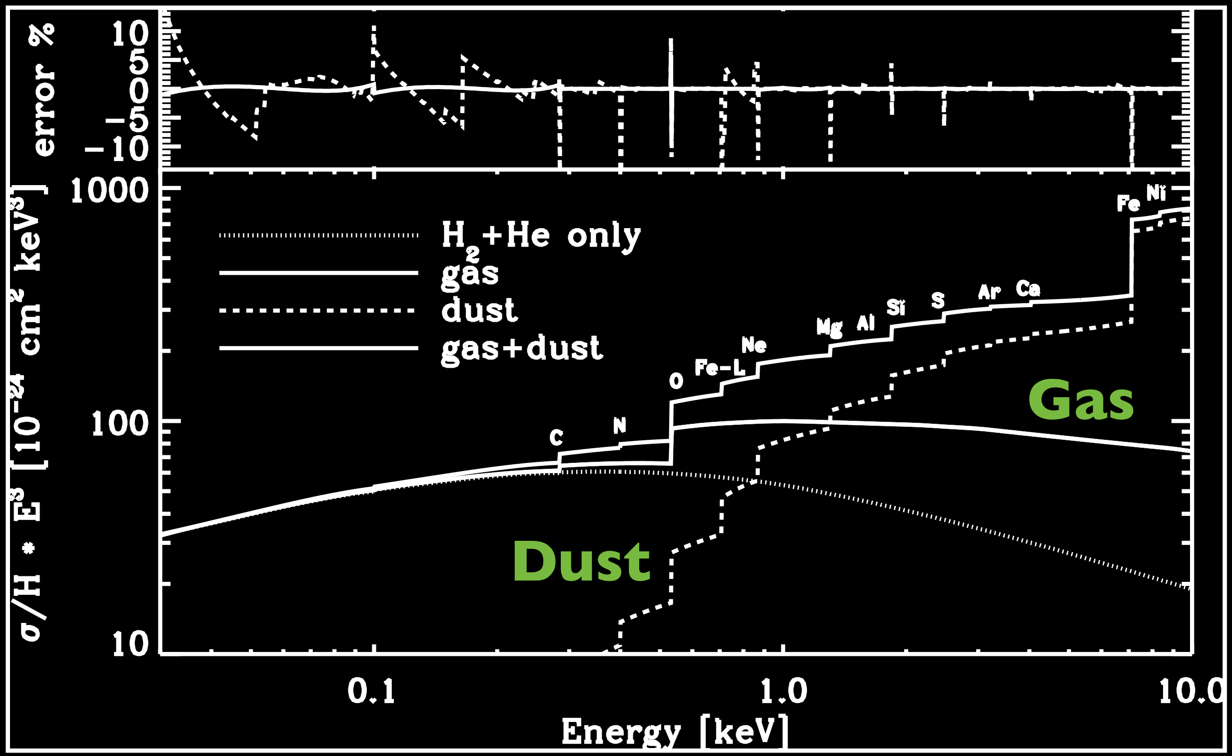


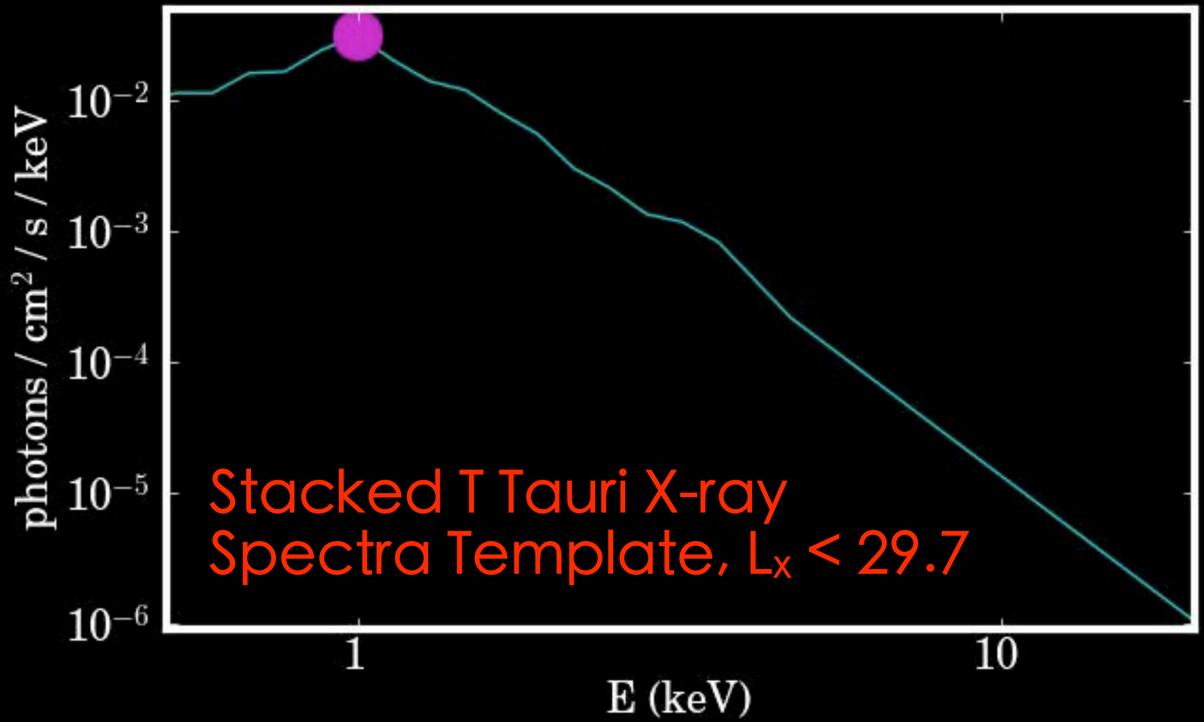


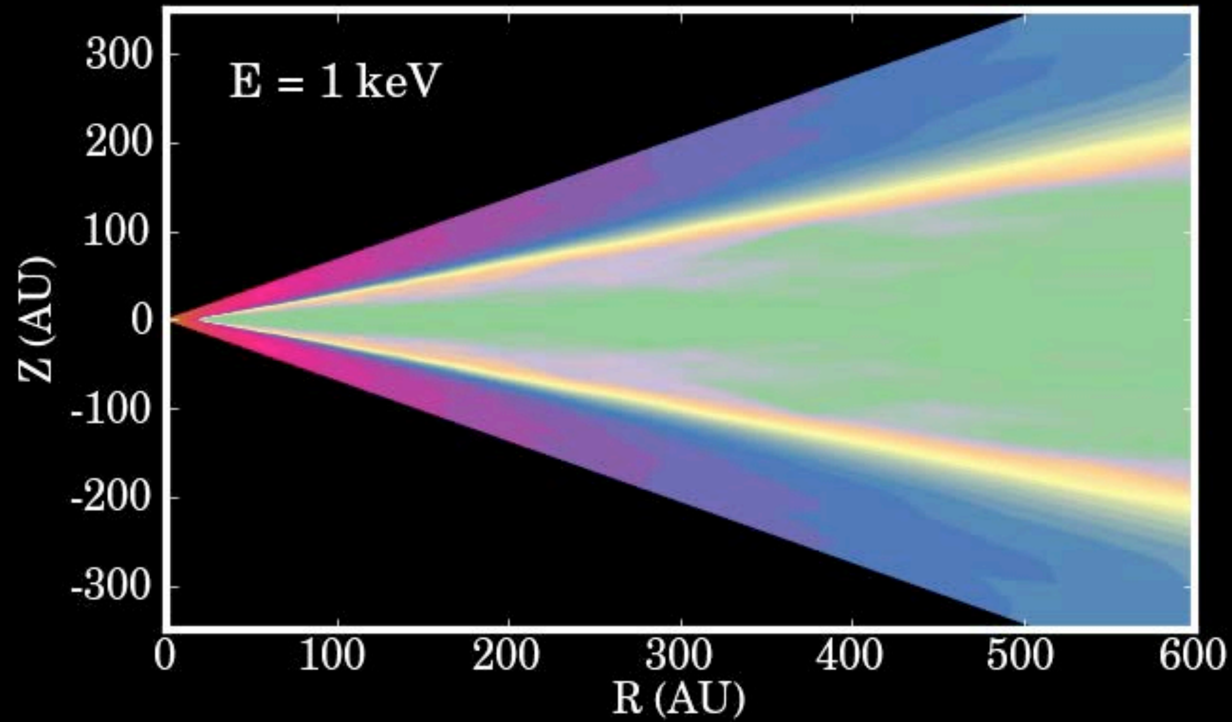
Model Radiative Transfer: Stellar X-rays

- X-ray scattering with cross sections from Bethell & Bergin 2011b.
  - Includes contributions from k & l-shell ionization cross-sections from both dust and gas components.

Sources of X-ray Opacity

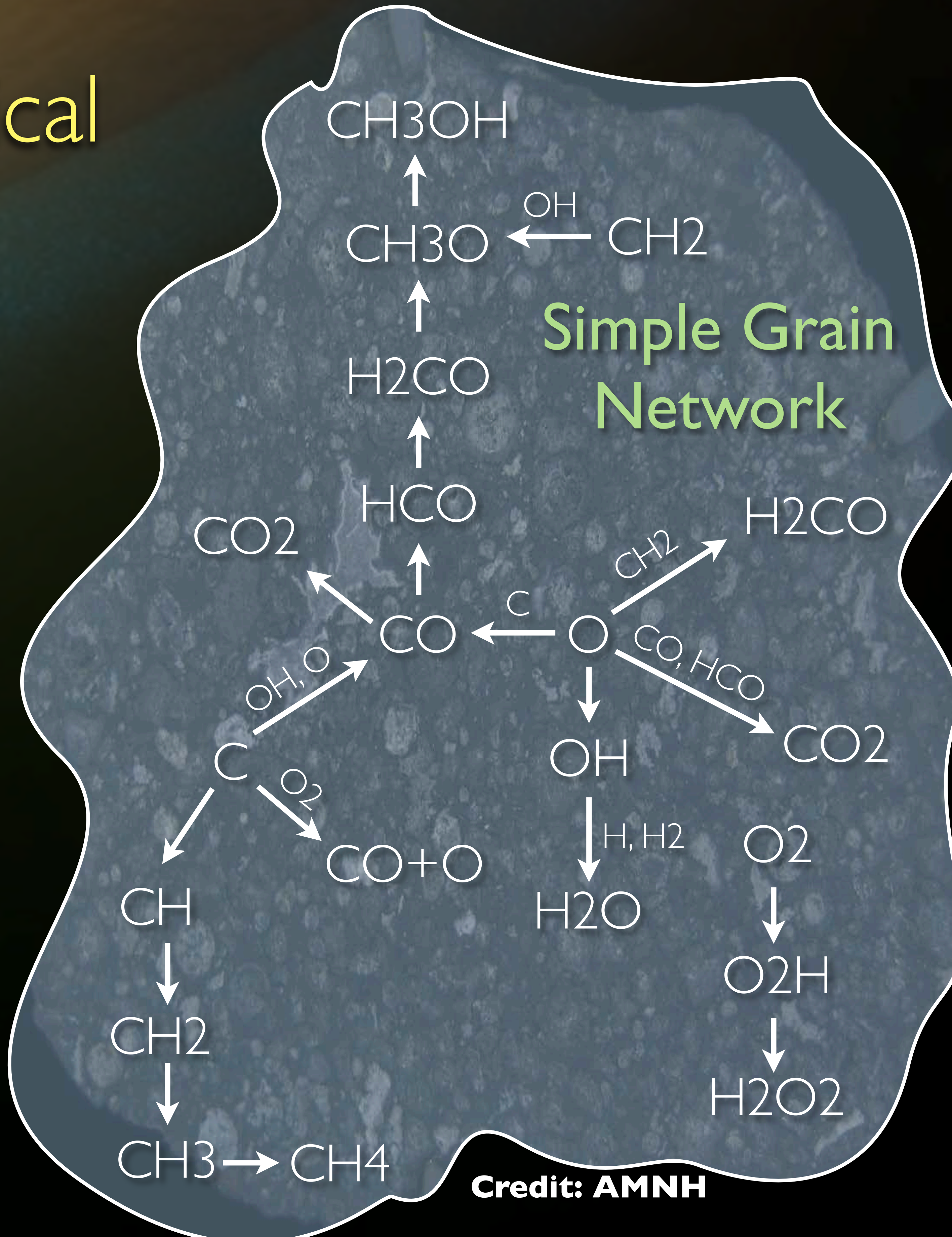






Model: The Chemical Network

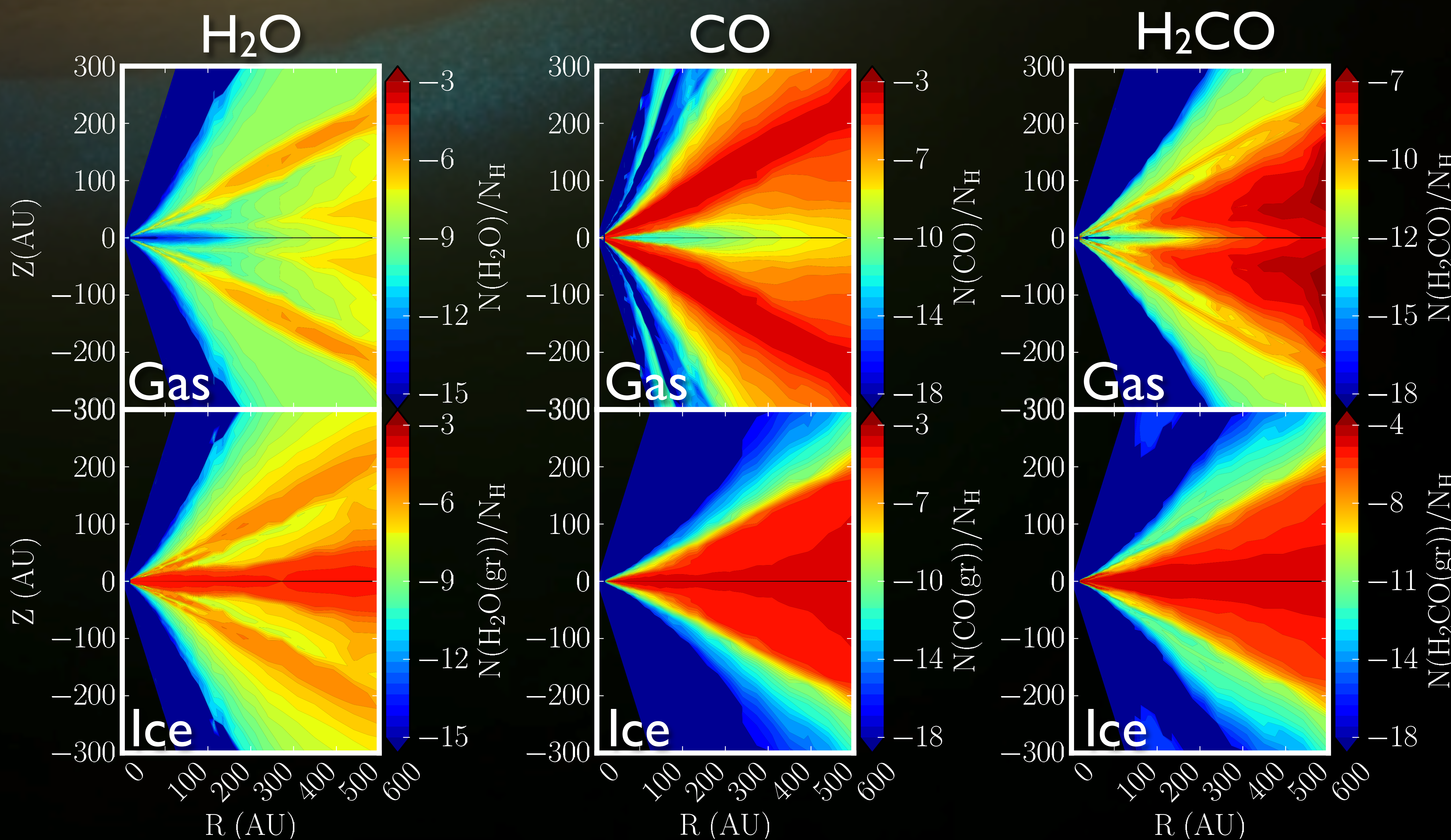
- Fogel et al. 2011 chemical network, 6084 reactions & 646 species.
  - Reactions included: photo-chemistry, UV/X-ray/CR ionization, ion-chemistry, neutral-neutral, CO and H2 self-shielding and more.
- Now with a simple grain chemical network (~30 reactions).
  - Motivated by Hasegawa, Herbst & Leung 1992, Garrod & Pauly 2011.
  - Tested under dark cloud conditions: 10K; n ~ 2×10^{4} cm^{-3}.



Modeling Results

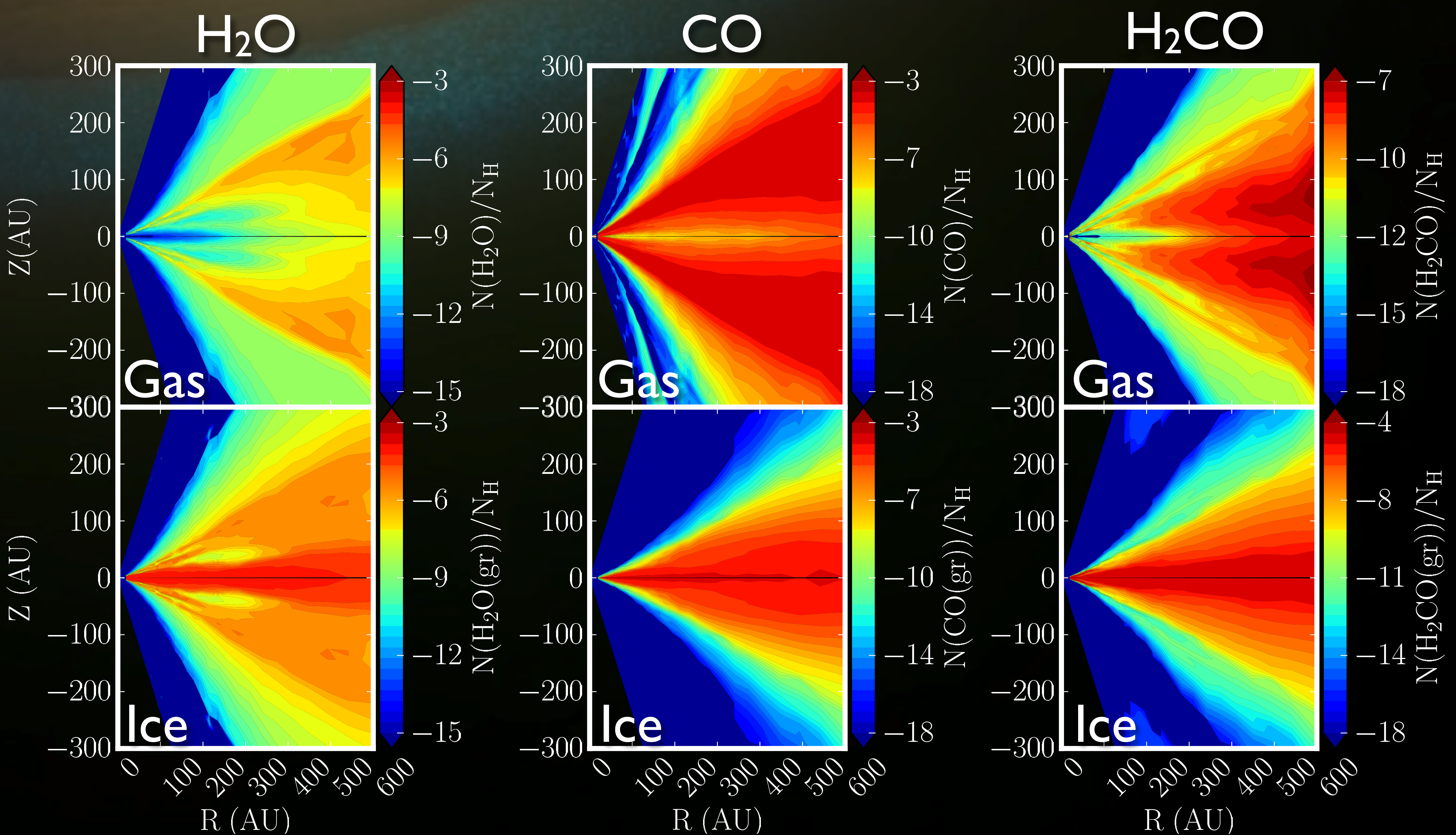
Chemical Results: 1) X-ray Desorption

No X-ray thermal desorption



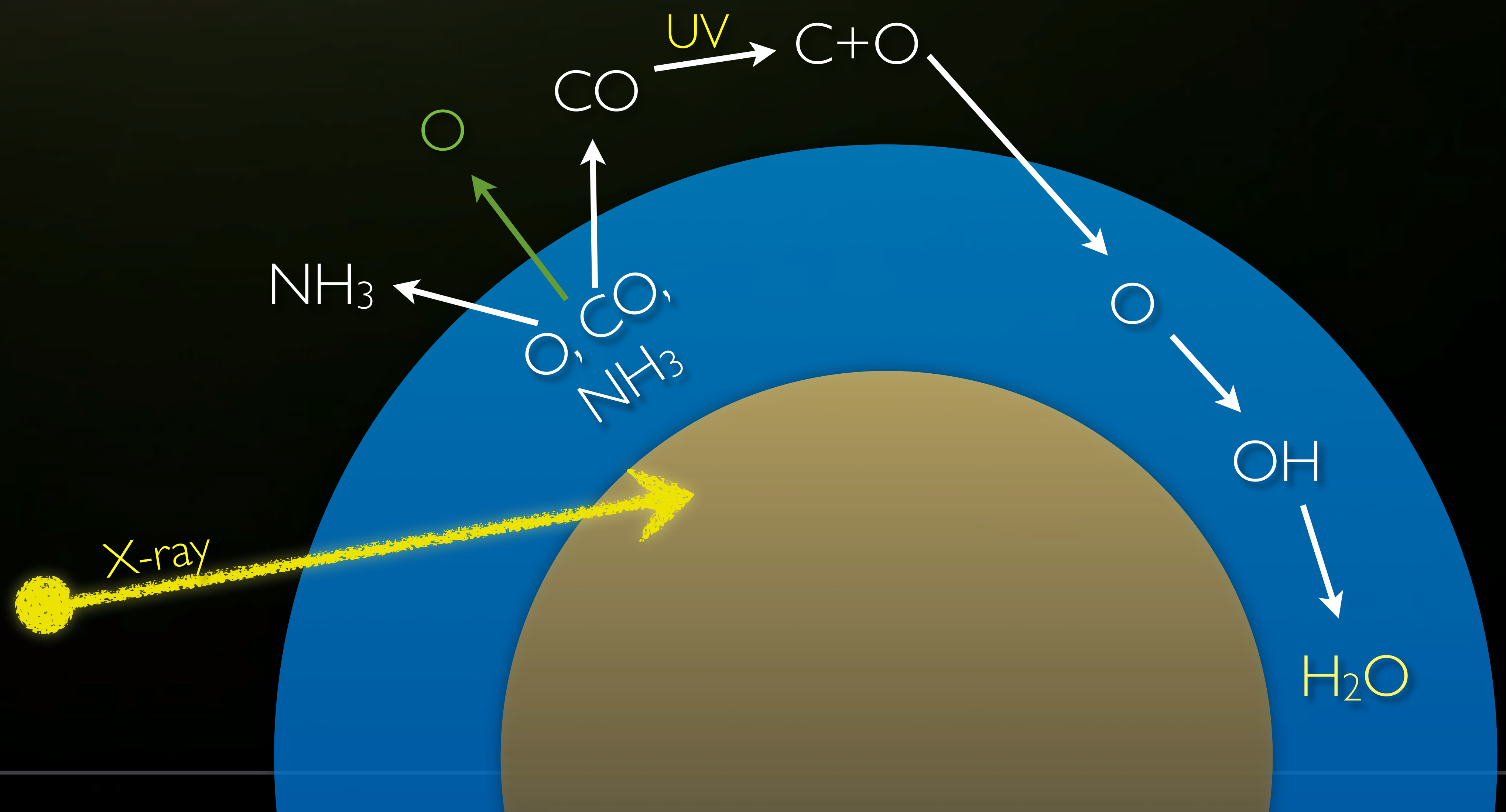
Chemical Results: 1) X-ray Desorption

X-ray thermal desorption



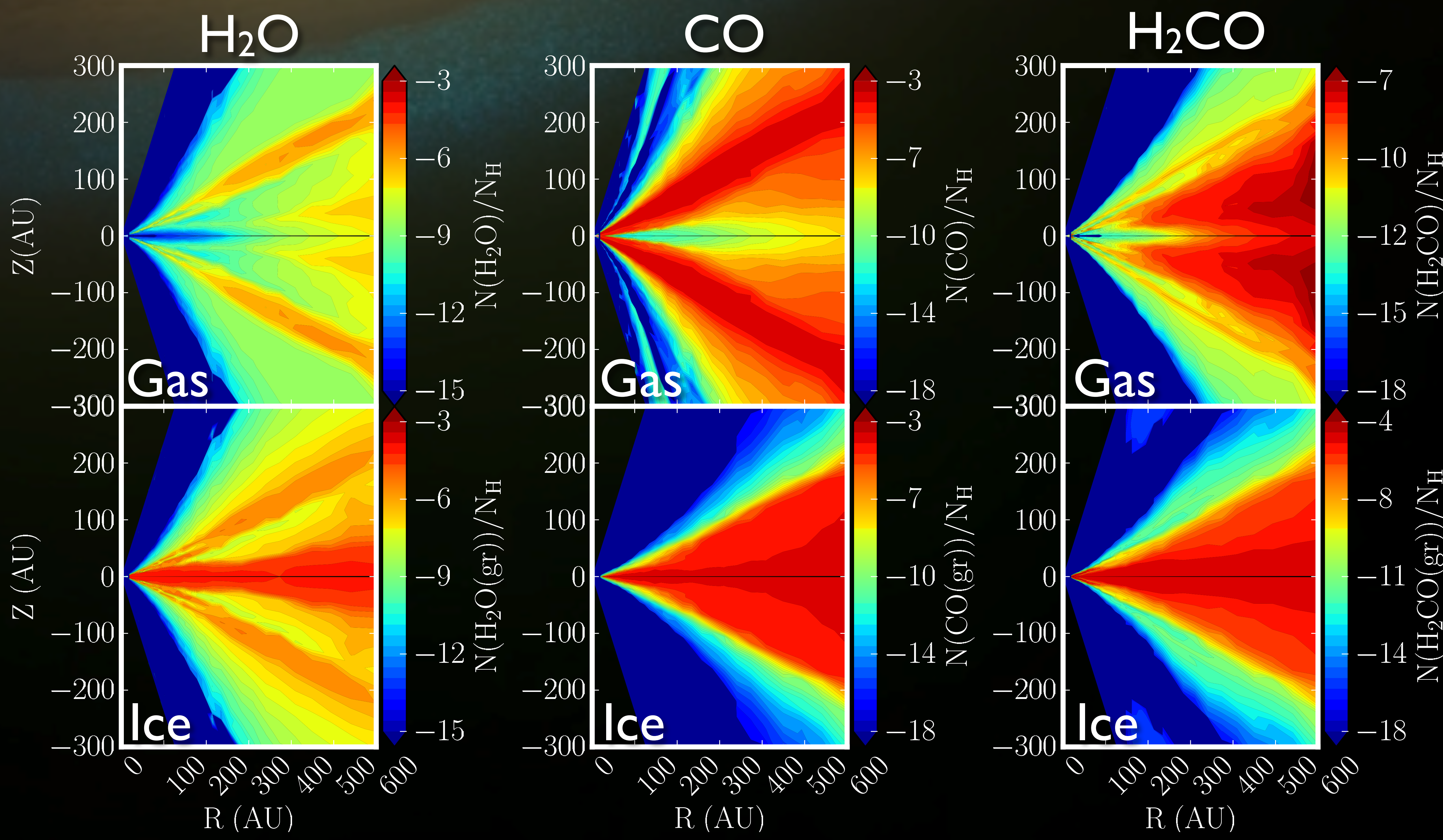
Chemical Results: 1) X-ray Desorption

- *More* water? We presumably remove oxygen from the grains, inhibiting water formation, so where is this excess originating?
- Reason: X-rays remove O, but that isn't all: NH_3, CO and C are simultaneously desorbed efficiently.
- Newly desorbed CO photo-dissociates, enhancing the gas-phase atomic oxygen content, pushing the system to form *more* water, rather than less.



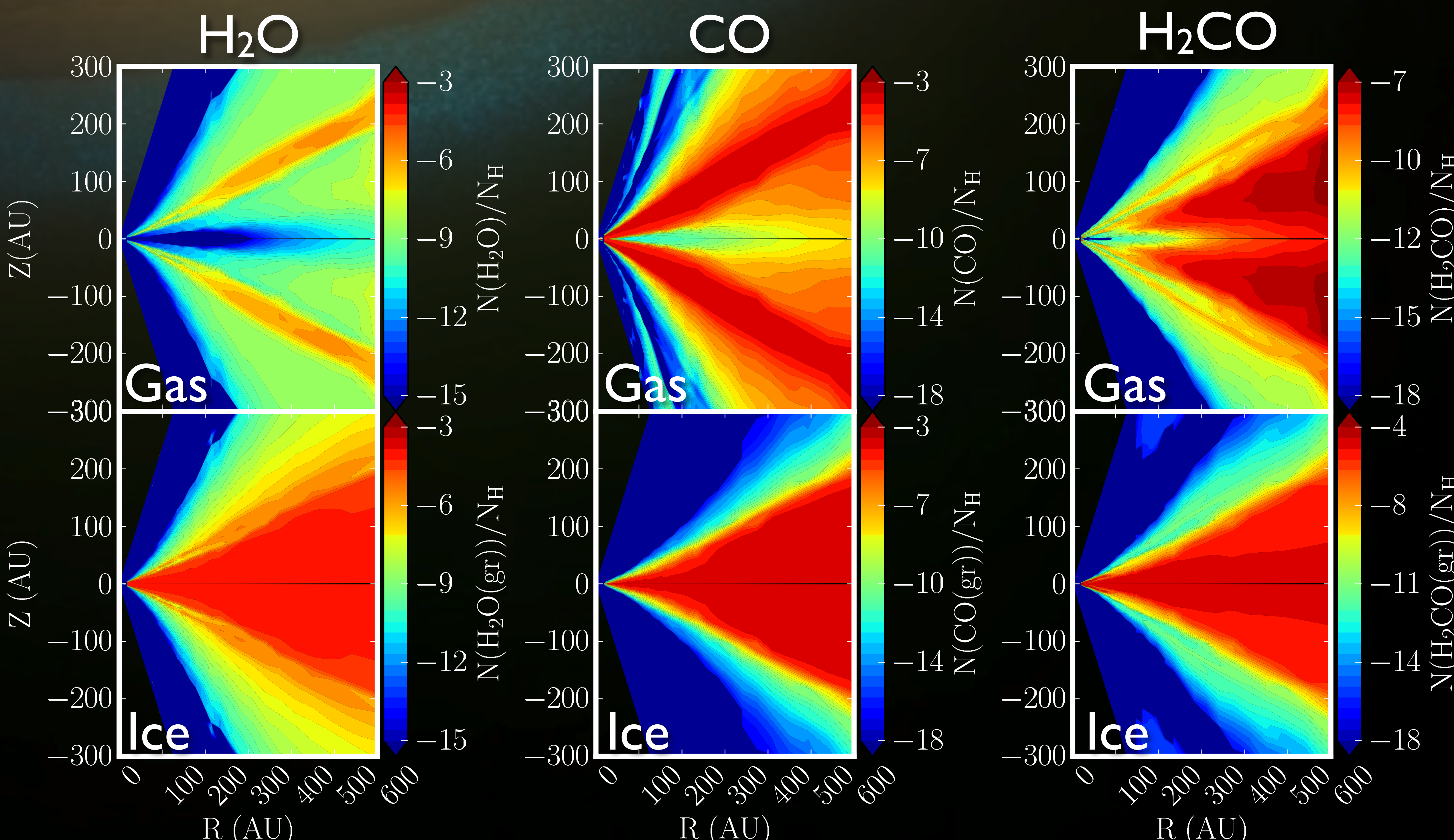
Chemical Results: 2) Carbon-'goo'

Without 'goo' effects



Chemical Results: 2) Carbon-'goo'

Reduced H_2O UV-desorption efficiency due to carbon ices.



Results: Molecular Emission

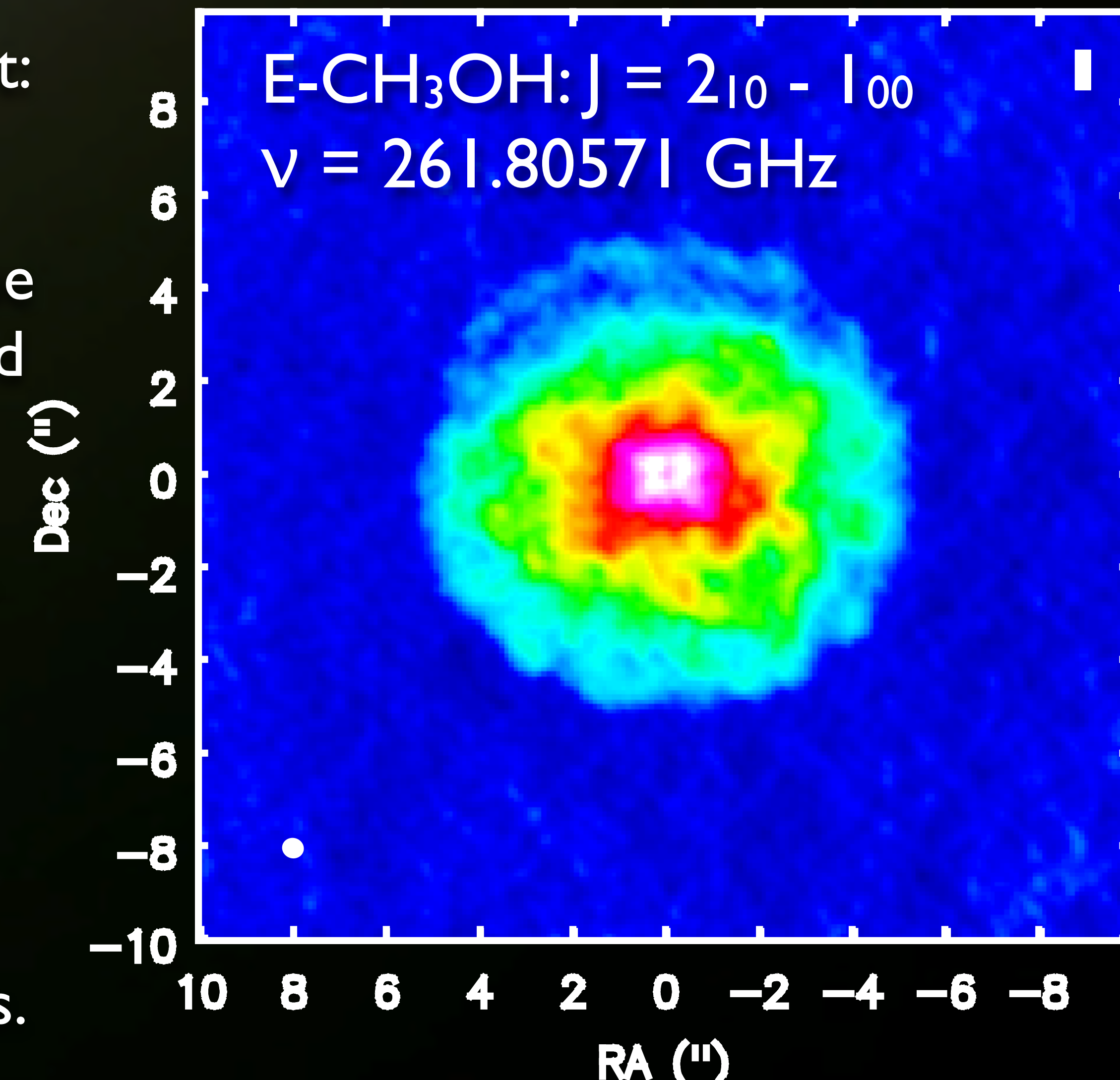
- Using the non-LTE code LIME (Line Modeling Engine, Brinch & Hogerheijde 2010)
  - Adding the more robust grain network helps reduce the H_2O problem
  - H_2CO consistently too strong - likely the result of an incomplete grain network.
  - Model assumes $T_{gas} = T_{dust}$ → but goo heads in right direction.
  - Not including UV ice-photodissociation (more frequent) rather than pure desorption (e.g. H2CO(gr) + hv → HCO(gr) + H).

	o-H_2O $1_{10} - 1_{01}$ (mK km/s)	p-H_2CO $3_{03} - 2_{02}$ (Jy km/s)	o-H_2CO $4_{14} - 3_{13}$ (Jy km/s)	CO 2 – 1 (Jy km/s)
Observed	16[2]	0.35[0.03]	0.29[0.11]	14.87[0.12]
Original Model	28.1	0.7	0.5	22.7
Grain Chemistry	22.7	7.2	5.1	22.5
Grain + Goo	18.3	4.5	2.1	22.5

Conclusions + The Future

- X-ray desorption adds $CO \rightarrow C + O \rightarrow H_2O$: more water, not less.
- More sophisticated grain chemistry is important: competition for hydrogenation.
- Reduced UV photo-desorption yield of H_2O due to goo is a potential solution to the missing cold water.
- H_2CO grain/photo-chemistry likely incomplete.

- H_2O collision rates - perhaps overestimated <50K? (Dick et al. 2010)
- Models: different fits to same SED and $T_g \neq T_d$.
  - Explore different/more sophisticated models.
- Resolved observations with ALMA of carbon-ices can be used to test the 'goo' scenario.
- Herschel OT2 → Catch H_2O in absorption!



CASA *simdata* ALMA simulation of methanol. Antenna config. 10; Band 6; t = 8h.