The Physics and Chemistry of the Interstellar Medium
Avignon - September 2019

Modelling of the chemistry of protoplanetary disks

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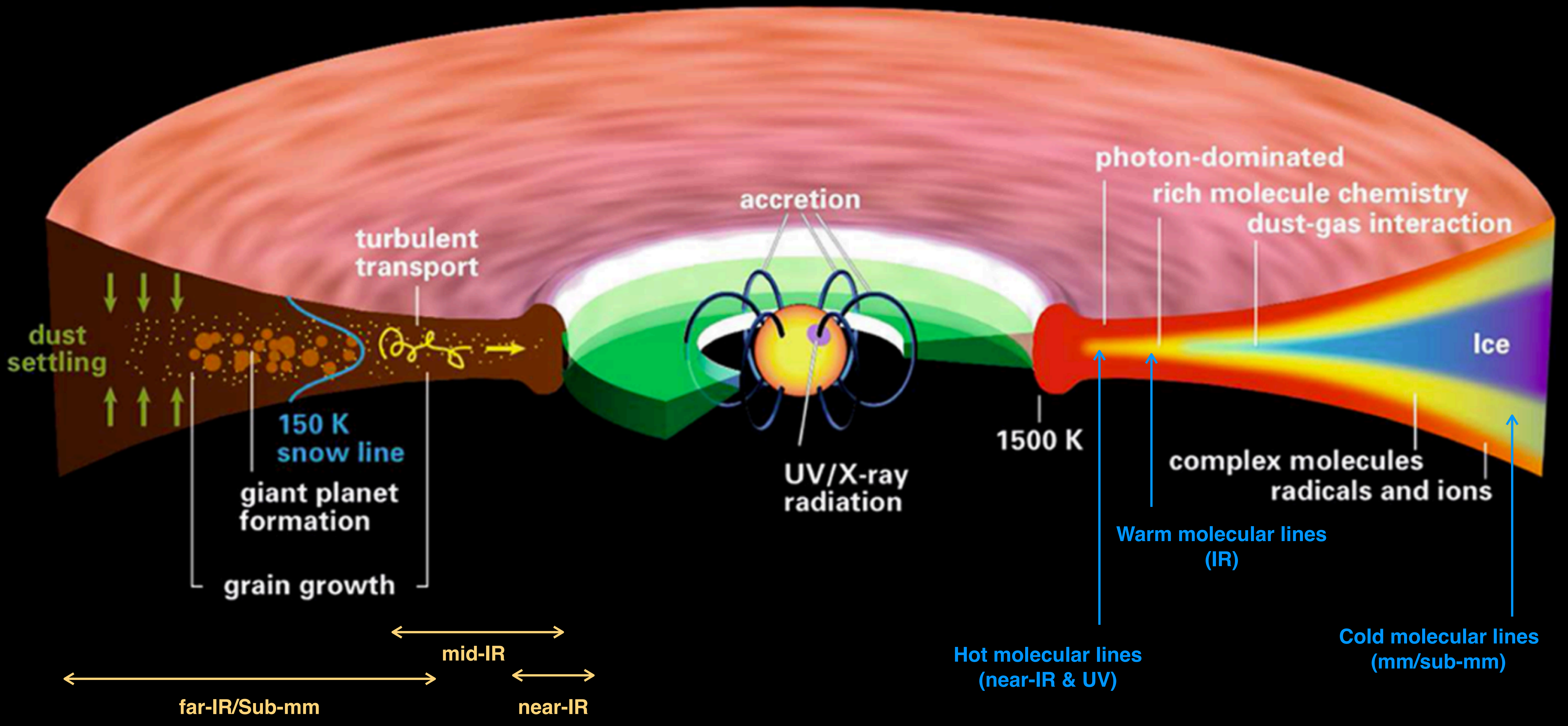
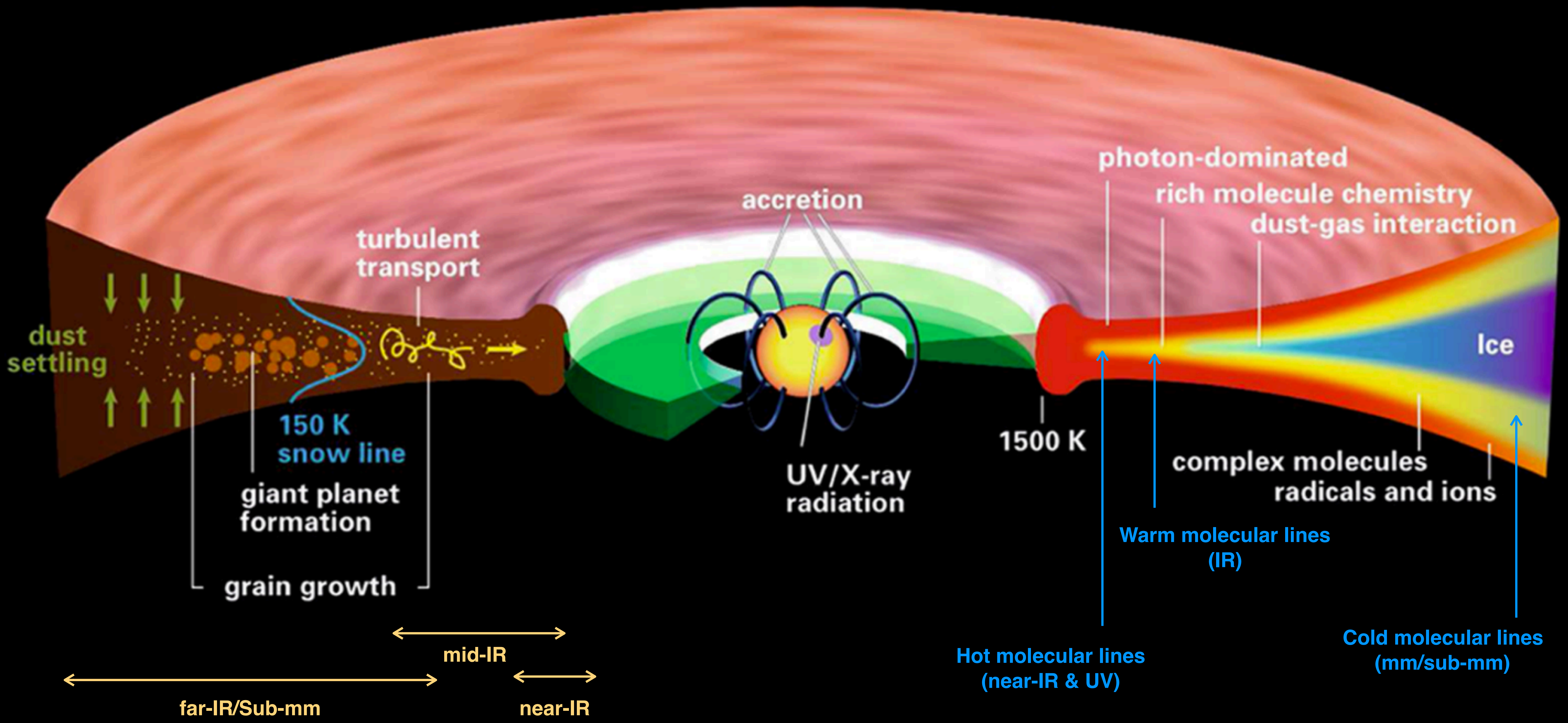
Introduction



Adapted from Semenov & Henning 2013

Introduction



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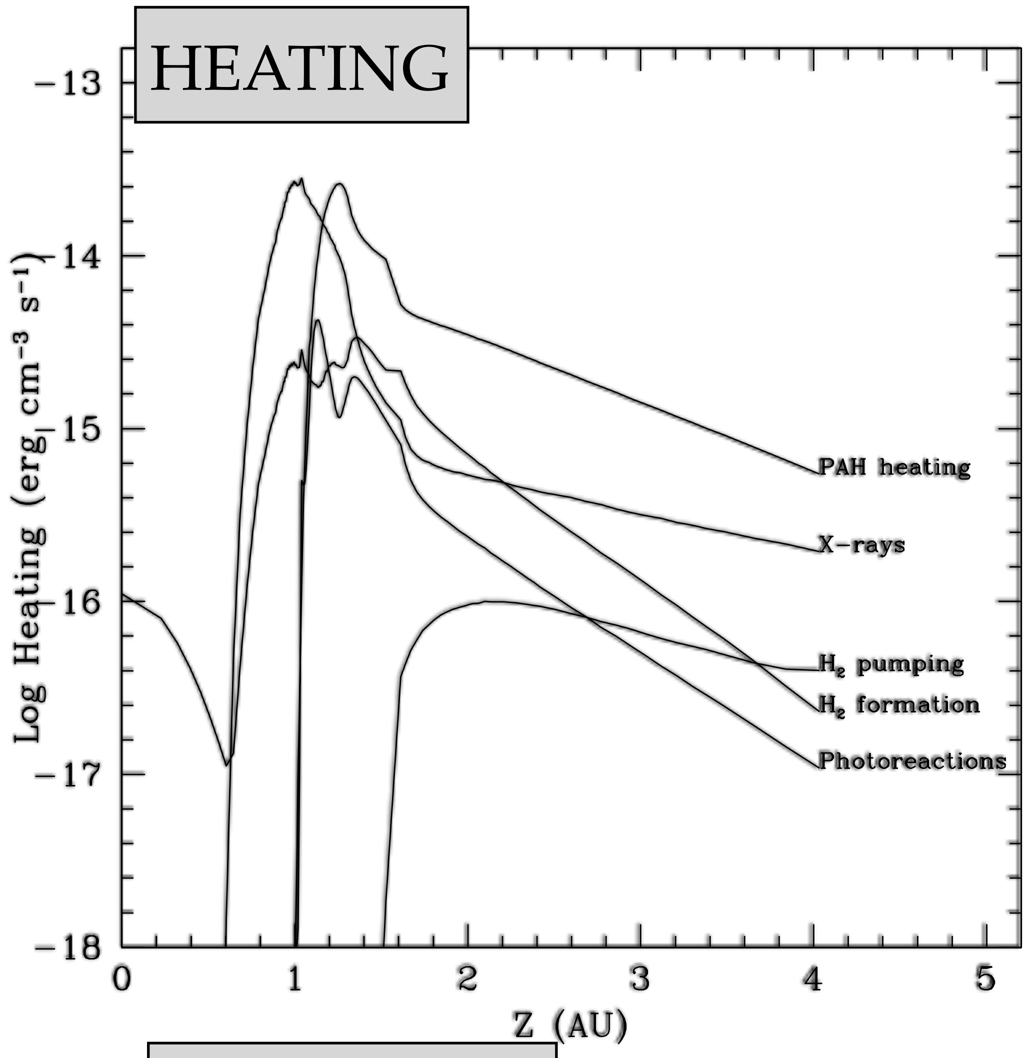
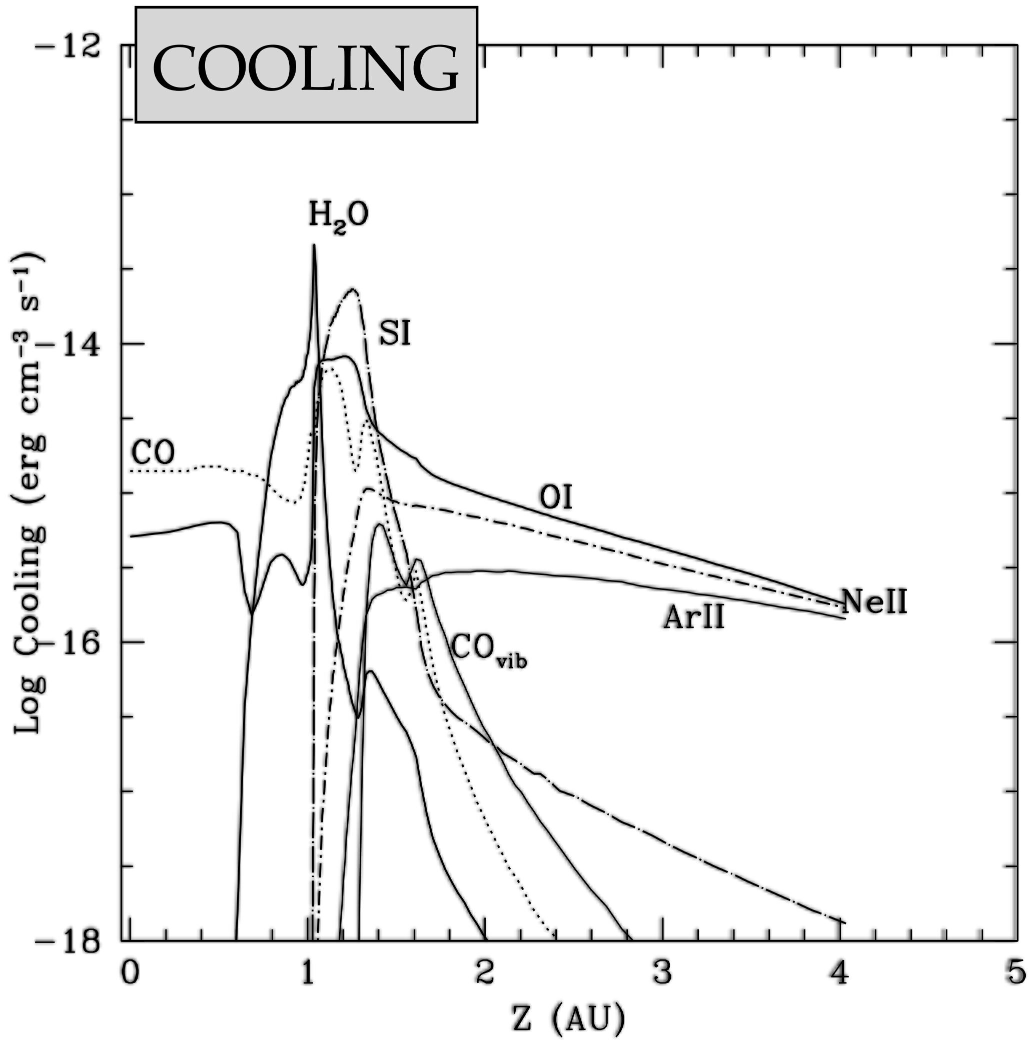
New framework which combines a thermo-chemical disk model and an full gas-grain chemical model (Ruaud & Gorti, submitted to ApJ)

Thermo-chemical disk model

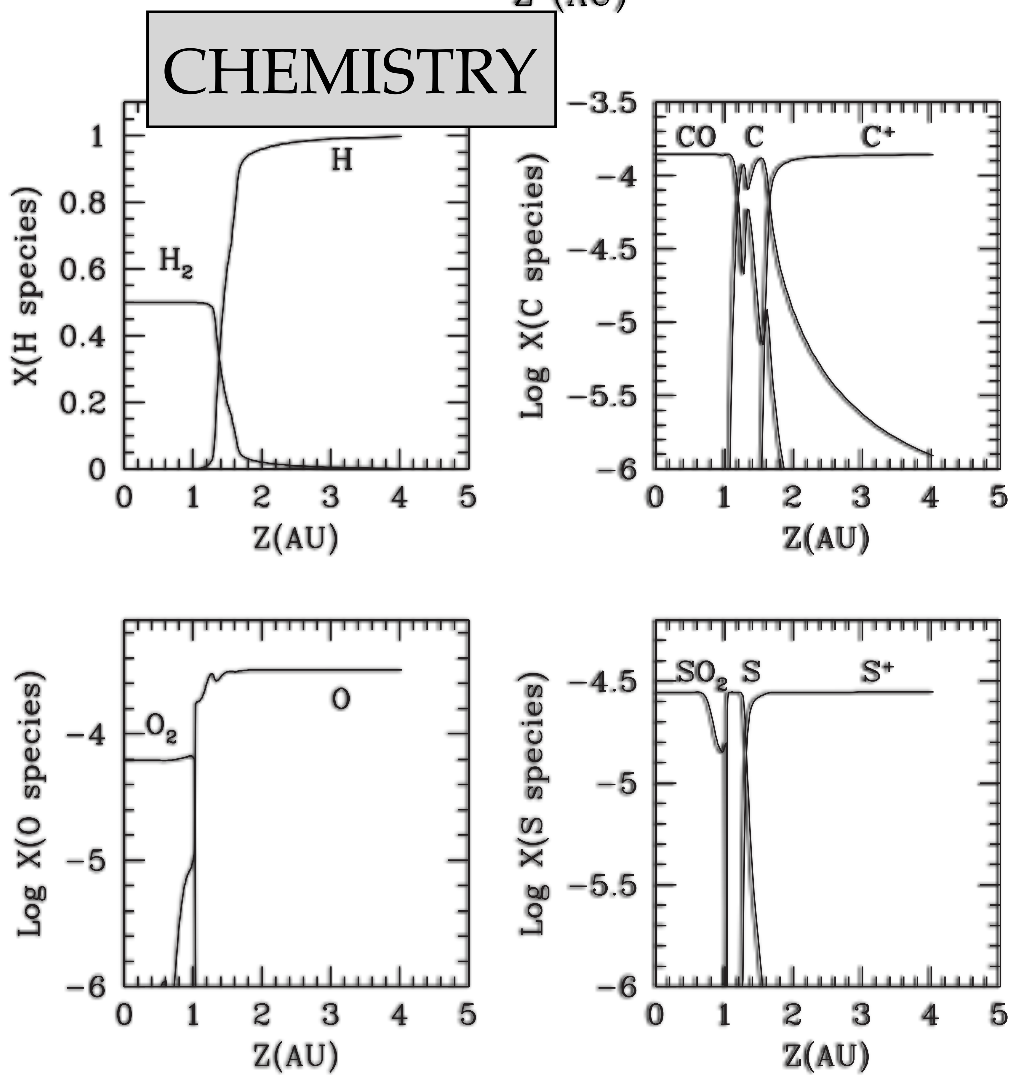
Iterations to get **density and temperature structure** at **vertical hydrostatic equilibrium**

- Dust collisions
- X-rays & UV
- H_2 pump/form
- Chemical reactions
- …

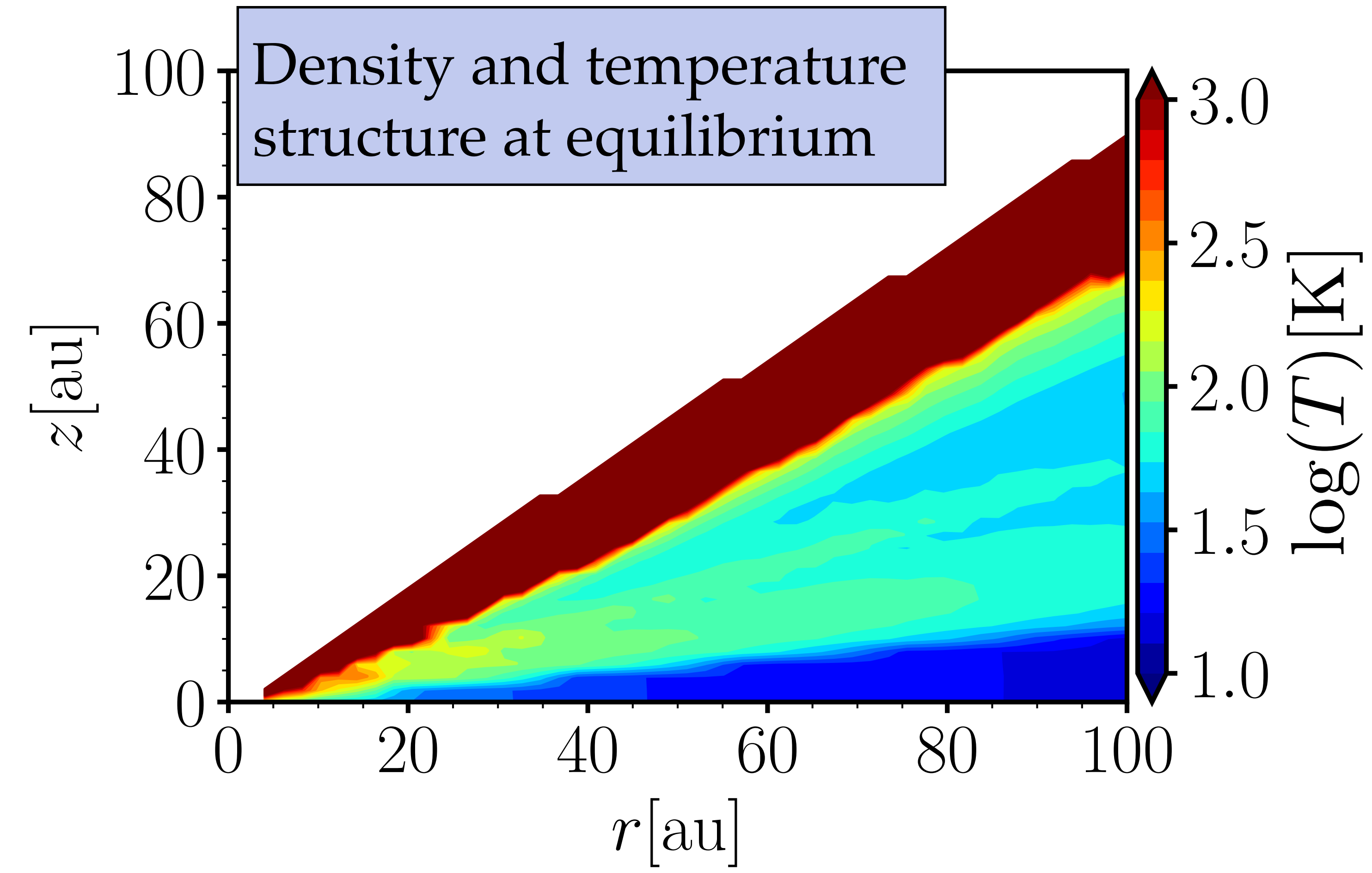




- Line emission from atoms, ions & molecules
- Dust continuum



- Ion-neutral
- Neutral-neutral
- Photoreactions
- 3-Body reactions

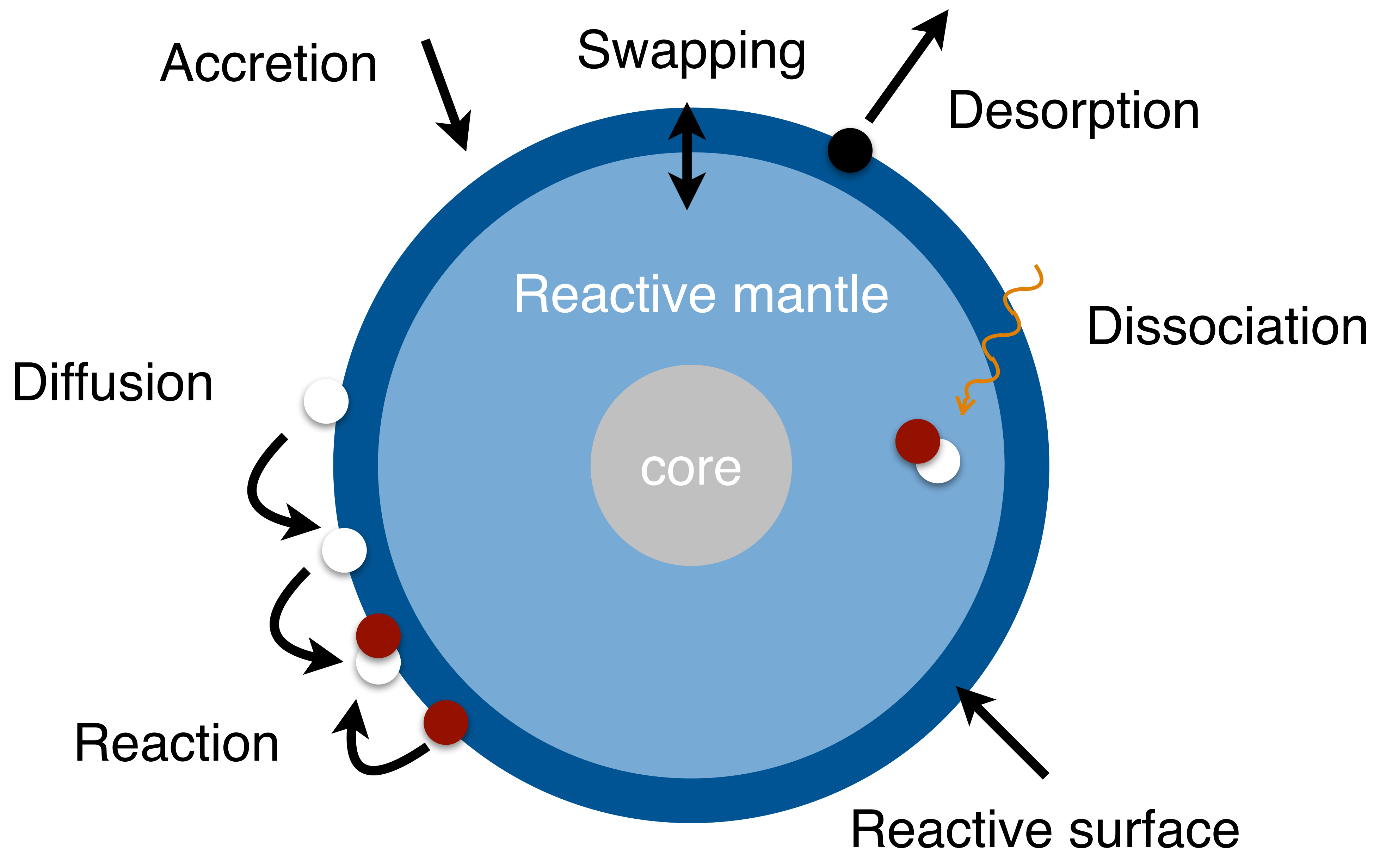


Gorti & Hollenbach 2008, 2009, 2011

Gas-grain chemical model

Time-dependent three-phase chemical model (~500 species and ~7000 reactions)

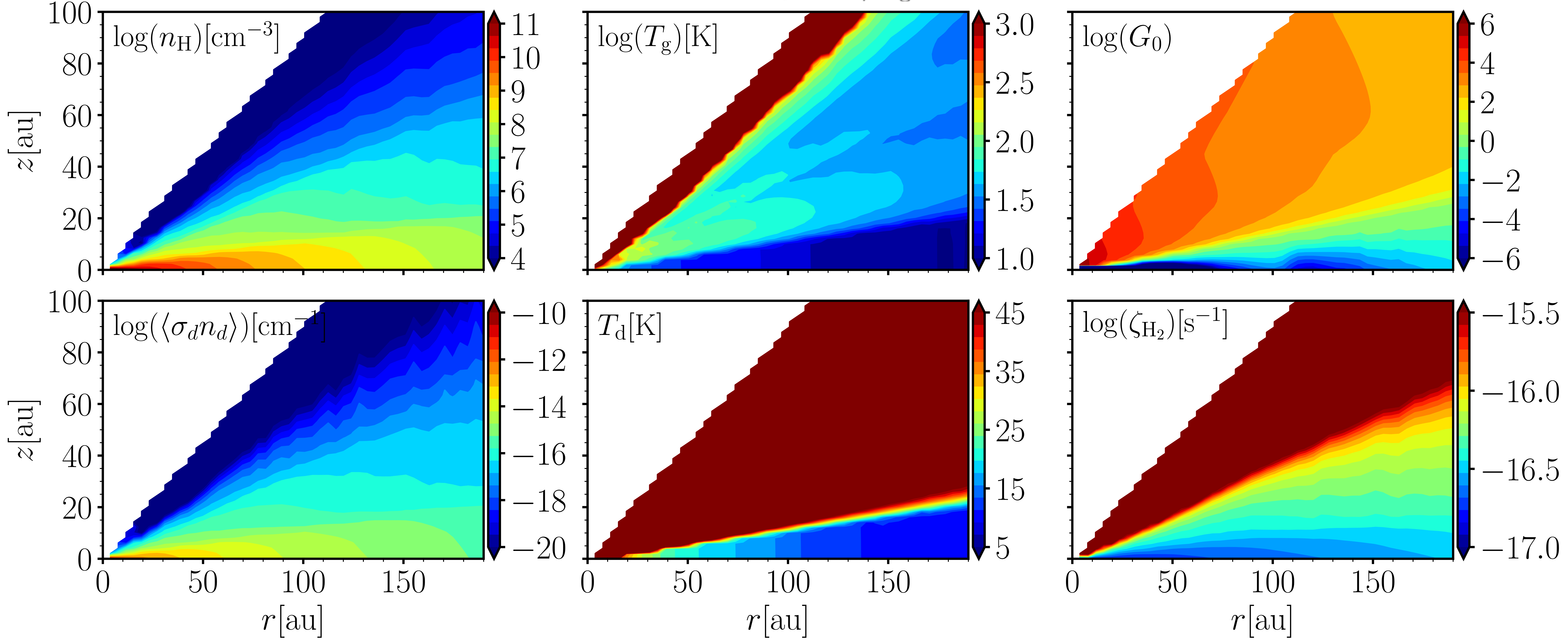
- **Surface** and **mantle** diffusion
- **Reactions** through the Langmuir-Hinshelwood process
- **Surface** and **sub-surface photoprocessing** by stellar and interstellar photons and cosmic-rays generated photons
- **Desorption** restricted to the **top two monolayers** (thermal desorption, chemical desorption and photodesorption)
- **Grain growth** by accretion of molecules



Three phase model:
gas, ice surface and ice mantle
(Ruaud et al. 2016)

Results obtained with a typical disk

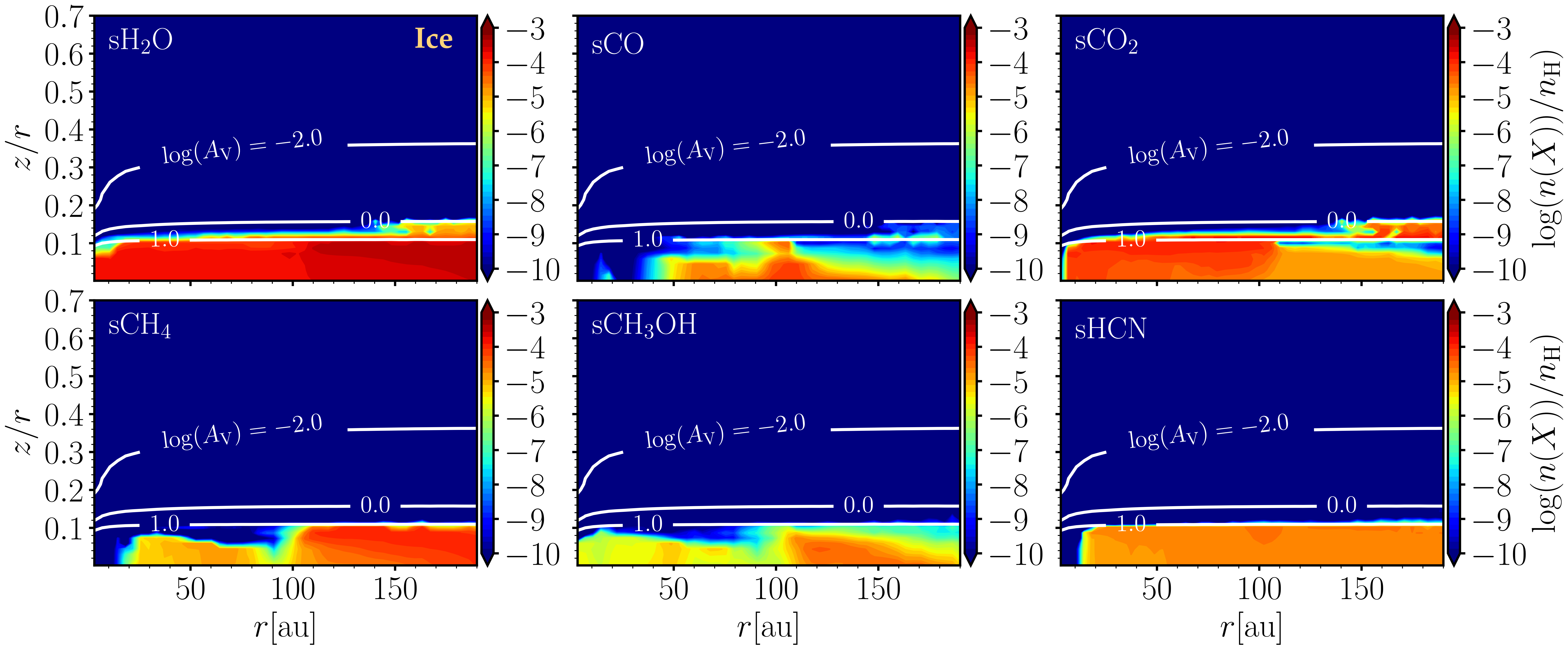
$M_{\rm disk} = 0.005 M_\odot$ - $\Sigma_d/\Sigma_g = 0.01$



$M_{\rm disk}$ ~ mean disk mass derived from surveys in Taurus and Lupus regions (Ansdell et al. 2016)

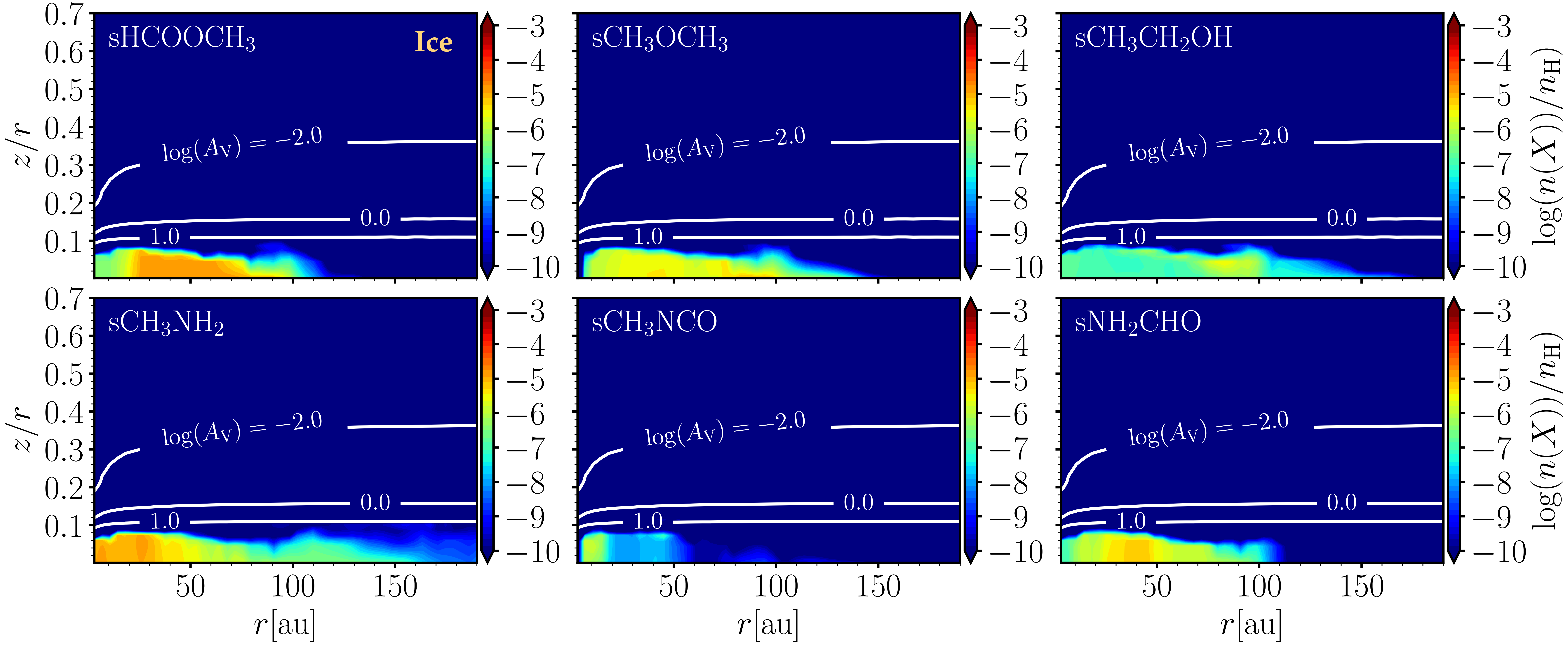
Predicted ice composition

Ice mainly consists of simple molecules: H_2O, CO, CO_2, CH_4, CH_3OH, HCN, …



Predicted ice composition

Complex molecules efficiently form in the inner disk



~0.1-1% relative to water

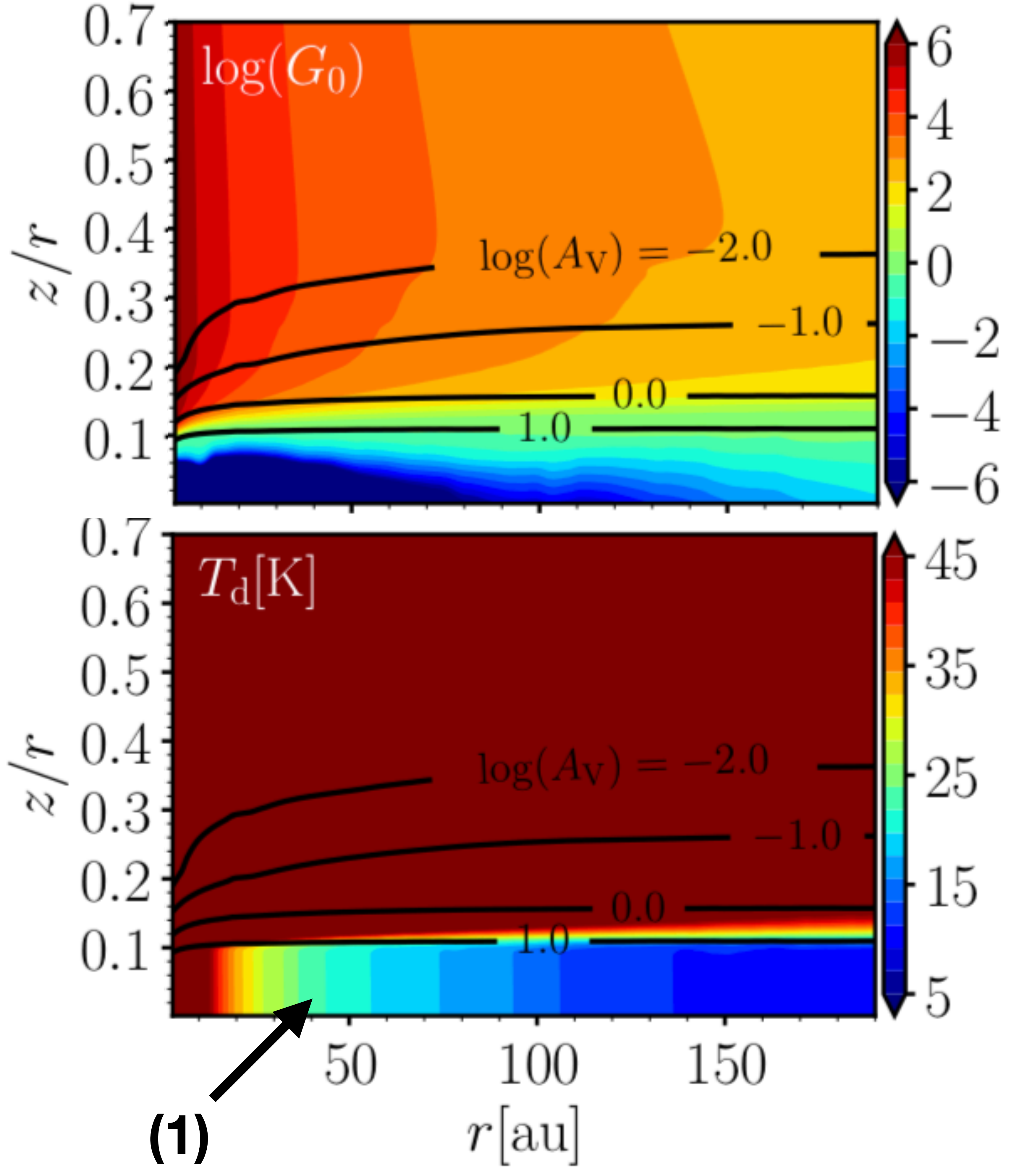
Chemistry of the midplane

Three chemically distinct regions in the disk midplane:

(1) Inner disk midplane (r<100 au):

- low UV flux
- T_d>15 K

➜ Efficient formation of COMs: radicals diffuse at the surface of grains



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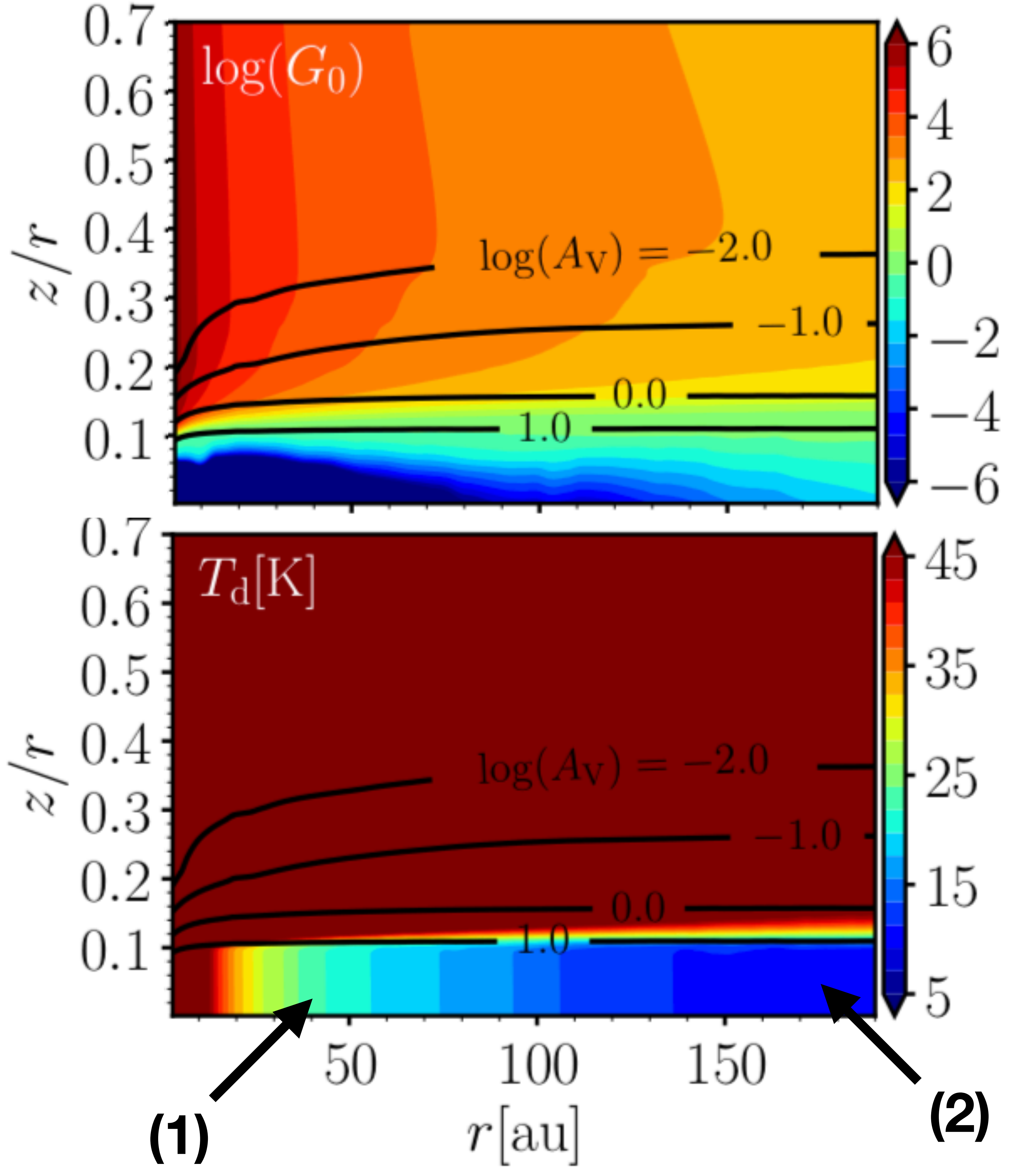

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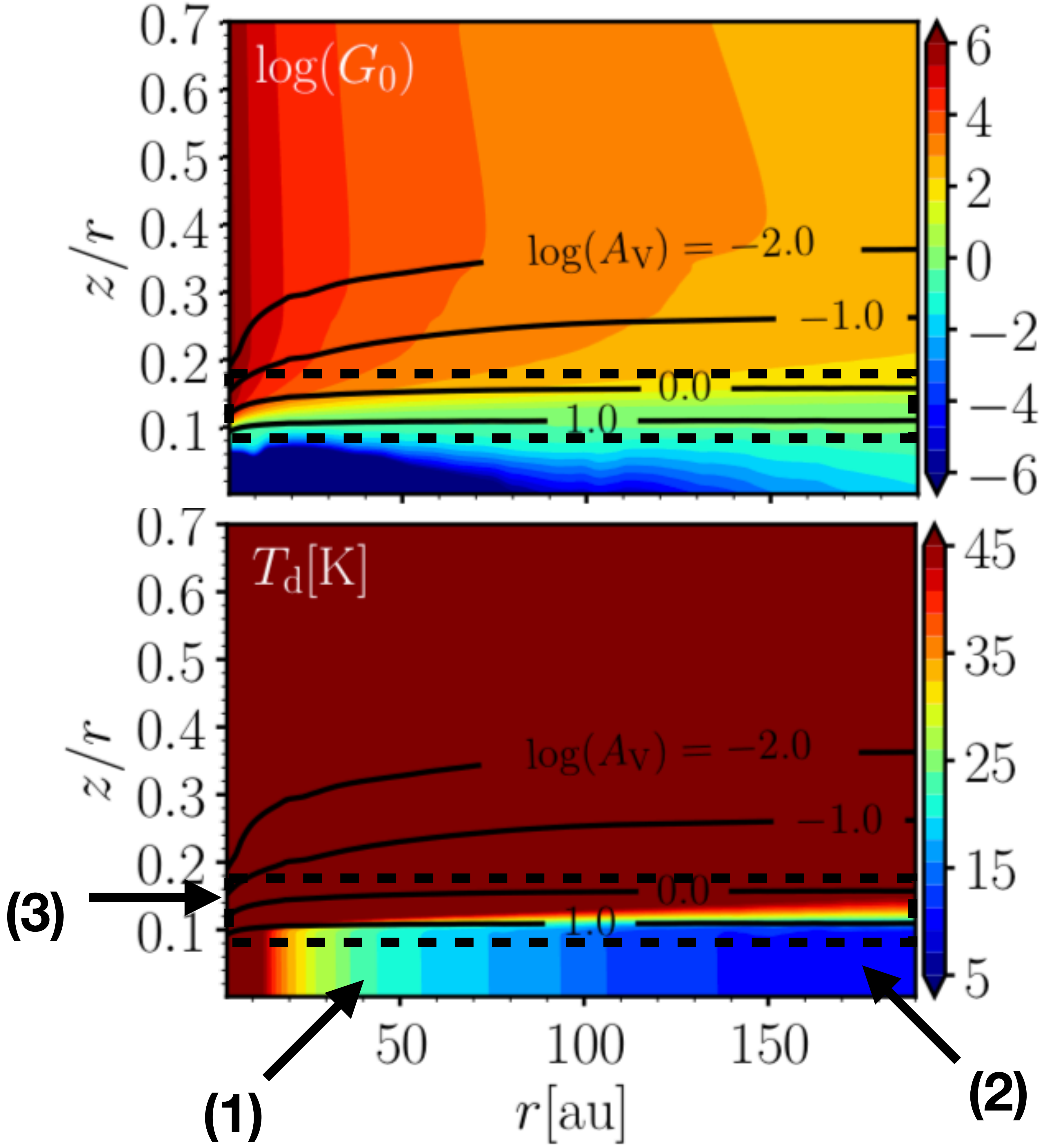
(3) Interface molecular layer / midplane or **water condensation front**:

- Important UV
- T_d≳15 K

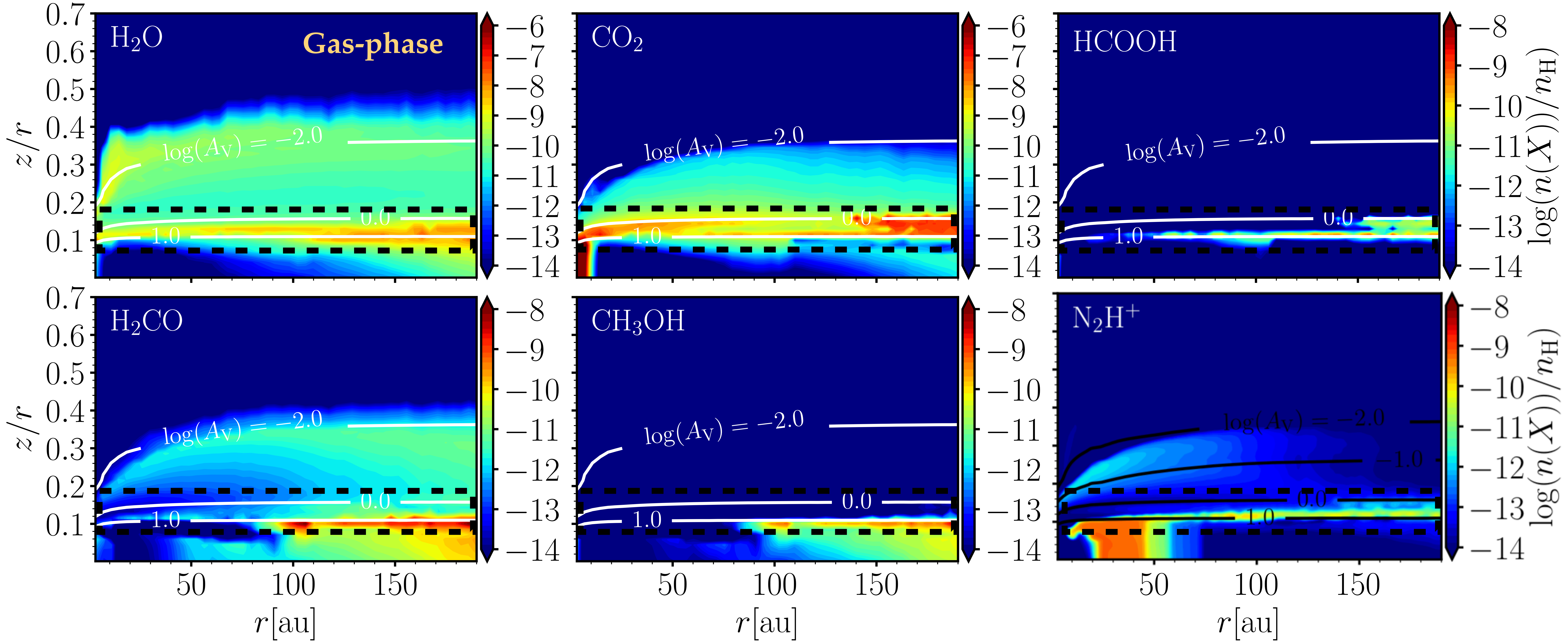
→ Important photoprocessing of the ice



Impact of ice photochemistry on gas-phase composition

Photo-processing of the ice near the water condensation front:

- Photodesorption
- Photodissociation and re-formation at the surface of the ice: promotes chemical desorption



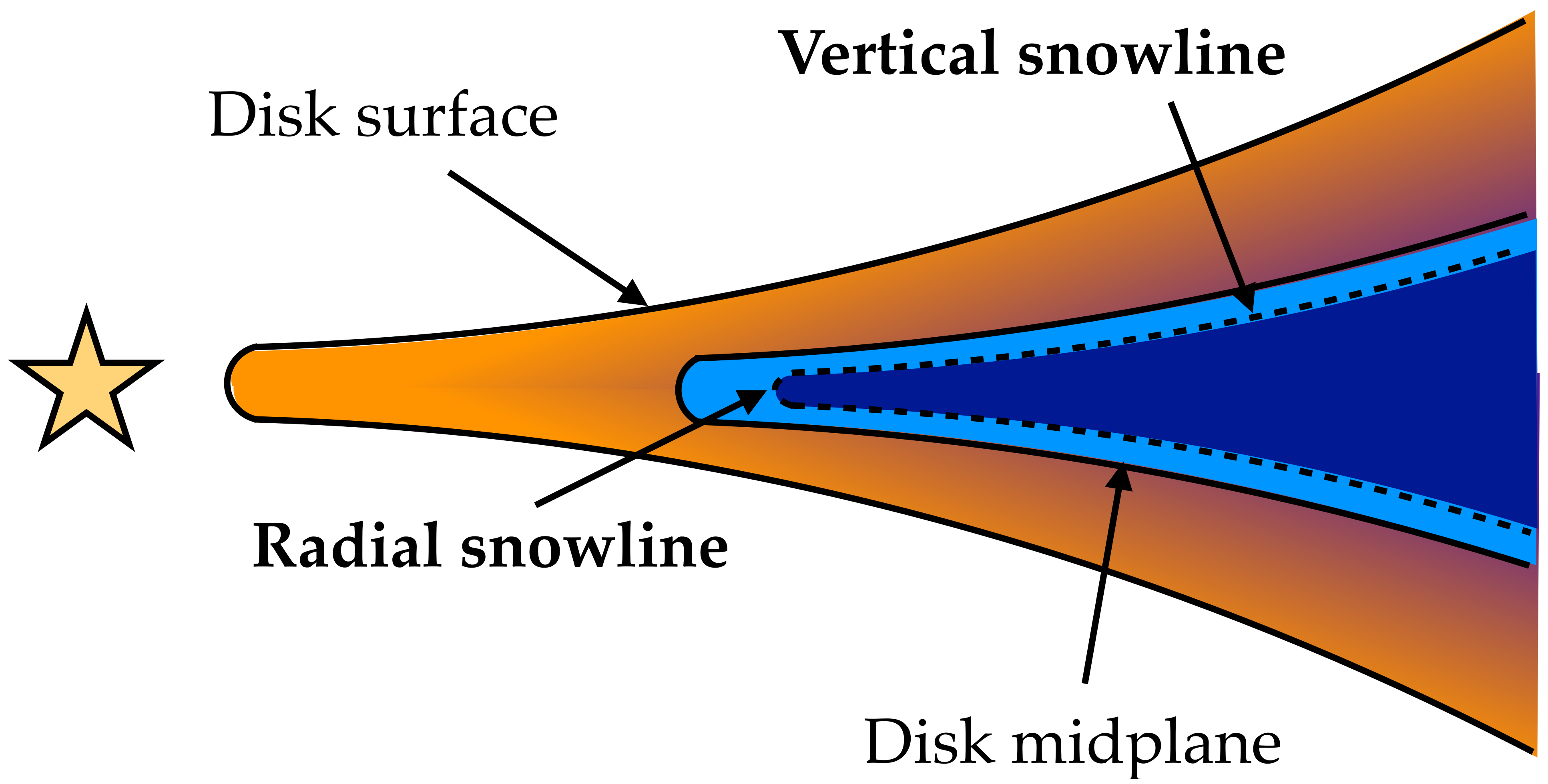
Impact on vertical CO snowline

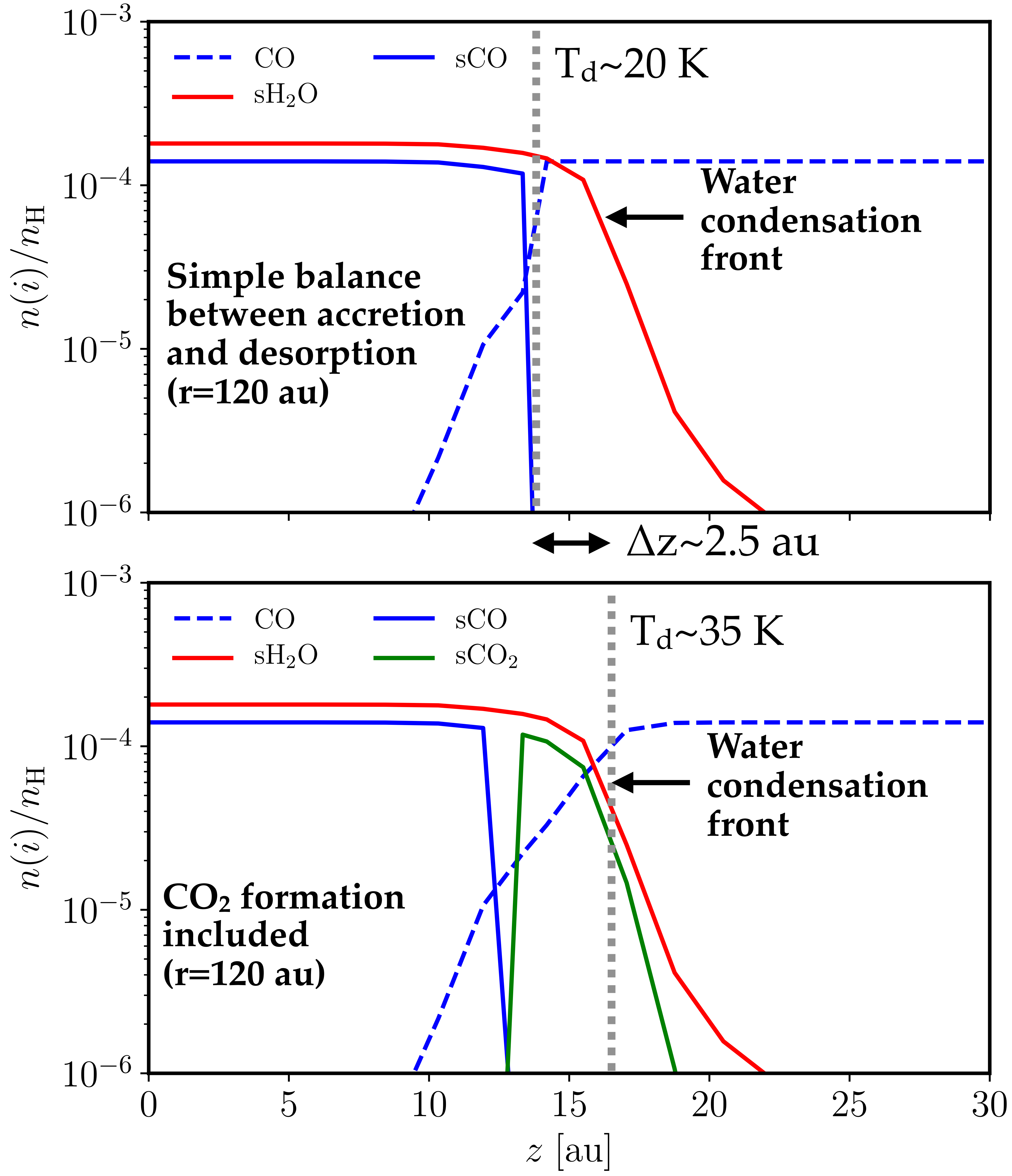
- **Efficient formation of sCO_2 near water condensation front impacts the location of the vertical CO snowline**: shifts higher up from the disk midplane

$$sH_2O + h\nu \rightarrow sOH + sH$$

$$sOH + sCO \rightarrow sCO_2 + sH \ (\Delta E = 150K)$$

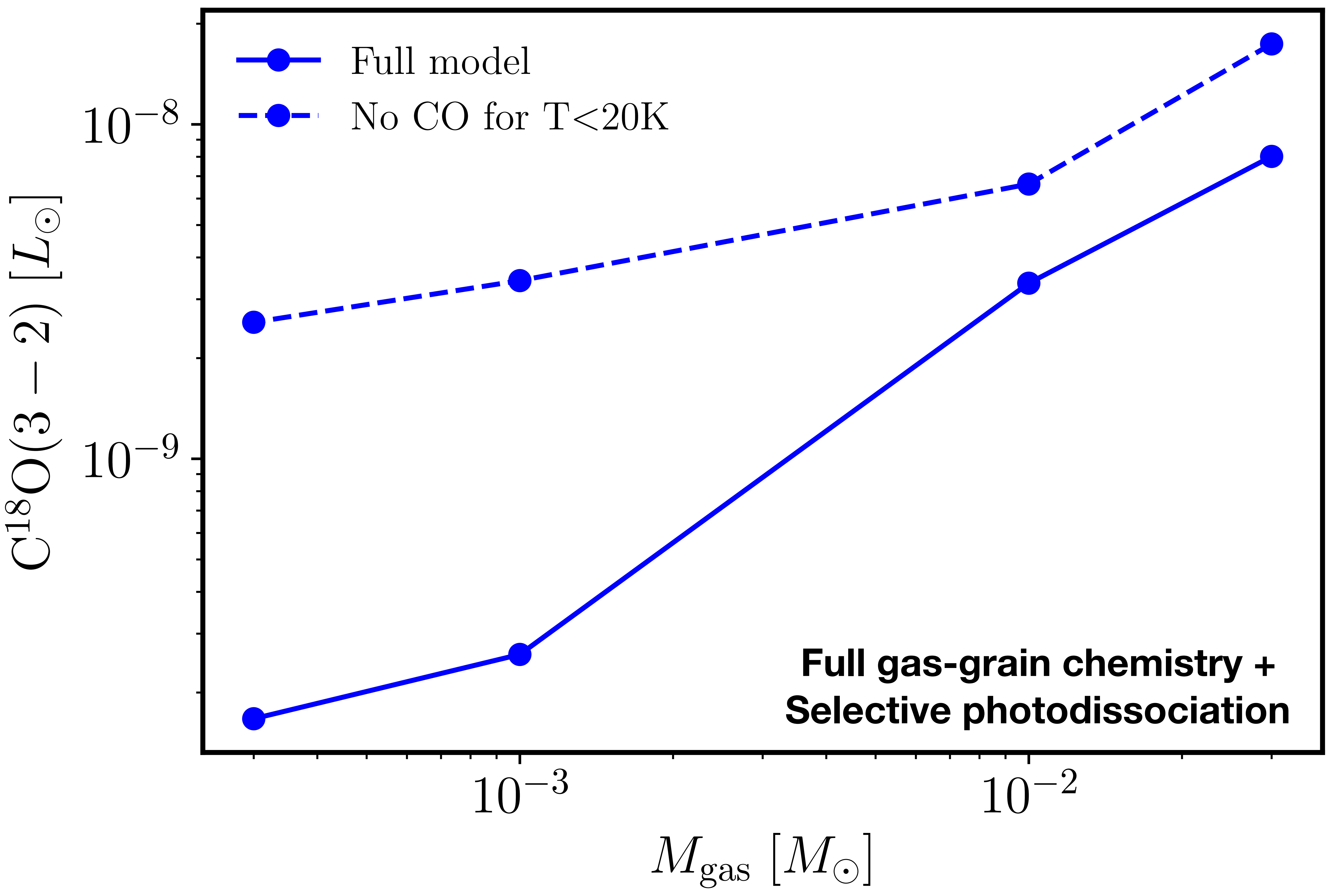
$$\rightarrow sHOCO \ (\Delta E = 150K)$$





Impact on the emission of CO isotopologues

Predicted line emissions can decrease by a factor of ~10
(work in progress)



Summary

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- **The disk interior can be divided into three chemically distinct regions**:

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(2) The outer disk midplane where hydrogenation reactions dominate the chemistry

(3) The interface between the molecular layer and the midplane where grain surface chemistry is driven by photoprocessing of ices

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- **Interface between the molecular layer and the midplane**:
  - **Photoprocessing of ices** has a significant **impact** on **the gas-phase abundance** of several molecules
  - **Efficient conversion of CO to CO_2 ice** which **impacts the location of the vertical CO snowline**: moves higher up in the disk midplane. **Important impact on the predicted emission lines of CO isotopologues**.

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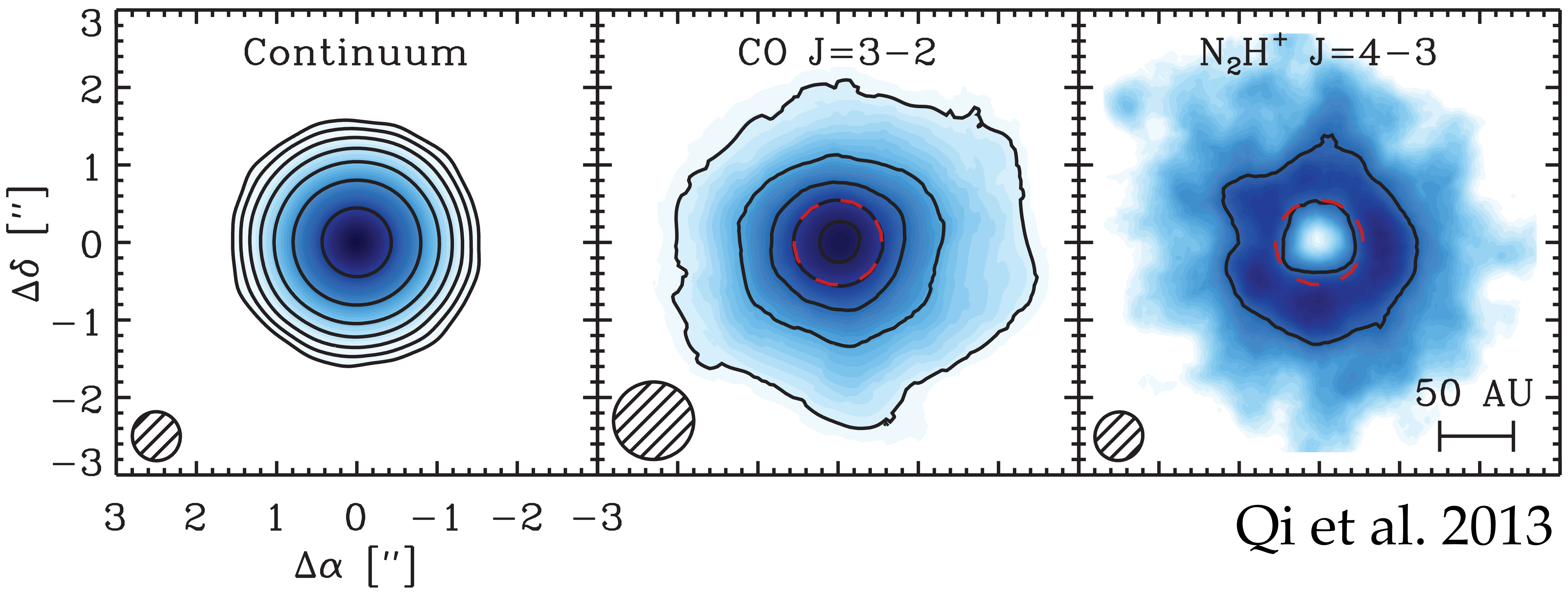
Thank you for your attention!

Chemistry of the midplane

- **Radial CO snowline also impacted**:
  - Move closer to the star as a function of time
  - Conversion driven by cosmic rays

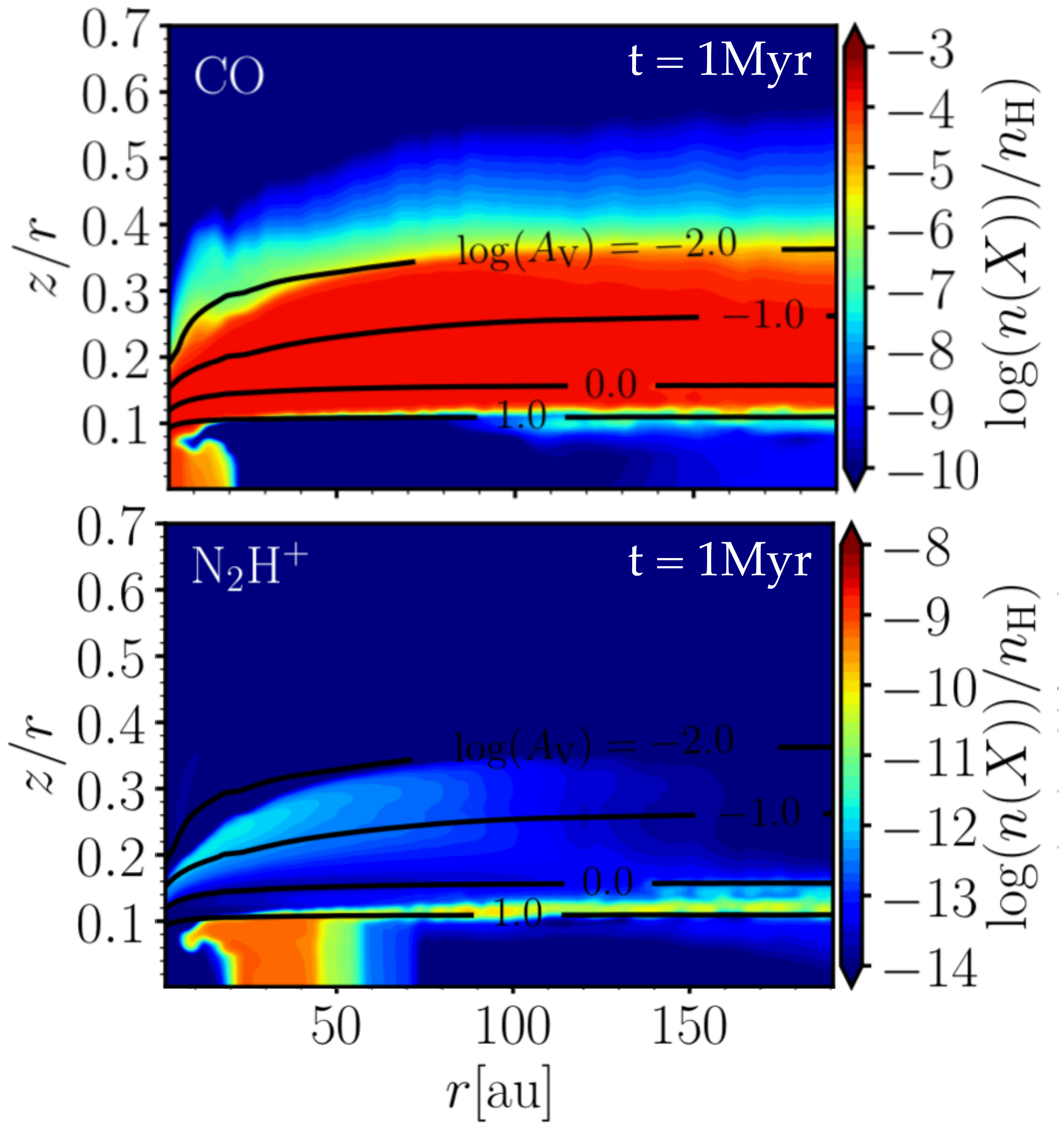
- **Impacts N_2H^+**: tracer of CO snowline

$$N_2 + H_3^+ \rightarrow N_2H^+ + H_2$$
$$CO + N_2H^+ \rightarrow HCO^+ + N_2$$



Qi et al. 2013

T_{kin}=39K from N_2H^+ J=1-0 and J=4-3
(Schwarz et al. 2019)



CO snowline

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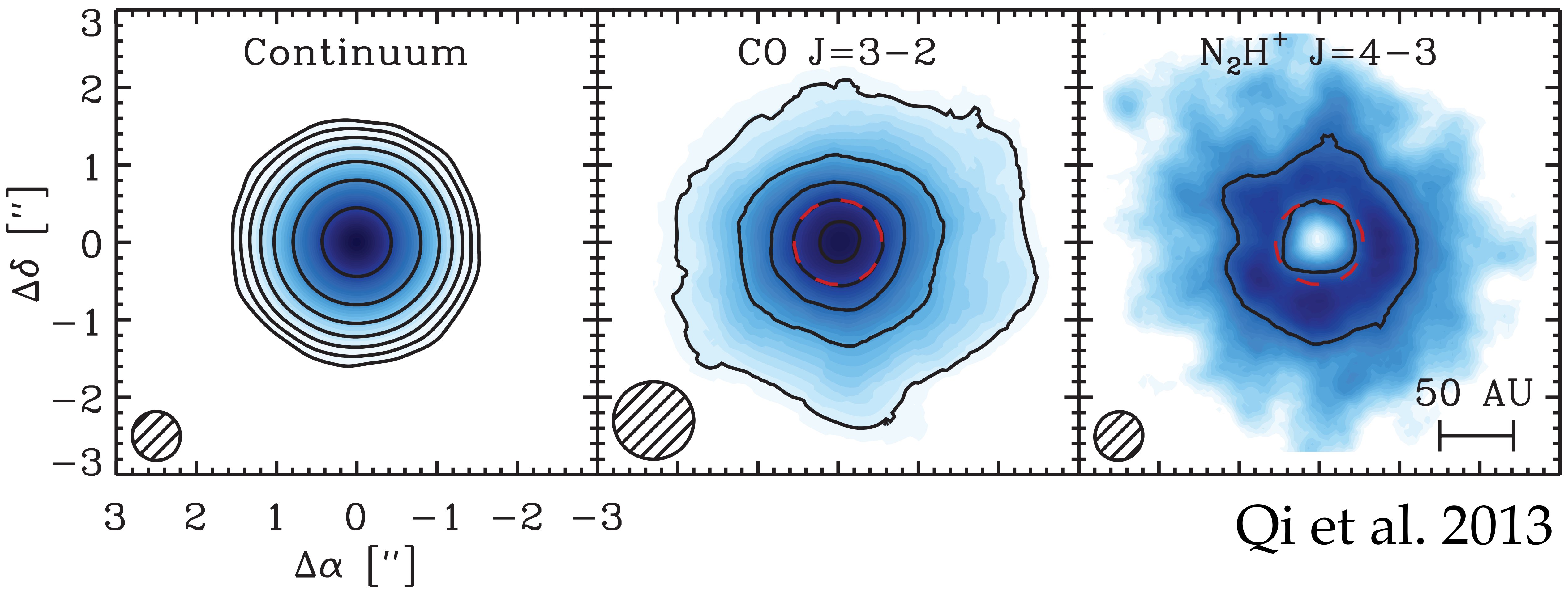

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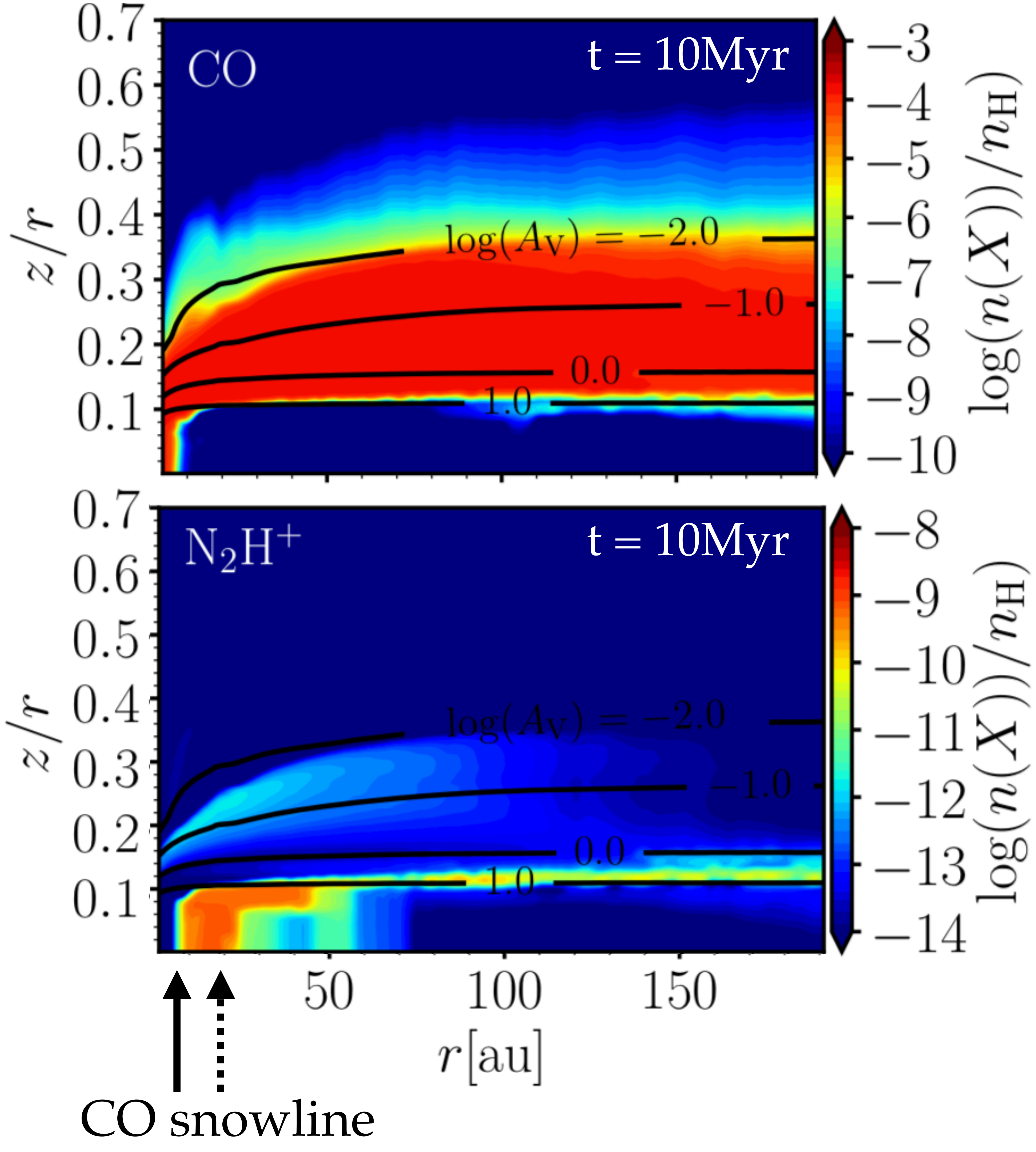
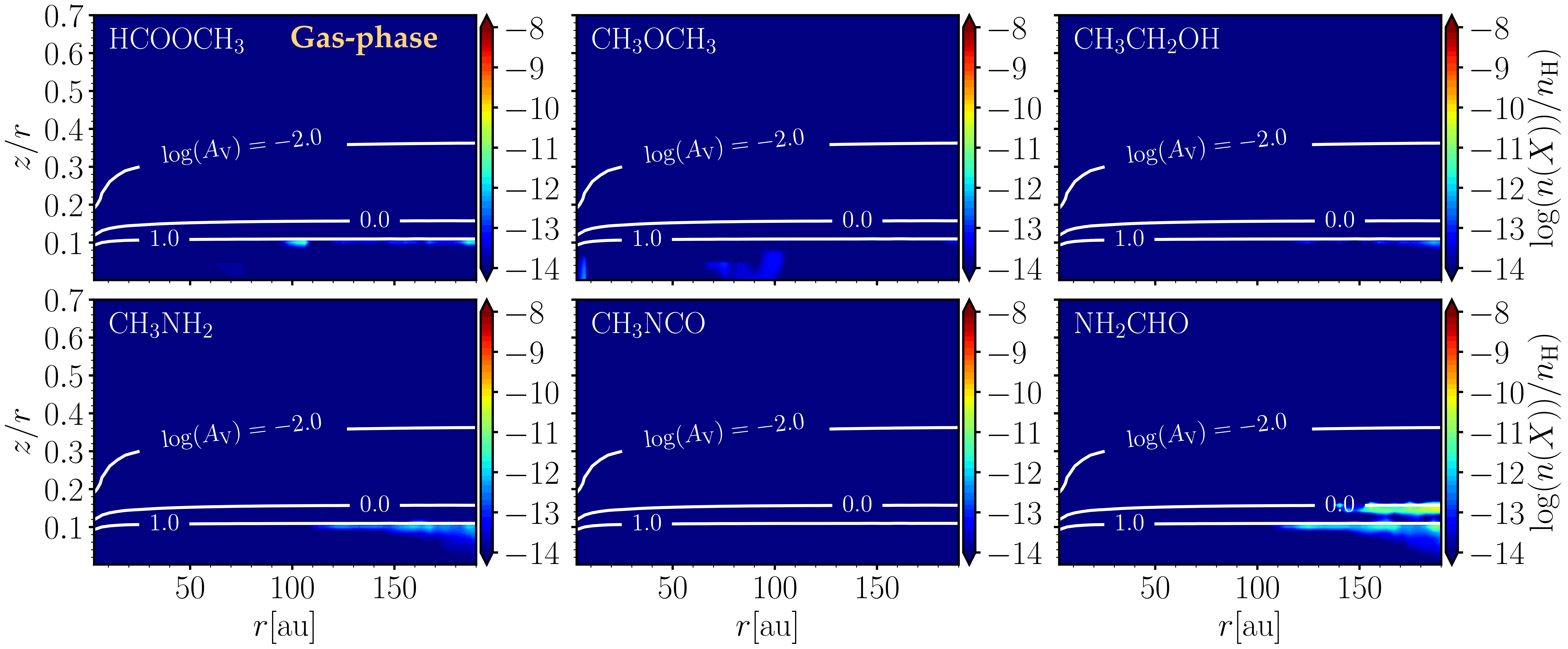


Impact on the composition of the gas



Two-phase vs three-phase approximation

- **Two-phase approximation over predicts gas-phase abundances**: all the mantle is available for desorption

- **Most disk chemical models use the two-phase approximation**

- Could explain the systematic overestimation of cold water lines as compared to observations: depletion factors of ~100 for oxygen have been invoked (Du et al. 2017)