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What do C_2H_2 and H_2O trace in planet-forming regions of disks ?

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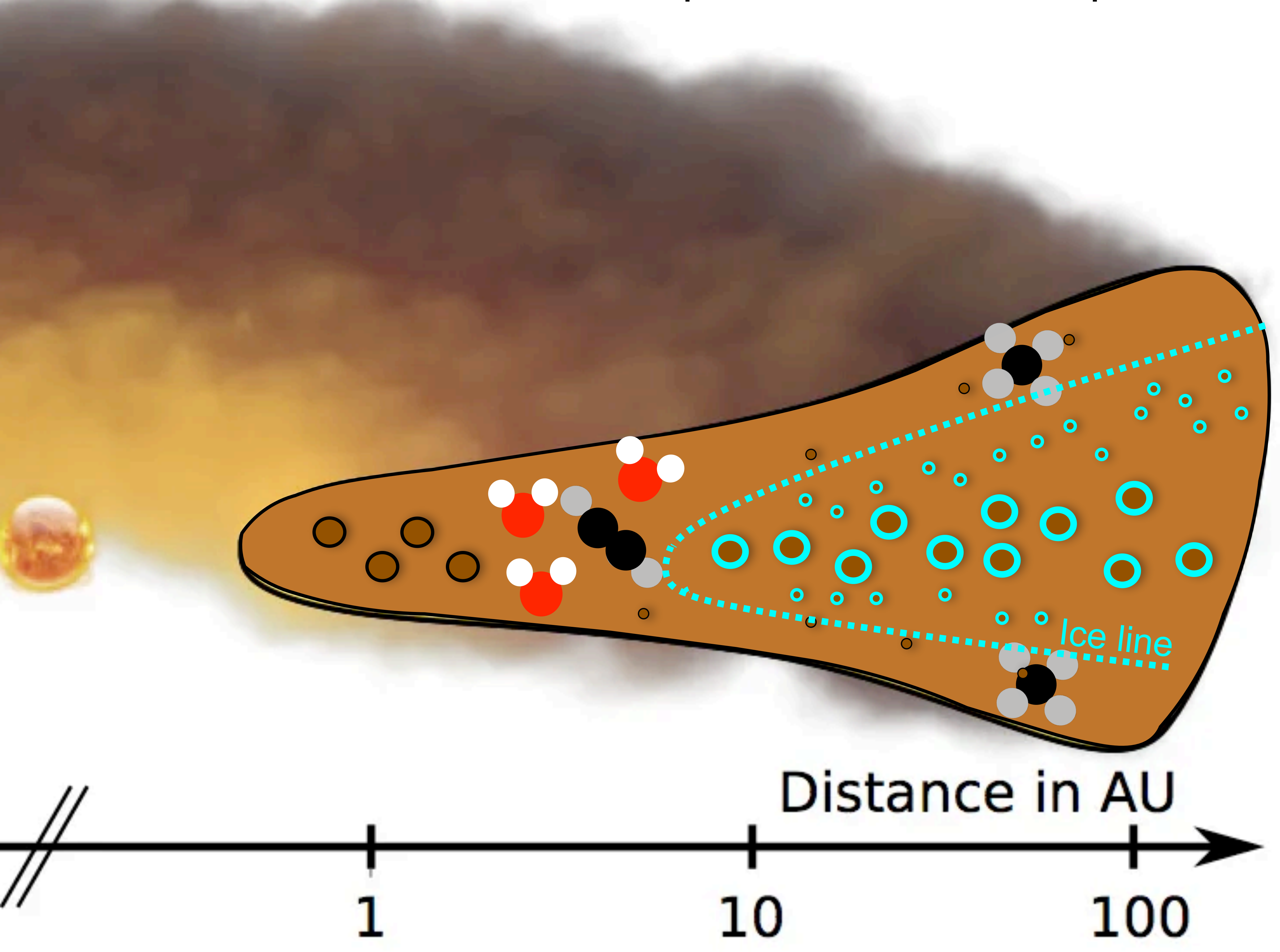
Context

Planet formation theories need constraints on disk properties to interpret the properties of exoplanets

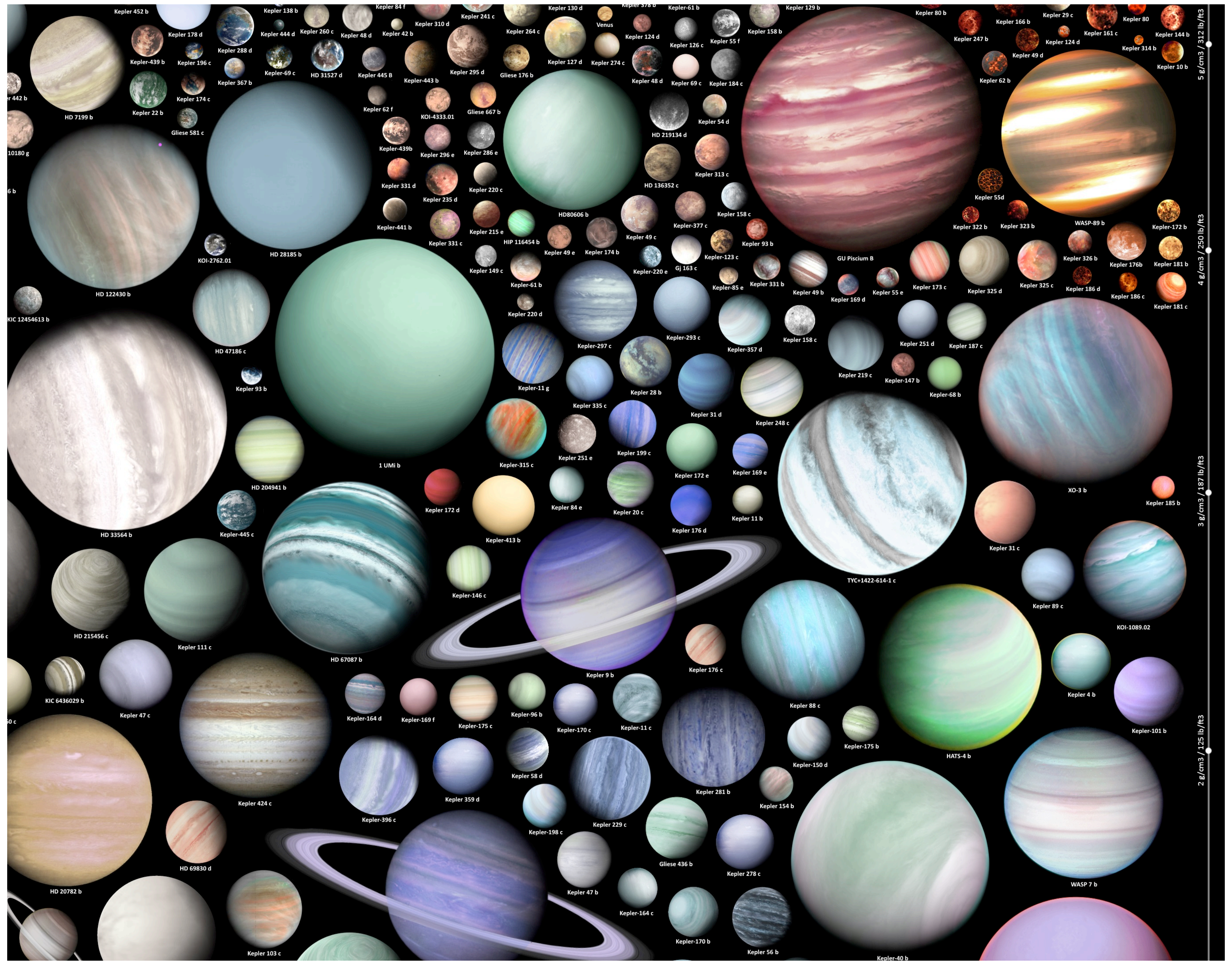
Chemical composition?

➡ Elemental composition of exoplanets



Planet formation models

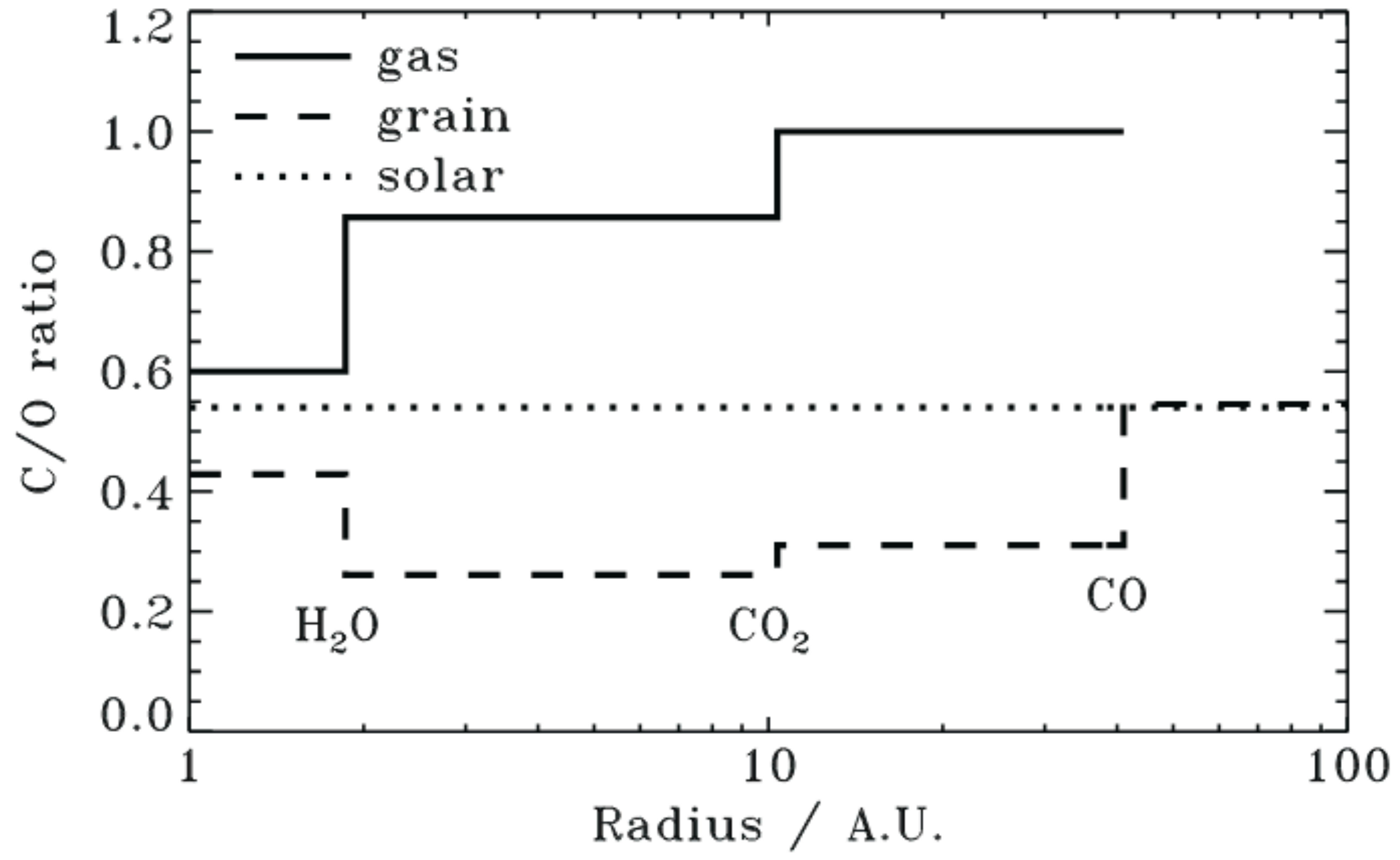
End-product: populations of exoplanets



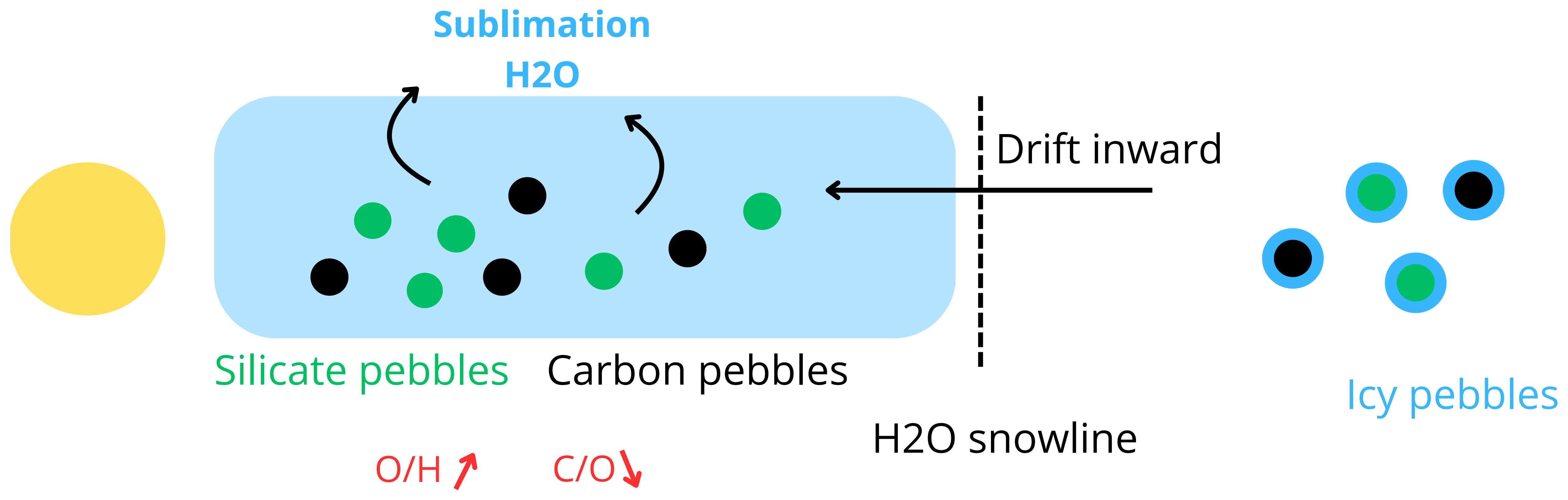
The C/O ratio and metallicity

- The C/O ratio and 'metallicity' ((C+O)/H) are key parameters to constrain planet formation *(Madhusudhan et al. 2016)*
- Indicator of when and where the accretion of gaseous planets starts *(Cridland et al. 2017)*
- Elemental abundances in disks set by complex processes

→ **Need observational constraints**



Evolution of the C/O ratio with radius. Öberg et al. 2011.

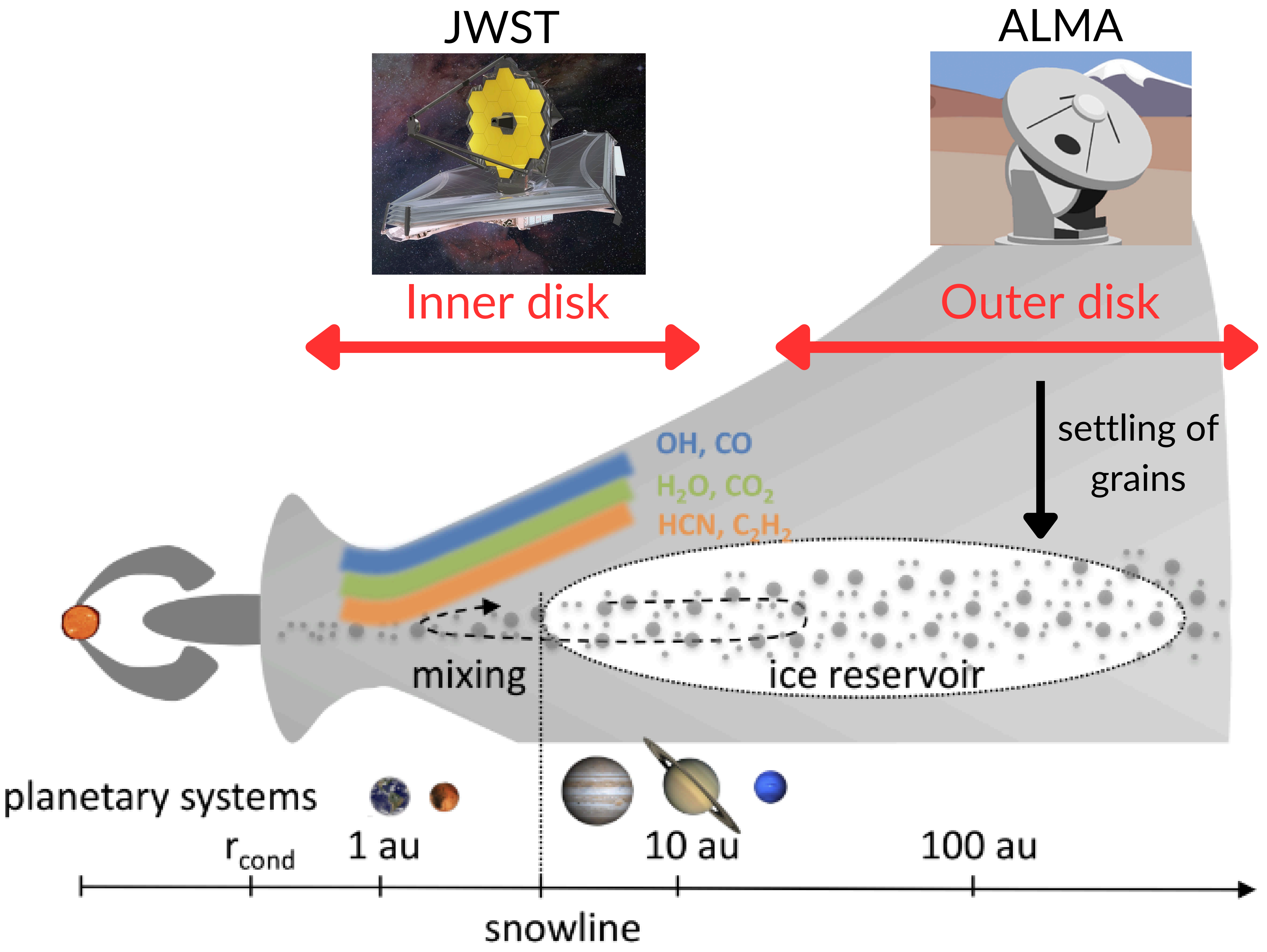


Sketch illustrating the pebble drift.

Context

→ JWST probe the thermal emission from the inner disk <10 au

- Disk composed of gas and dust
- $n_{gas} \sim 10^8 - 10^{15} cm^{-3}$
- $T \sim 50 - 1500$ K
- $R < 10$ au

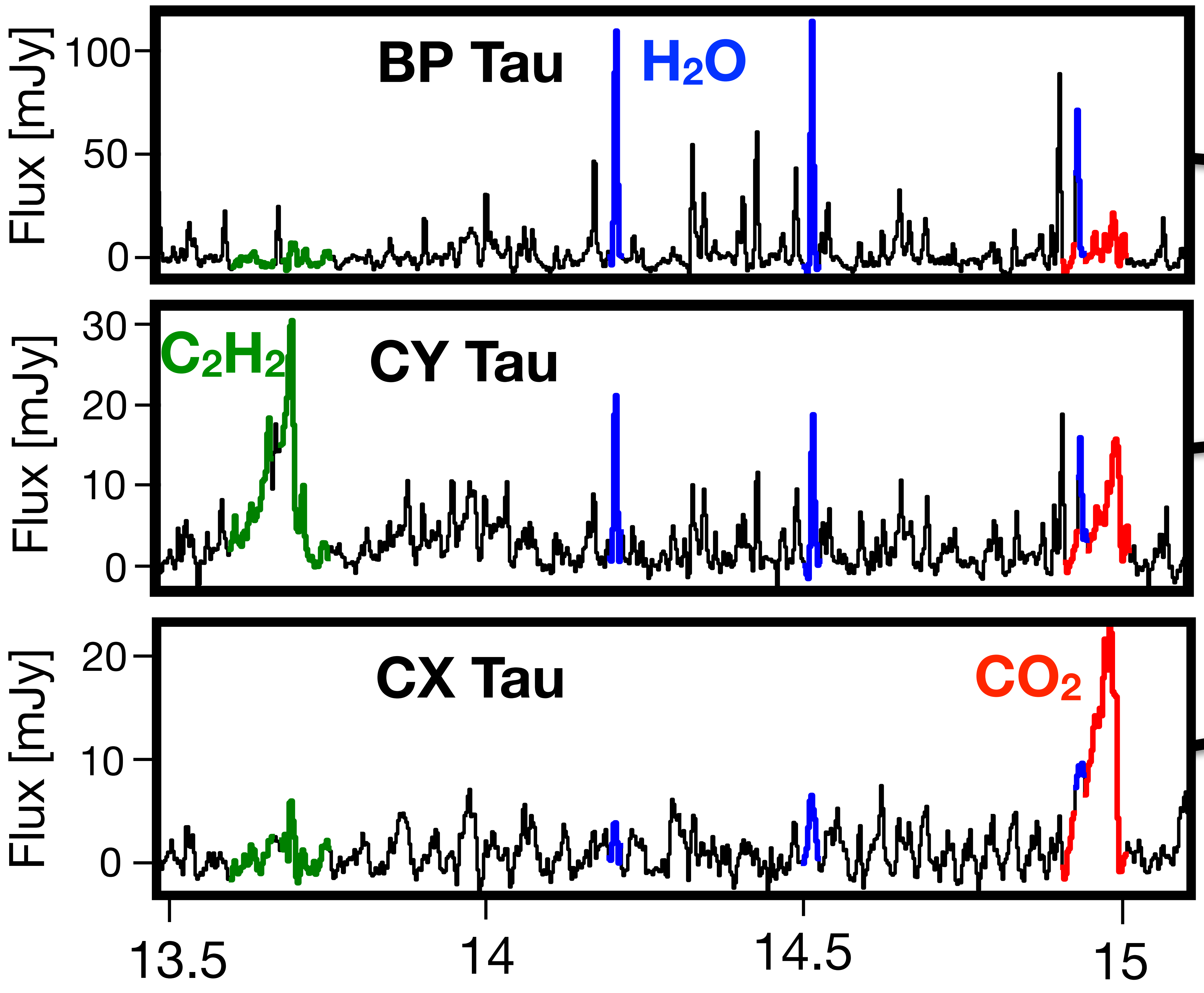


Schematic representation of a protoplanetary disk adapted from Kamp et al. 2023.

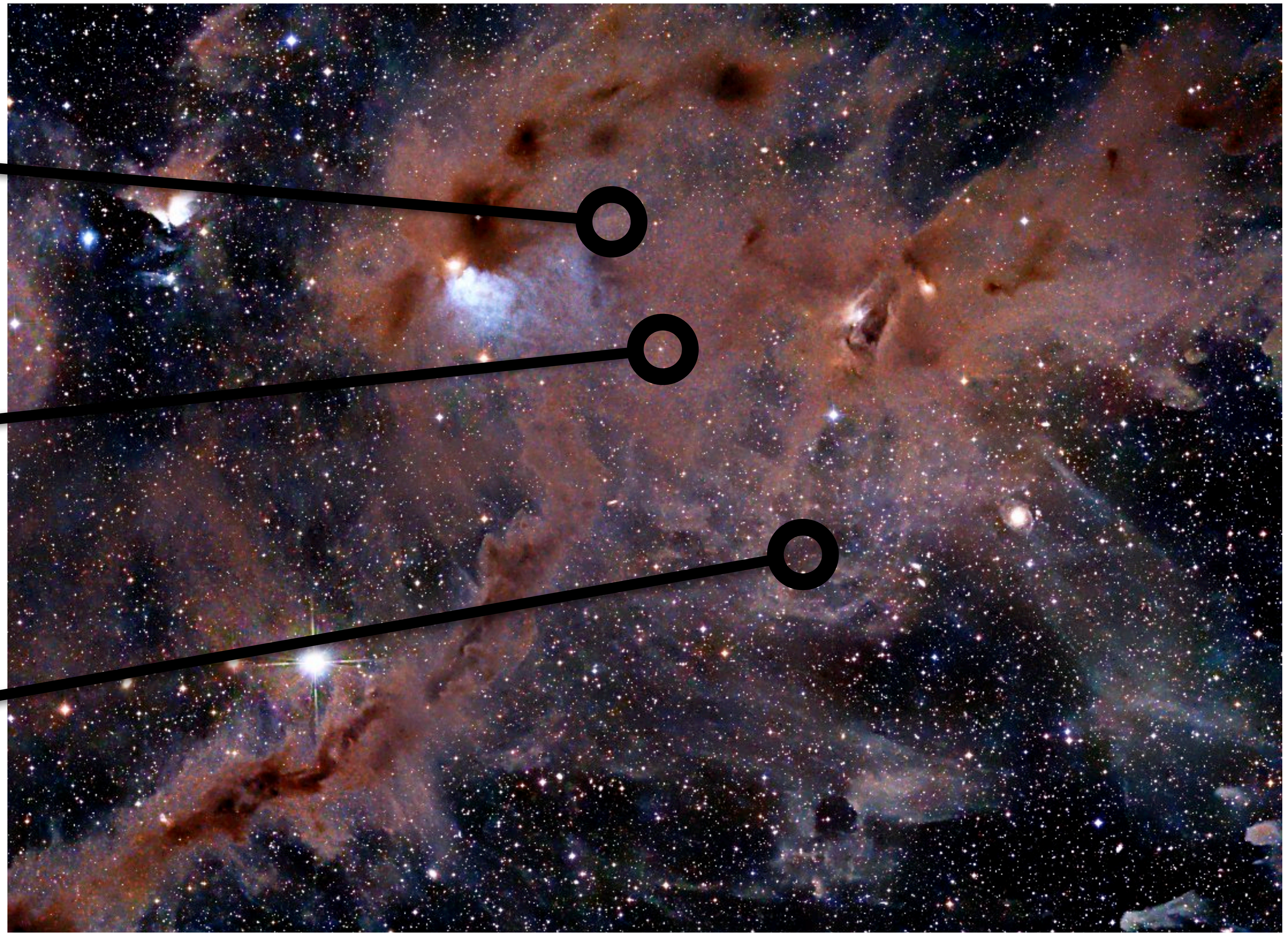
Context

- H_2O, C_2H_2, HCN, OH, CO_2, CO widely detected
- Diversity of JWST spectra of inner disks → Diversity of exoplanet atmospheres ?

JWST spectra of disks around 0.4 $M_\odot$ stars

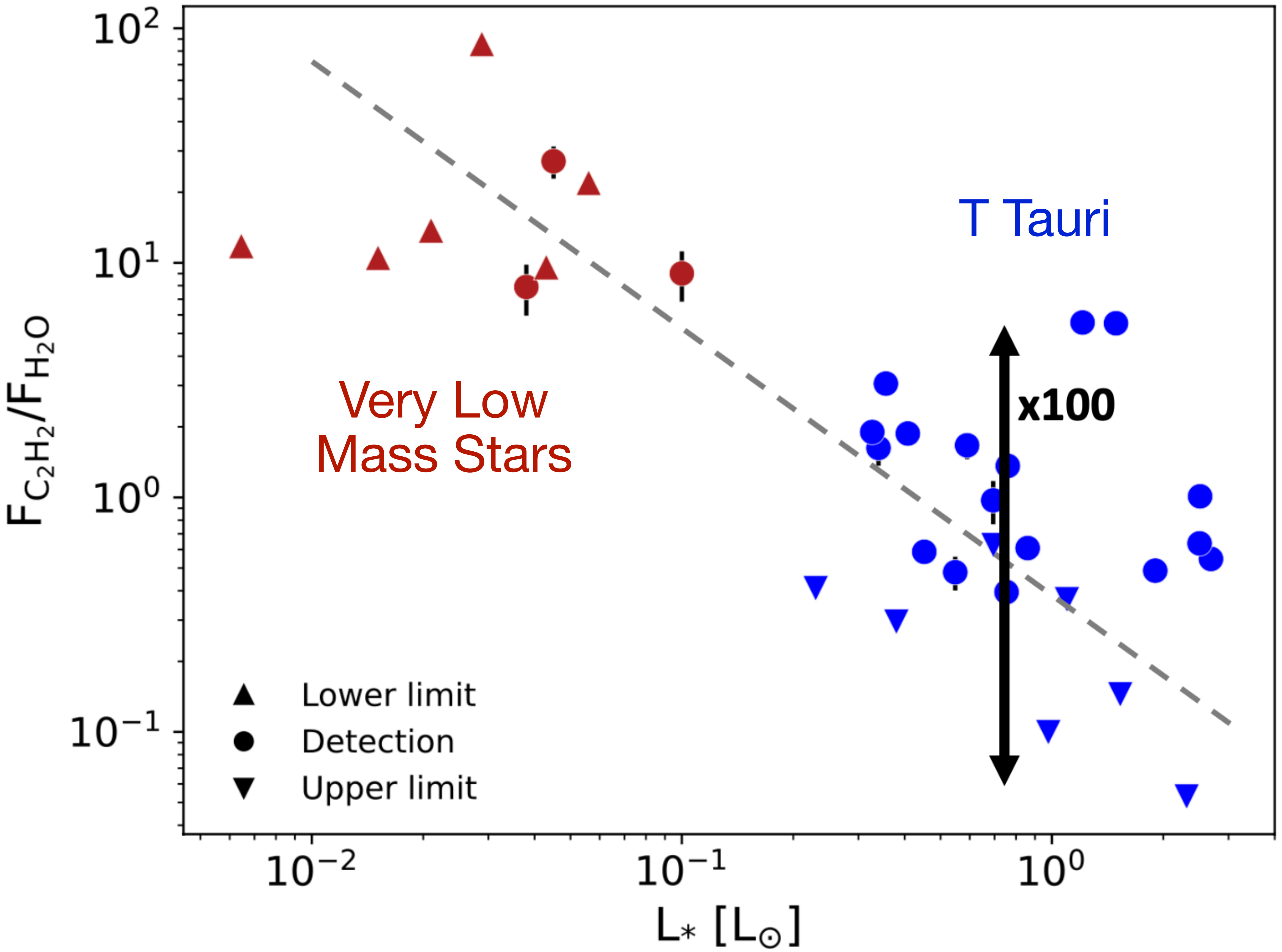


The Taurus molecular cloud



MINDS sources

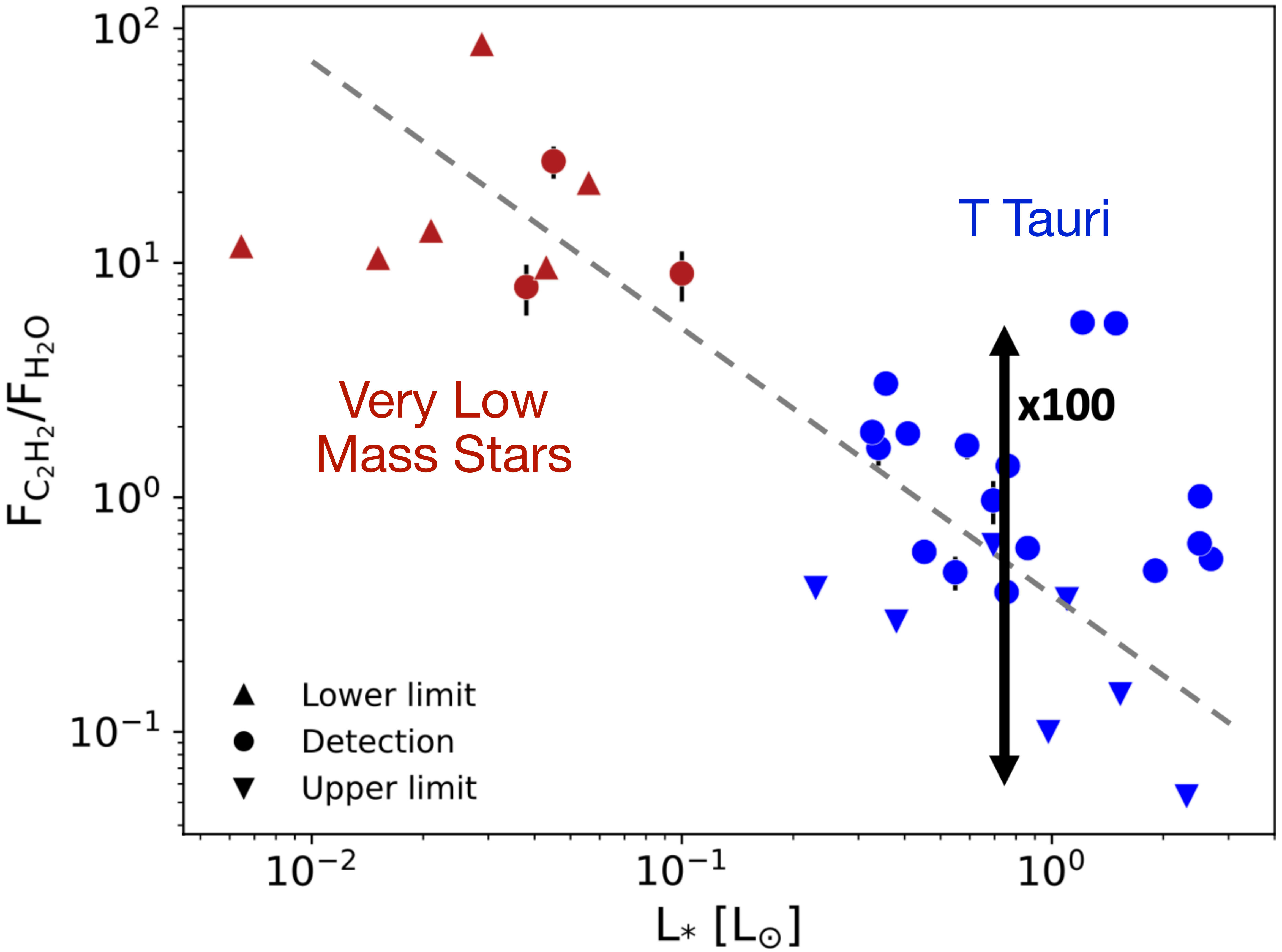
The diversity of C_2H_2 and H_2O emission



JWST spectra of disks (MINDS), Grant et al. subm.

- Strong correlation between H_2O and C_2H_2 emission with the stellar mass
- Large dispersion of $F_{C_2H_2}/F_{H_2O}$ for T Tauri stars

The diversity of C_2H_2 and H_2O emission



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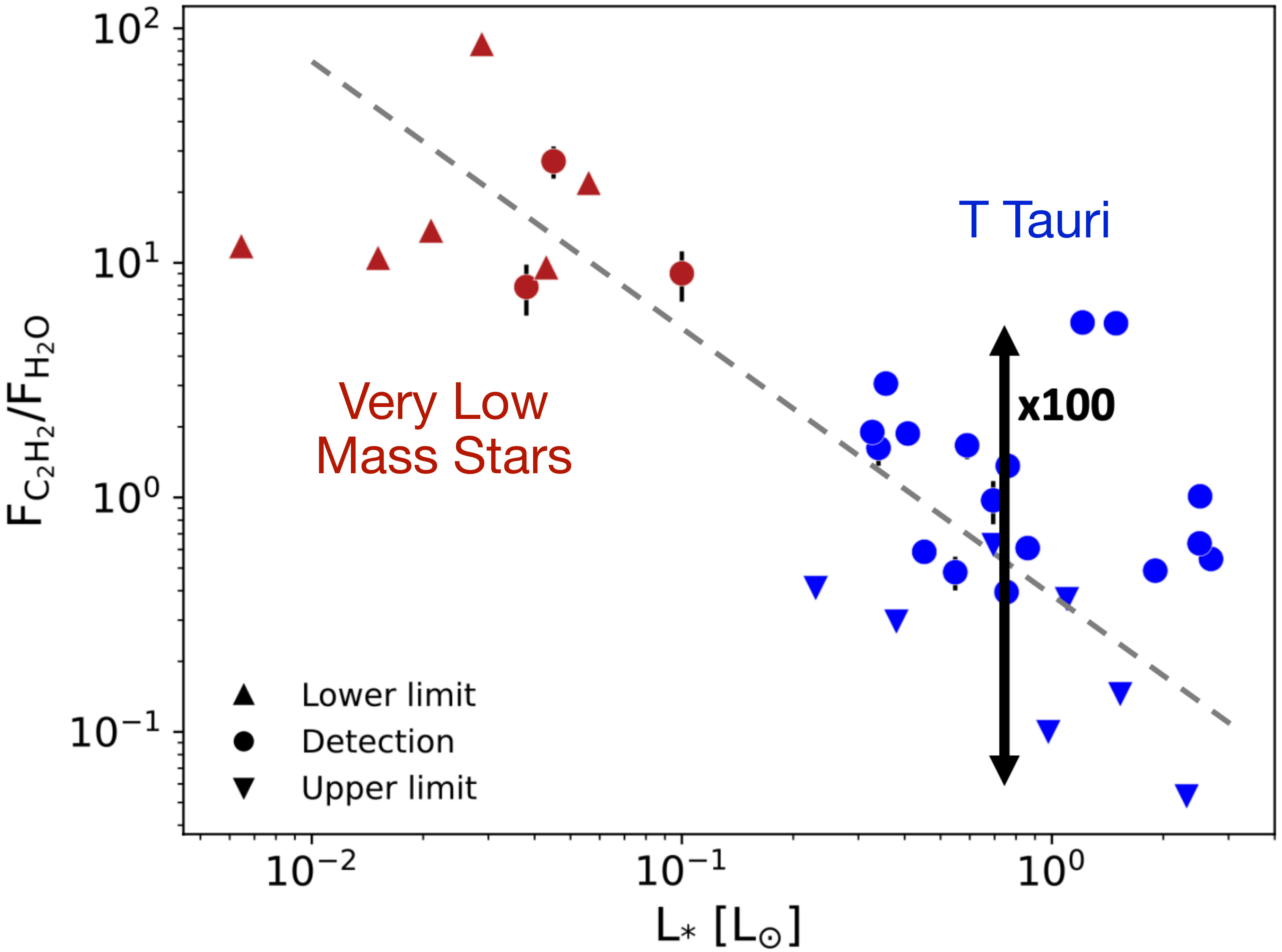
Where does that diversity come from ?

What drives the emission of C_2H_2 and H_2O in T Tauri disks ?

Does the ratio $F_{C_2H_2}/F_{H_2O}$ trace the C/O ratio in the inner disk ?

The diversity of C_2H_2 and H_2O emission



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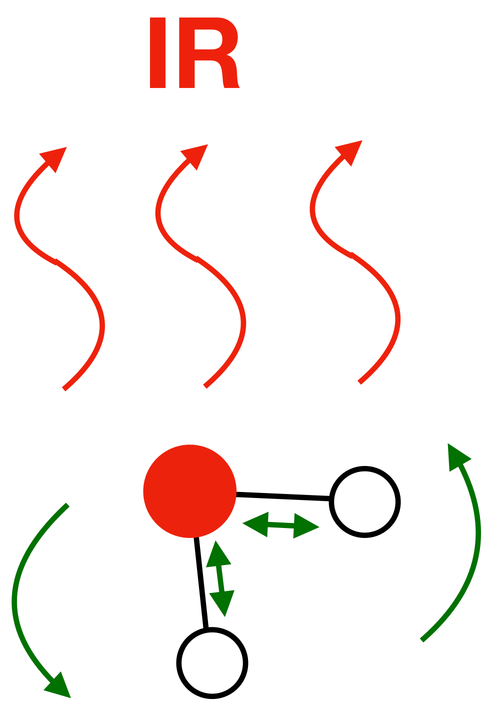
Does the ratio $F_{C_2H_2}/F_{H_2O}$ trace the C/O ratio in the inner disk ?

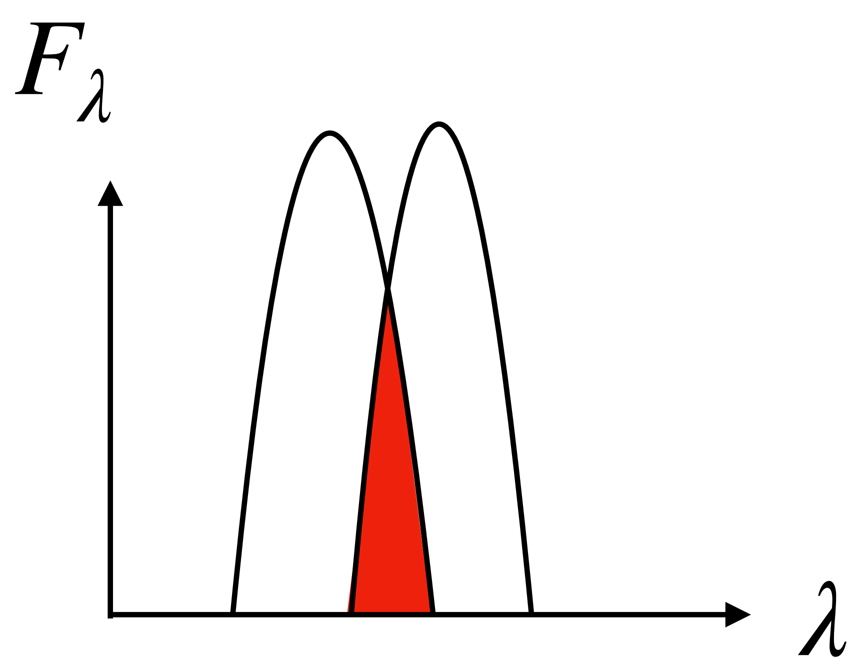
→ **We need thermo-chemical models**

Thermochemical models for inner disks

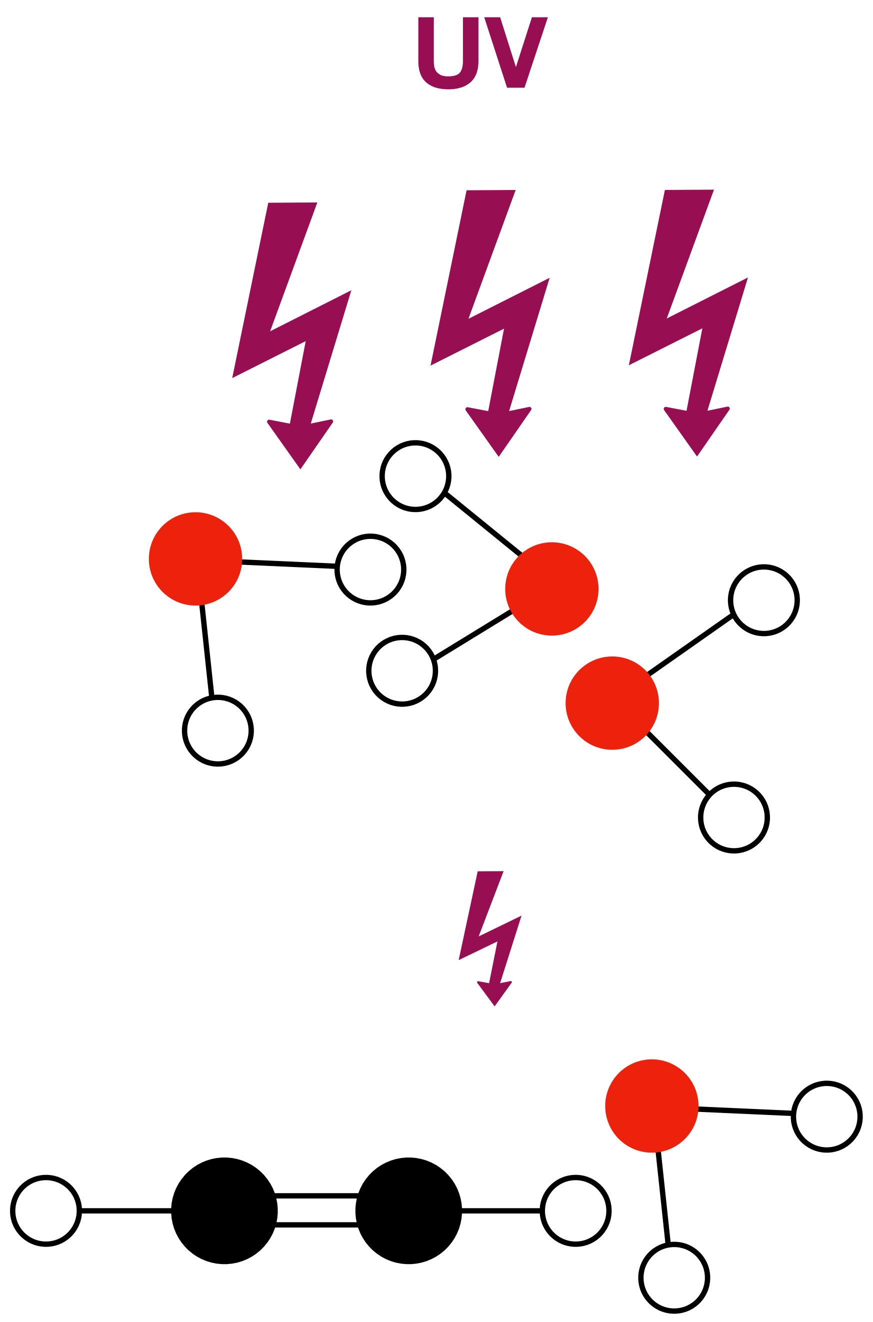
- Using the thermo-chemical model DALI (**D**ust **A**nd **Li**nes) *(Bruderer+2012, Bruderer2013)*
- Self-consistent solution : $T_{gas} \longleftrightarrow$ chemistry, according to a chemical network
- New processes added for inner disks: ro-vibrational cooling, line overlap, UV shielding; and new chemical network



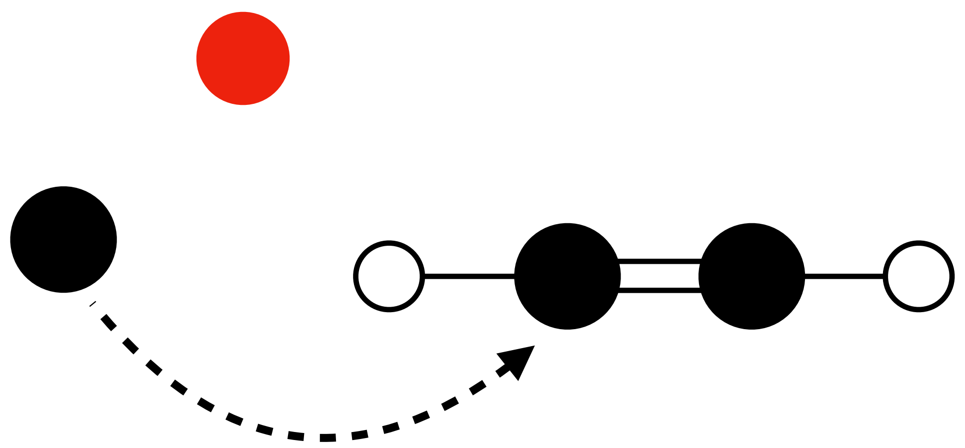
Ro-vibrational cooling



Line overlap



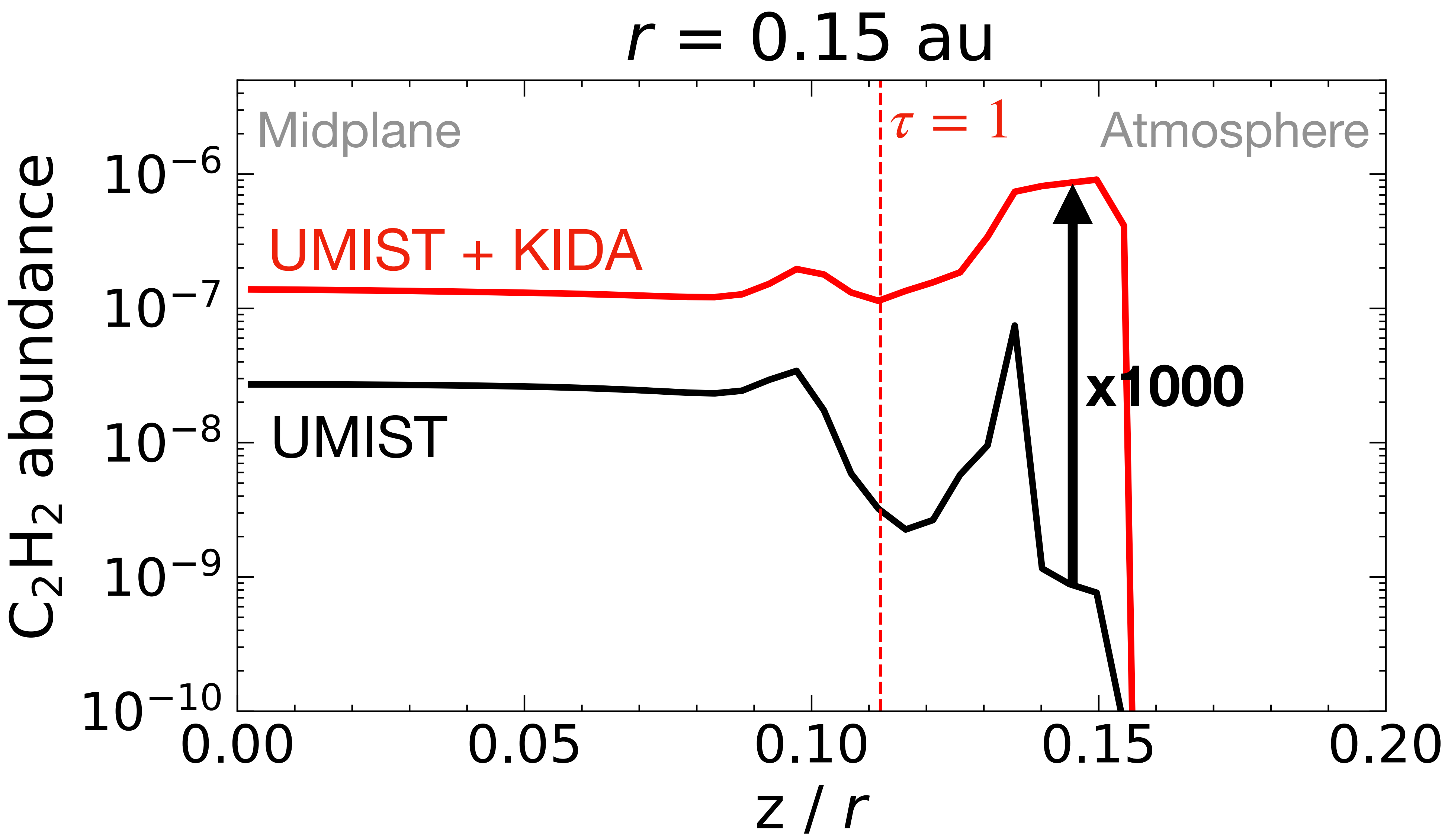
UV shielding

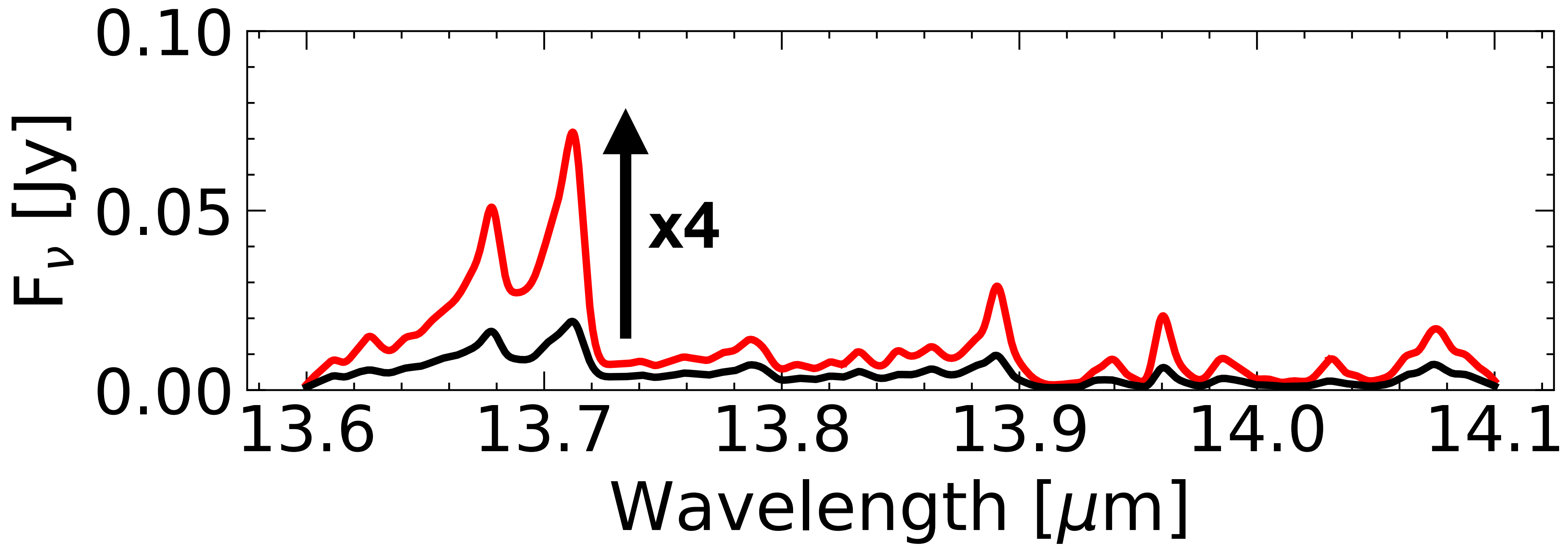


Chemical networks

UMIST vs UMIST + KIDA

- Reactions in KIDA, dramatically increases the abundance of C_2H_2 due to reactions with high activation barrier (not in UMIST)
- **Combining databases for inner disks is better to allow multiple formation and destruction pathways**





7 reactions are responsible for this 3 orders of magnitude difference:

$$C_2 + H_2 \rightarrow C_2H + H \;^{(1),(3)} \qquad E_{barrier} = 1420 \text{ K}$$

$$C_3H + H_2 \rightarrow C_3H_2 + H \;^{(1)} \qquad E_{barrier} = 950 \text{ K}$$

$$H_2CCC + H_2 \rightarrow CH_2CCH + H \;^{(1)} \qquad E_{barrier} = 8760 \text{ K}$$

$$C_4 + H_2 \rightarrow C_4H + H \;^{(1)} \qquad E_{barrier} = 1420 \text{ K}$$

$$C_4H + H_2 \rightarrow C_4H_2 + H \;^{(1)} \qquad E_{barrier} = 950 \text{ K}$$

$$N + CH_2CCH \rightarrow C_2H_2 + HCN \;^{(2)}$$

$$C_4H_3^+ + e^- \rightarrow C_2H_2 + C_2H \;^{(2)}$$

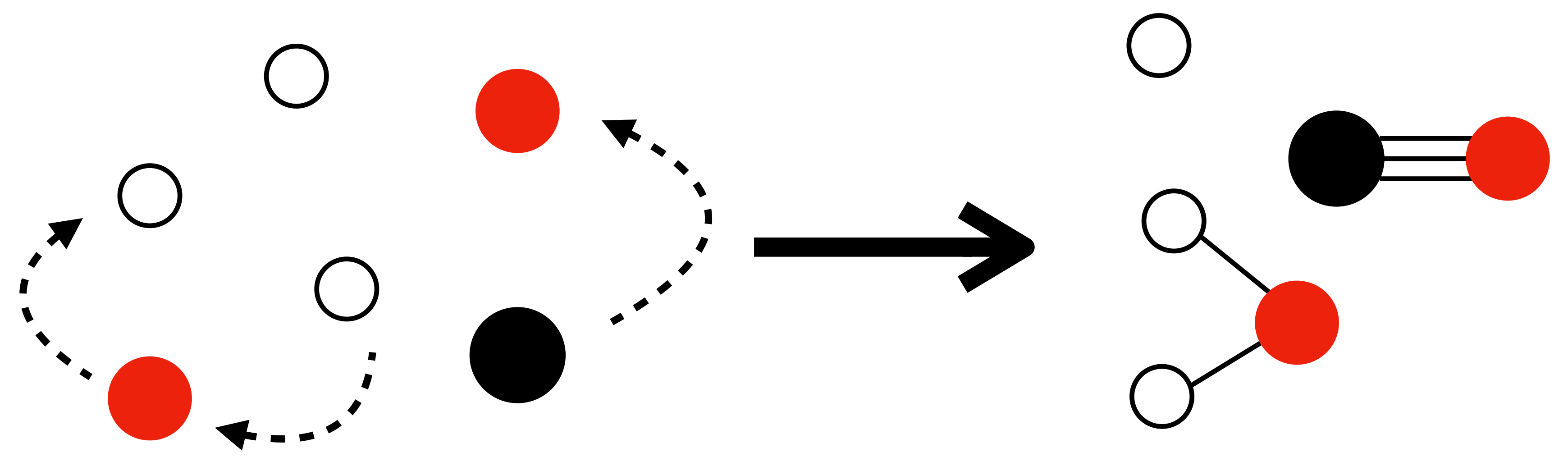
(1) Harada et al. 2010

(2) Loison et al. 2017

(3) Pitts et al. 1982

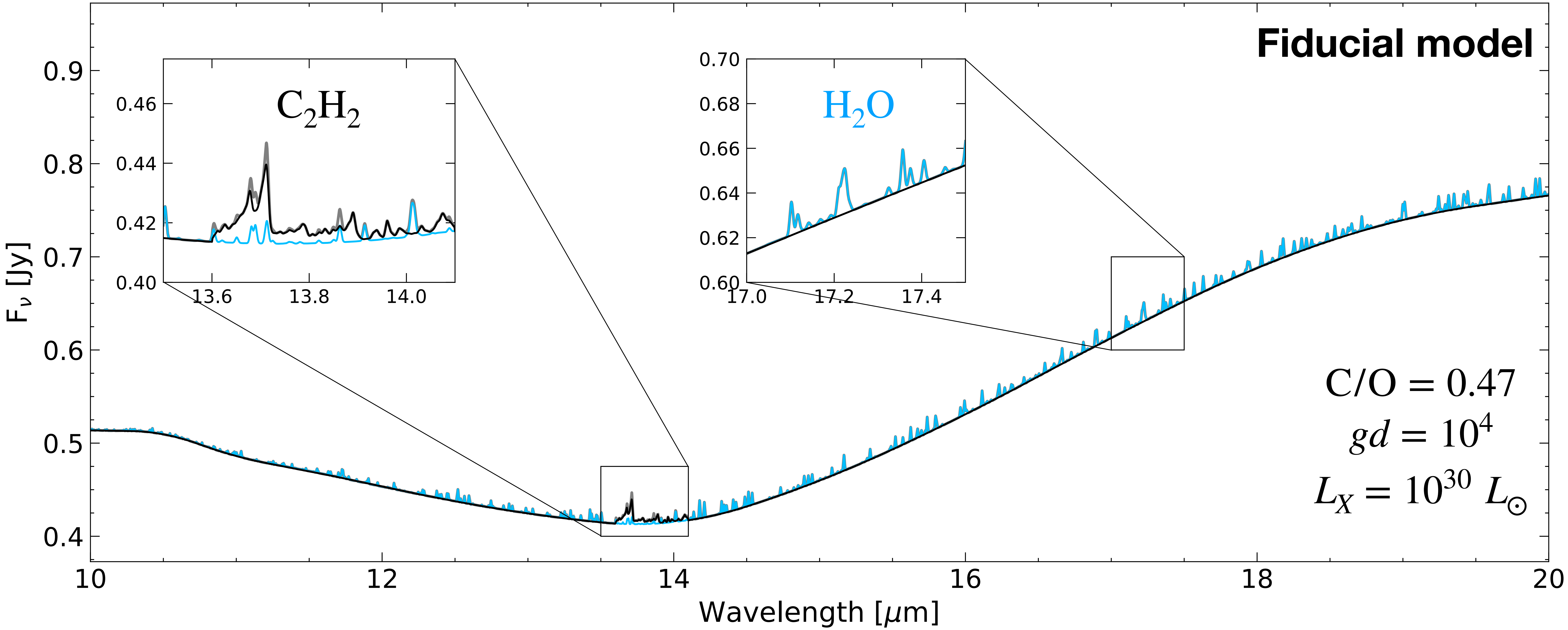
Carbon and Oxygen in T Tauri disks

- With a solar C/O (~0.45)
  - All carbon into CO
  - Excess of oxygen into H_2O



Brigthness of C_2H_2 in inner T Tauri disks

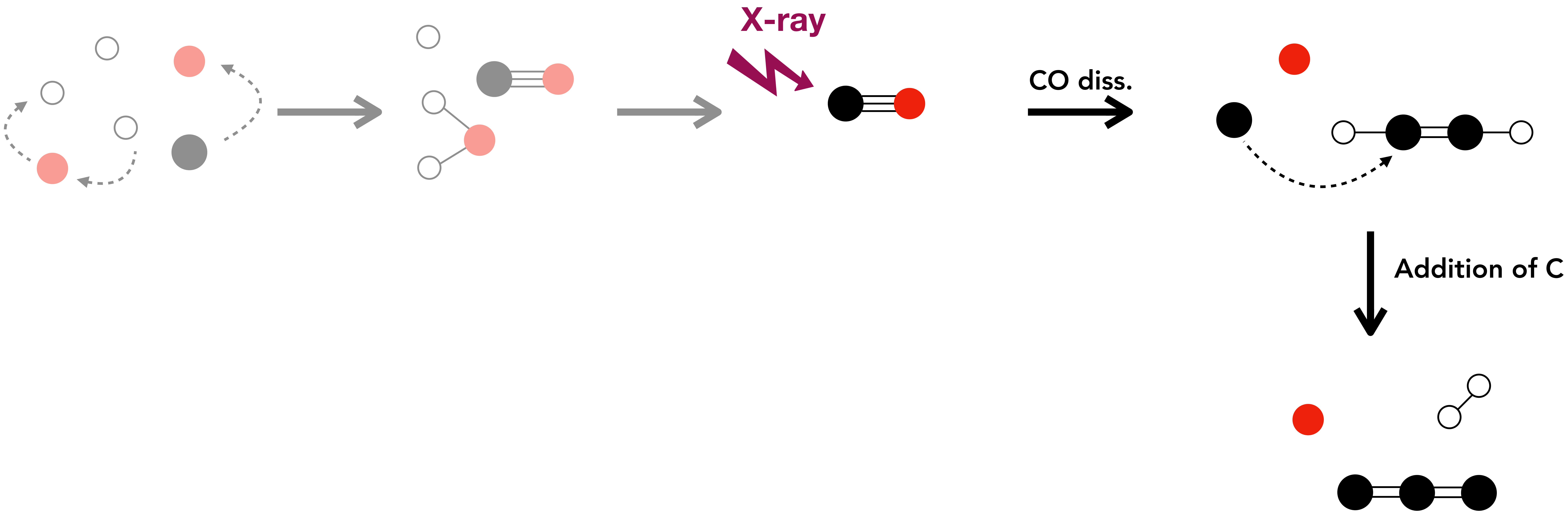
- Water creates a forest of rotational lines in the MIR
- The C_2H_2 feature at 13.7 um is bright, even with a solar C/O



DALI synthetic spectrum of the fiducial model.

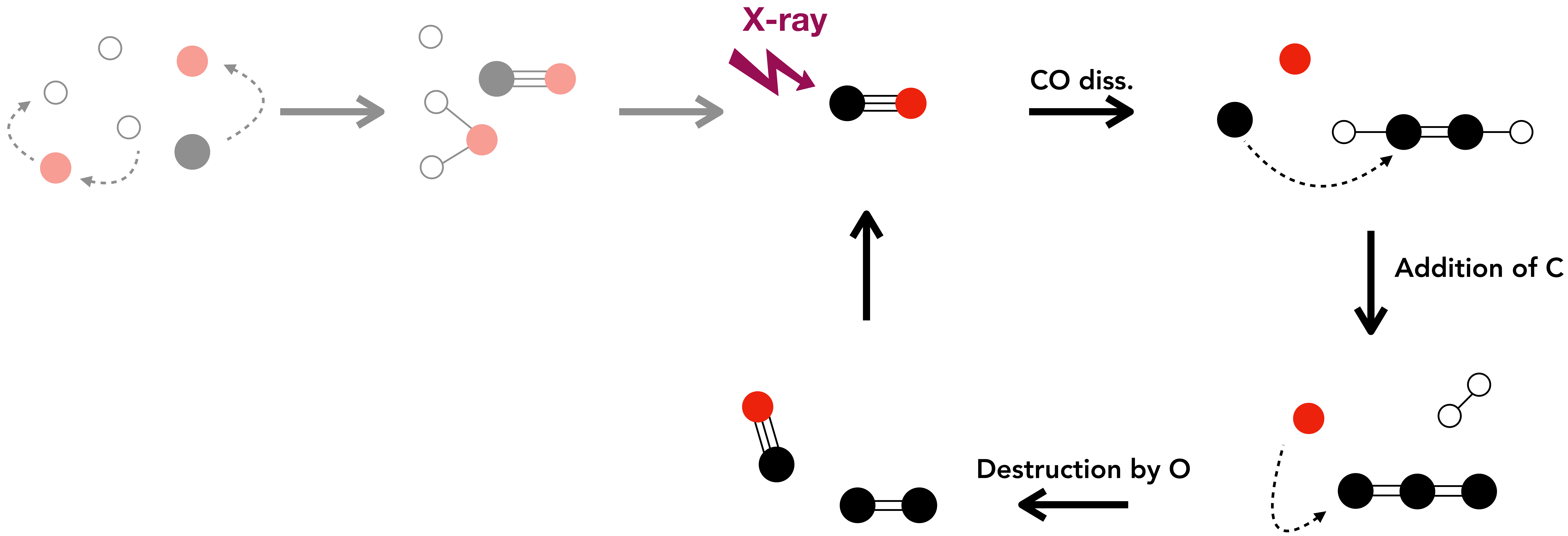
Where does the carbon come from ?

→ Dissociation of CO releases free carbon available for hydrocarbons



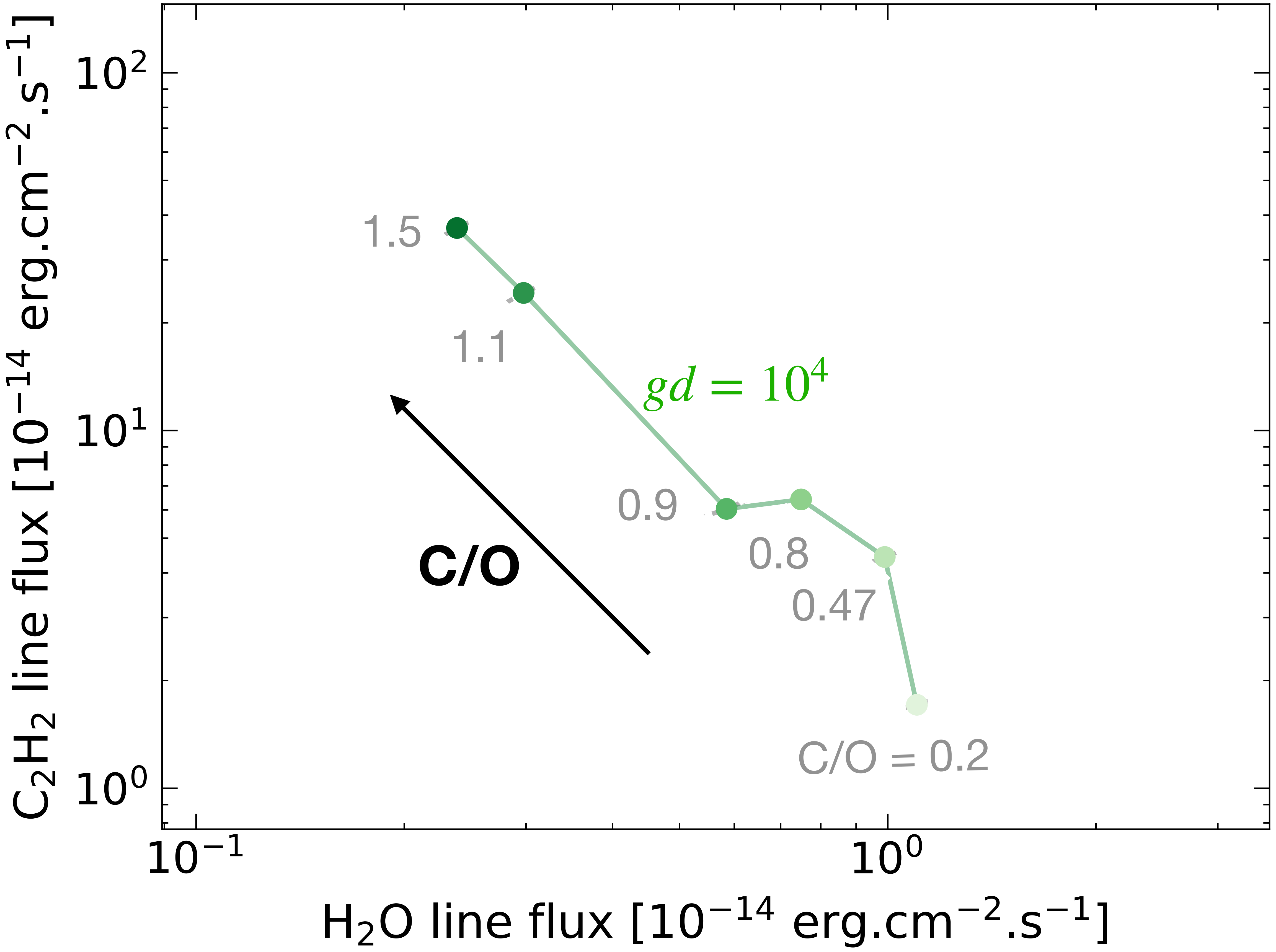
How are carbon chains destroyed ?

- Oxygen attacks carbon chains and form CO again
- **Missing reactions with O or OH : strongly impacts hydrocarbons**



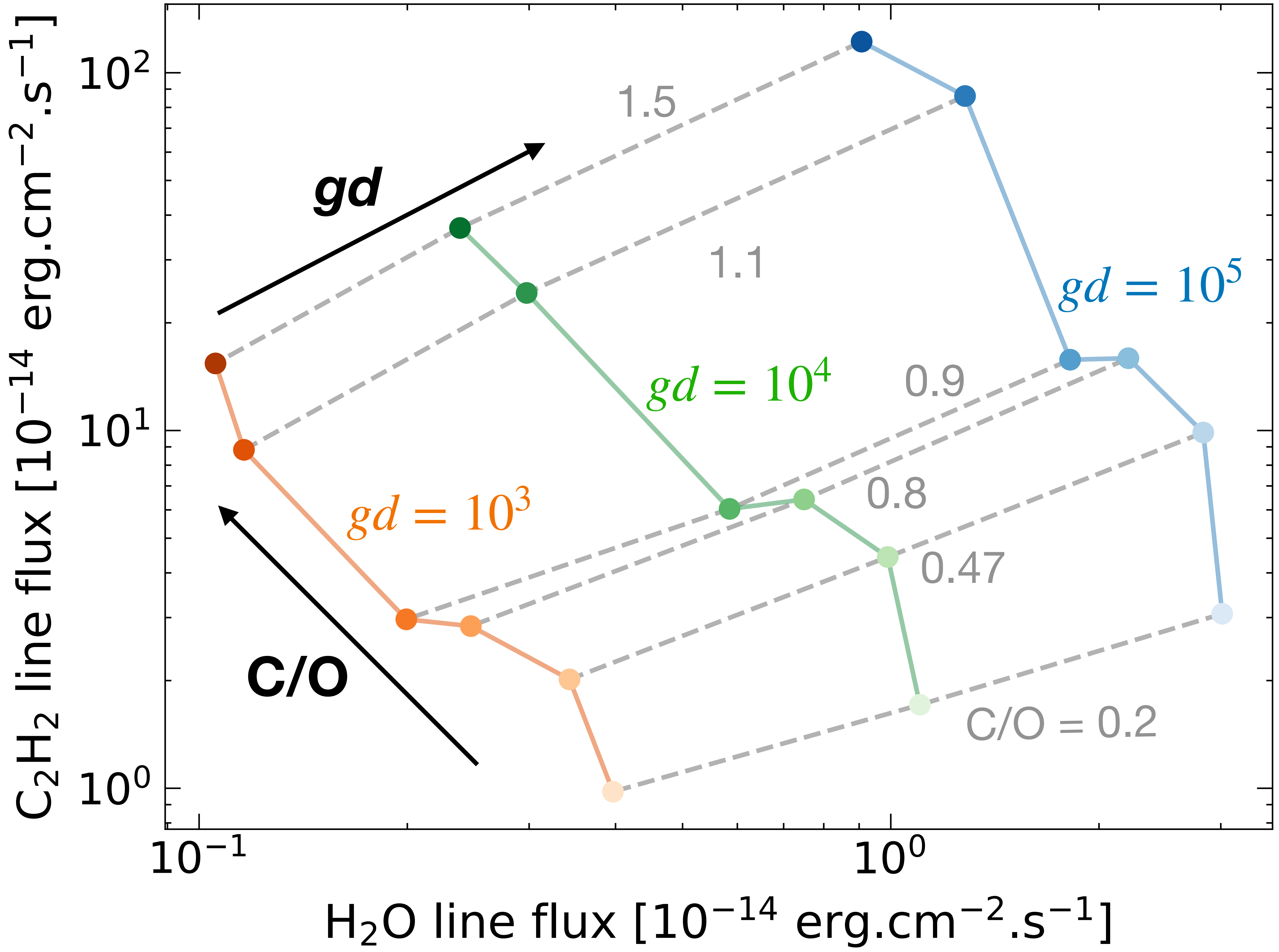
C/O ratio

- Significant difference of C_2H_2 emission with the C/O ratio, less significant for water
- Jump at C/O > 1 : free carbon available to built hydrocarbons!

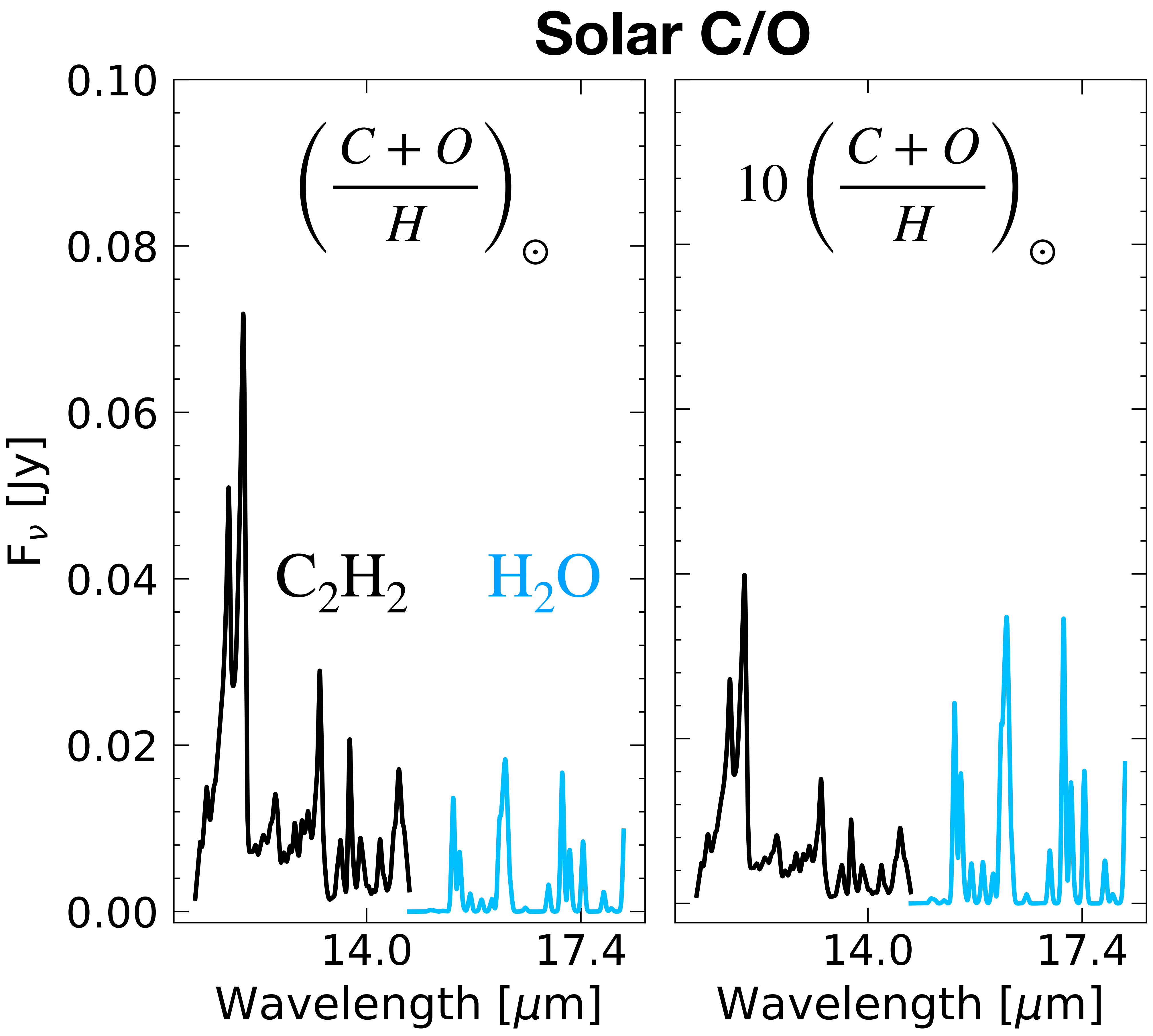


C/O ratio and gas-to-dust ratio

- Significant difference of C_2H_2 emission with the C/O ratio, less significant for water
- Jump at C/O > 1 : free carbon available to built hydrocarbons!
- The gd also strongly impacts molecular features, particularly water



Metallicity

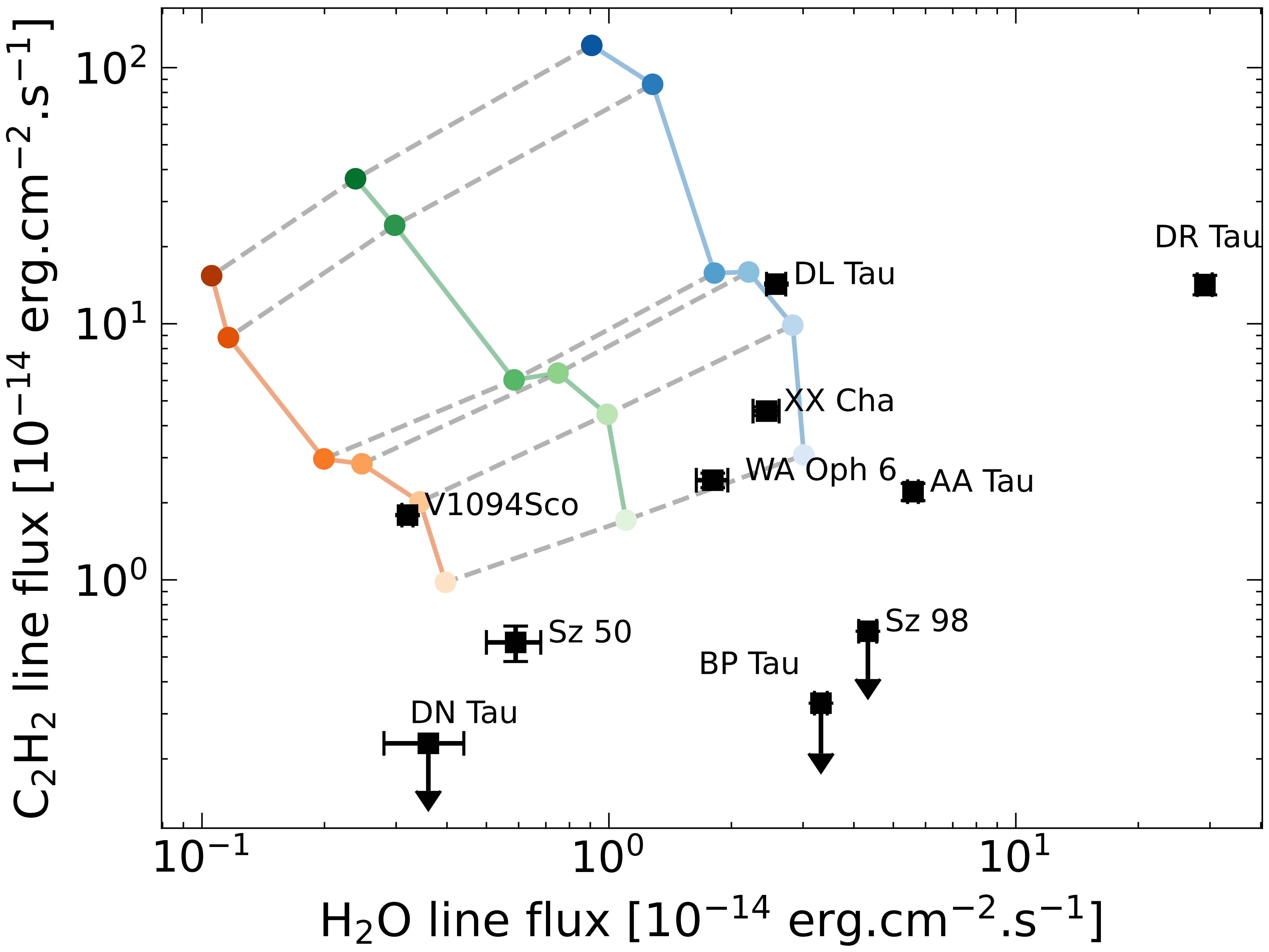


→ The amount of Oxygen and Carbon also influences the shape of the spectrum:

- Carbon-rich spectrum if: - High C/O
  - Low metallicity

JWST observations: non-solar abundances ?

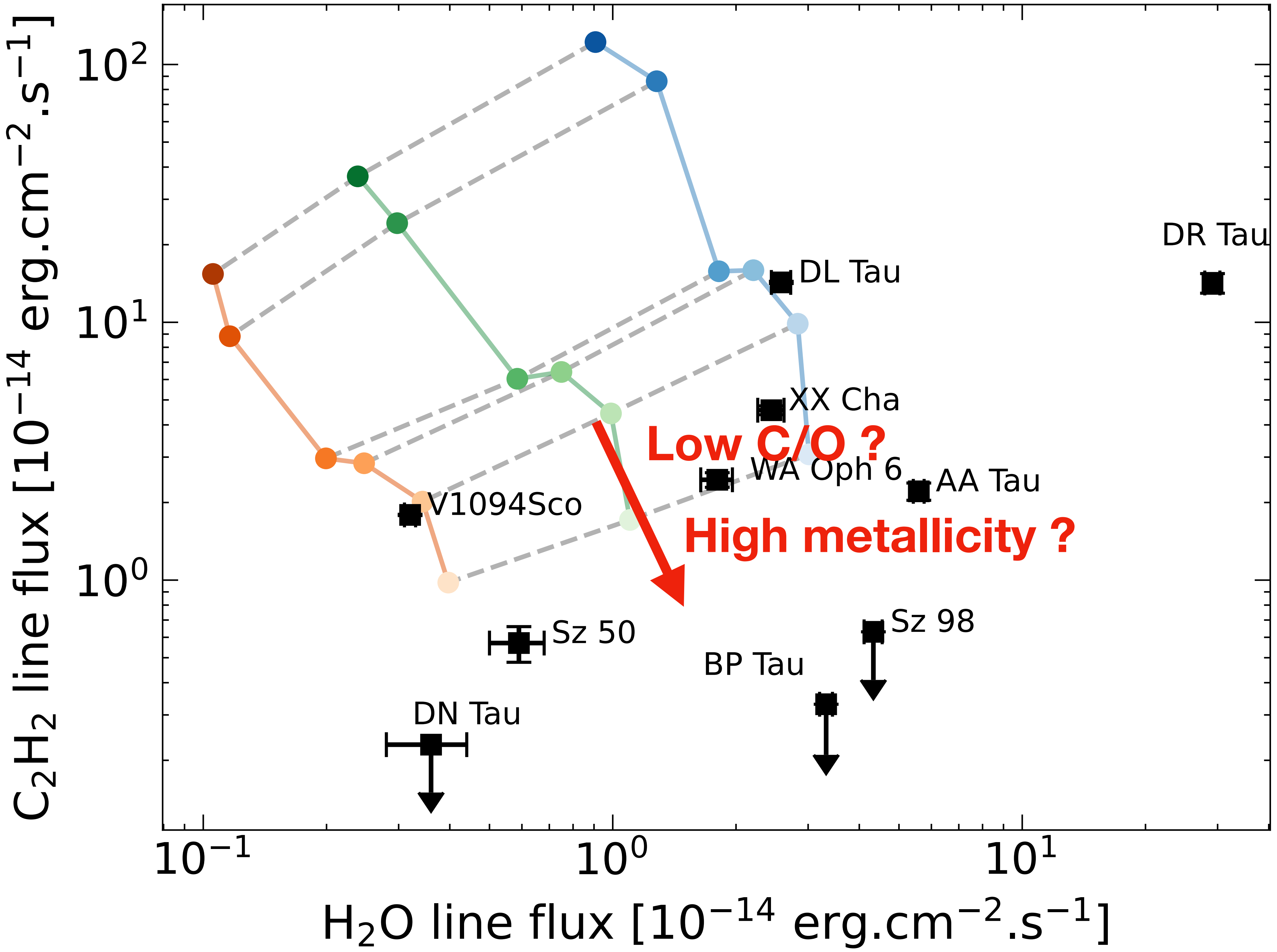
→ Acetylene emission overestimated:



JWST observations: non-solar abundances ?

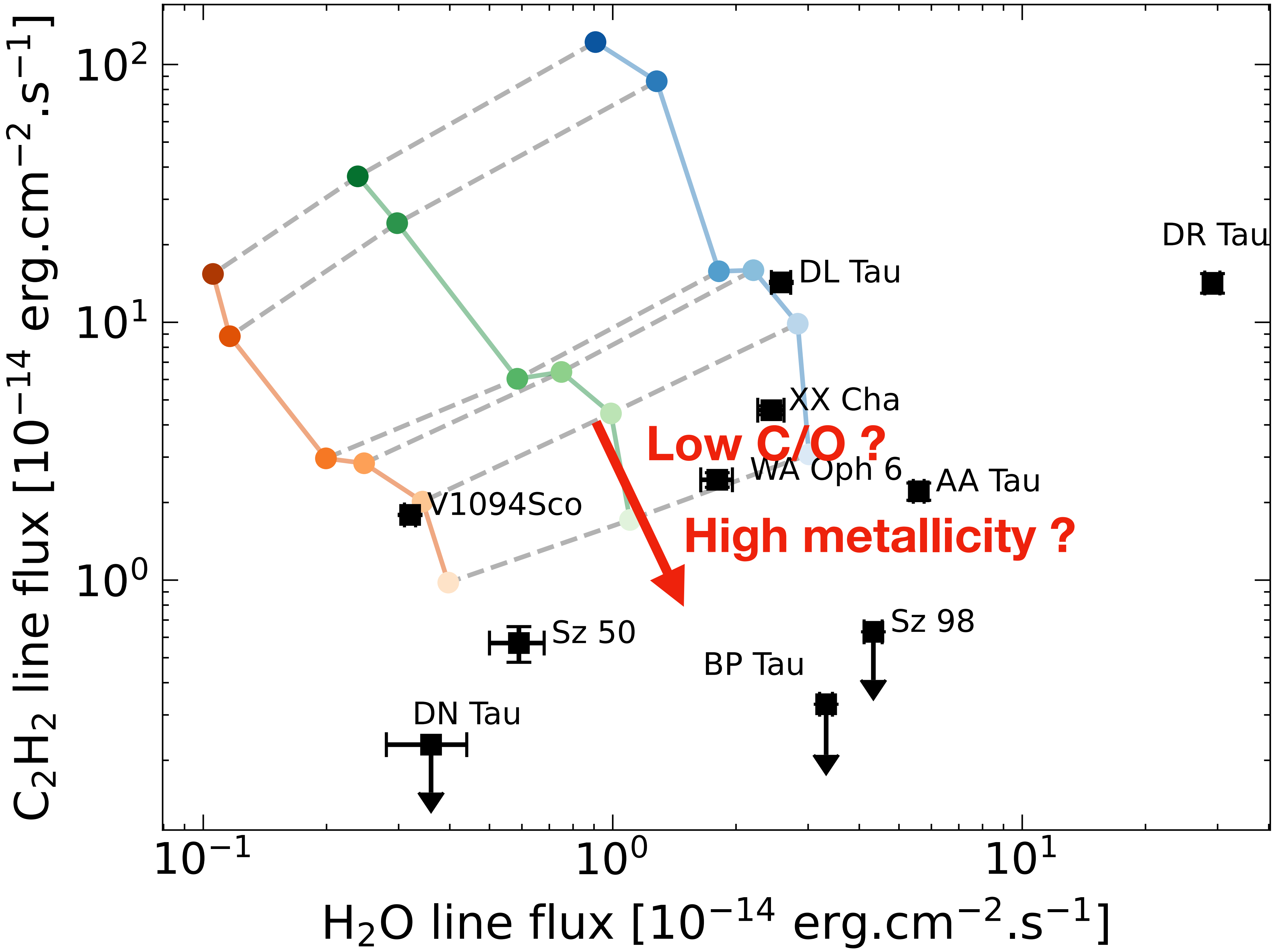
→ Acetylene emission overestimated:

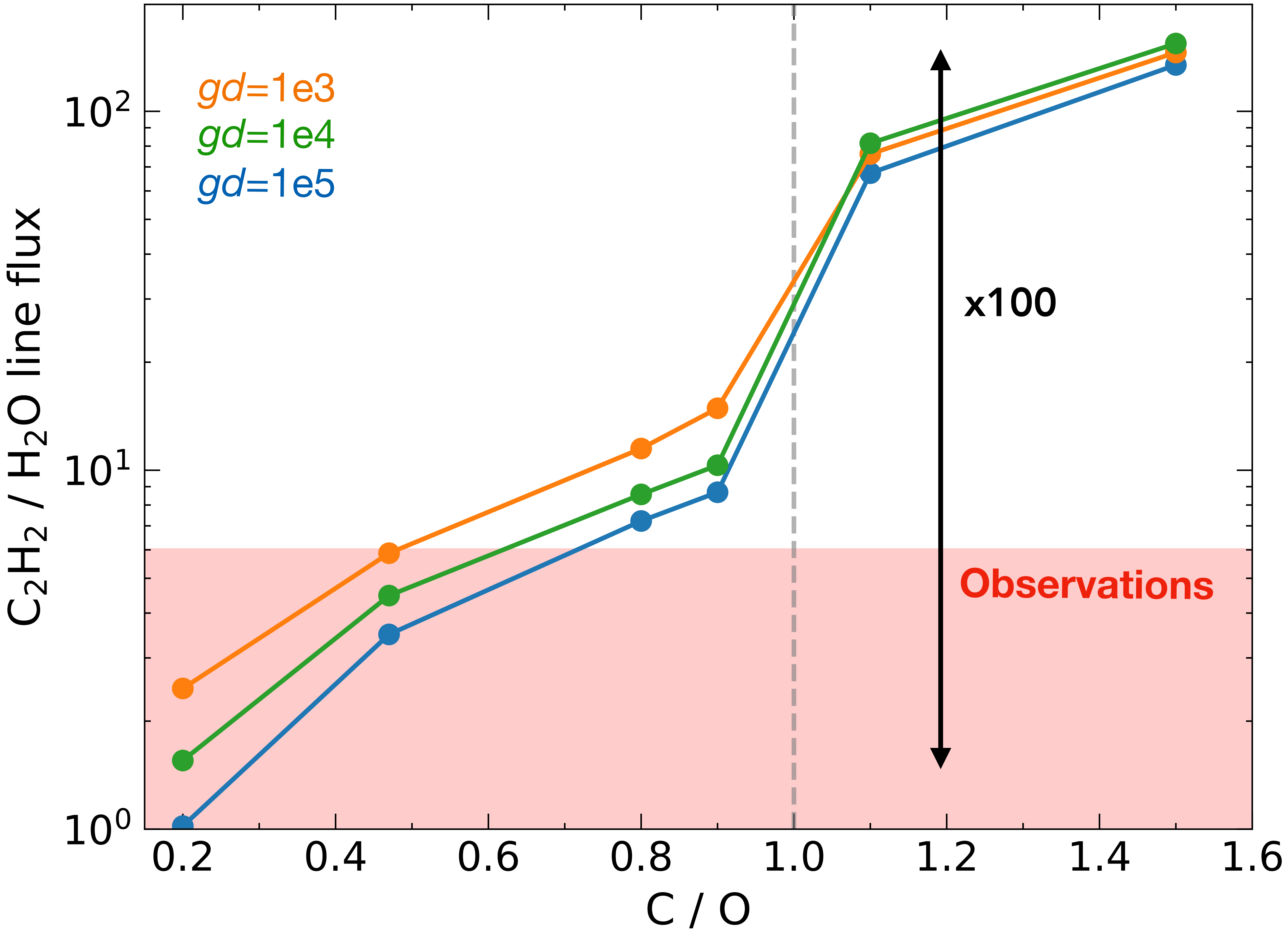
→ T Tauri inner disks either: - low C/O ?
- high metallicity ?



JWST observations: non-solar abundances ?

- Acetylene emission overestimated:
  - T Tauri inner disks either: - low C/O ?
    - high metallicity ?
- $F_{C_2H_2}/F_{H_2O}$ seems a good tracer of C/O but affected by the gas-to-dust ratio



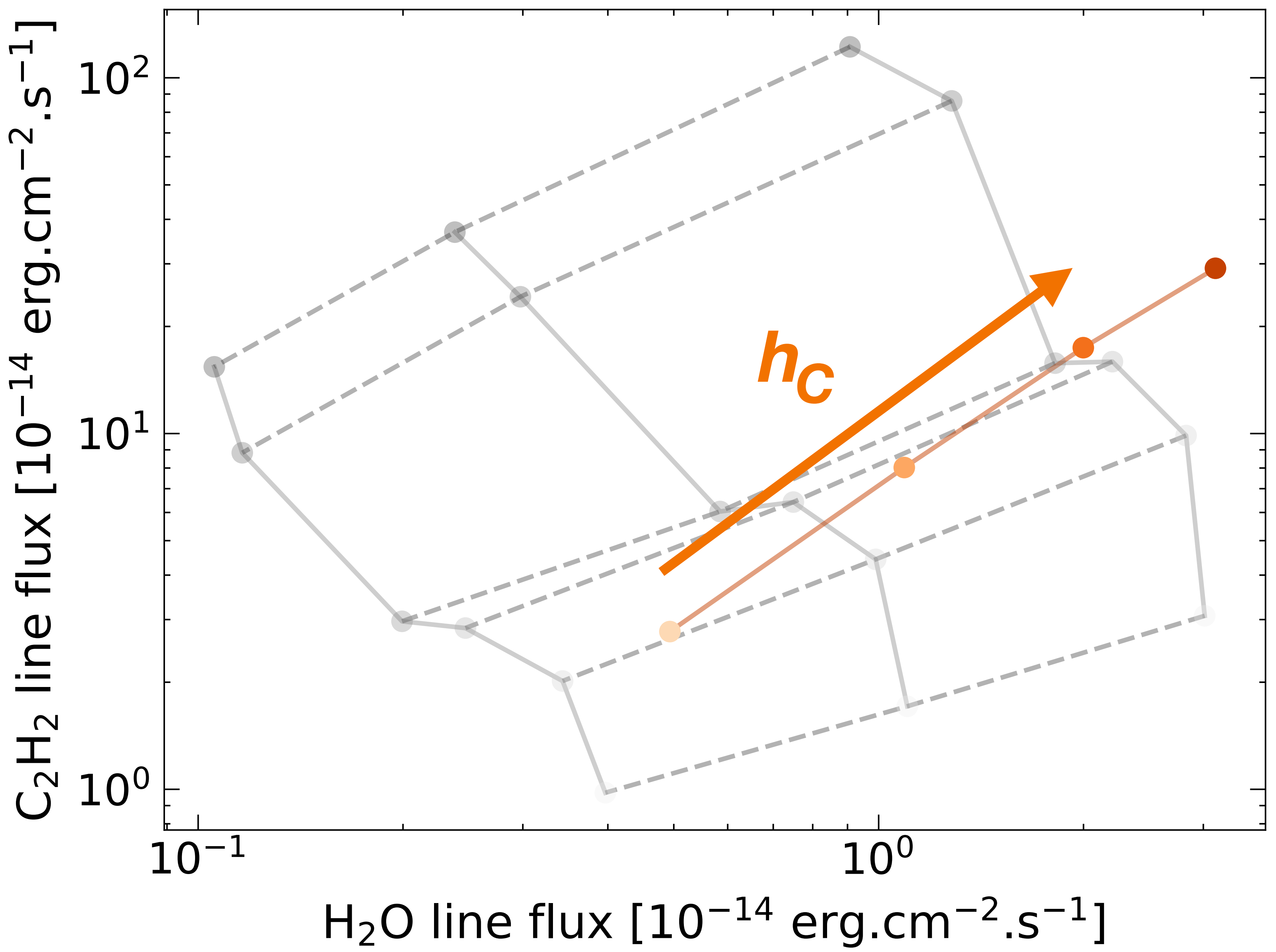


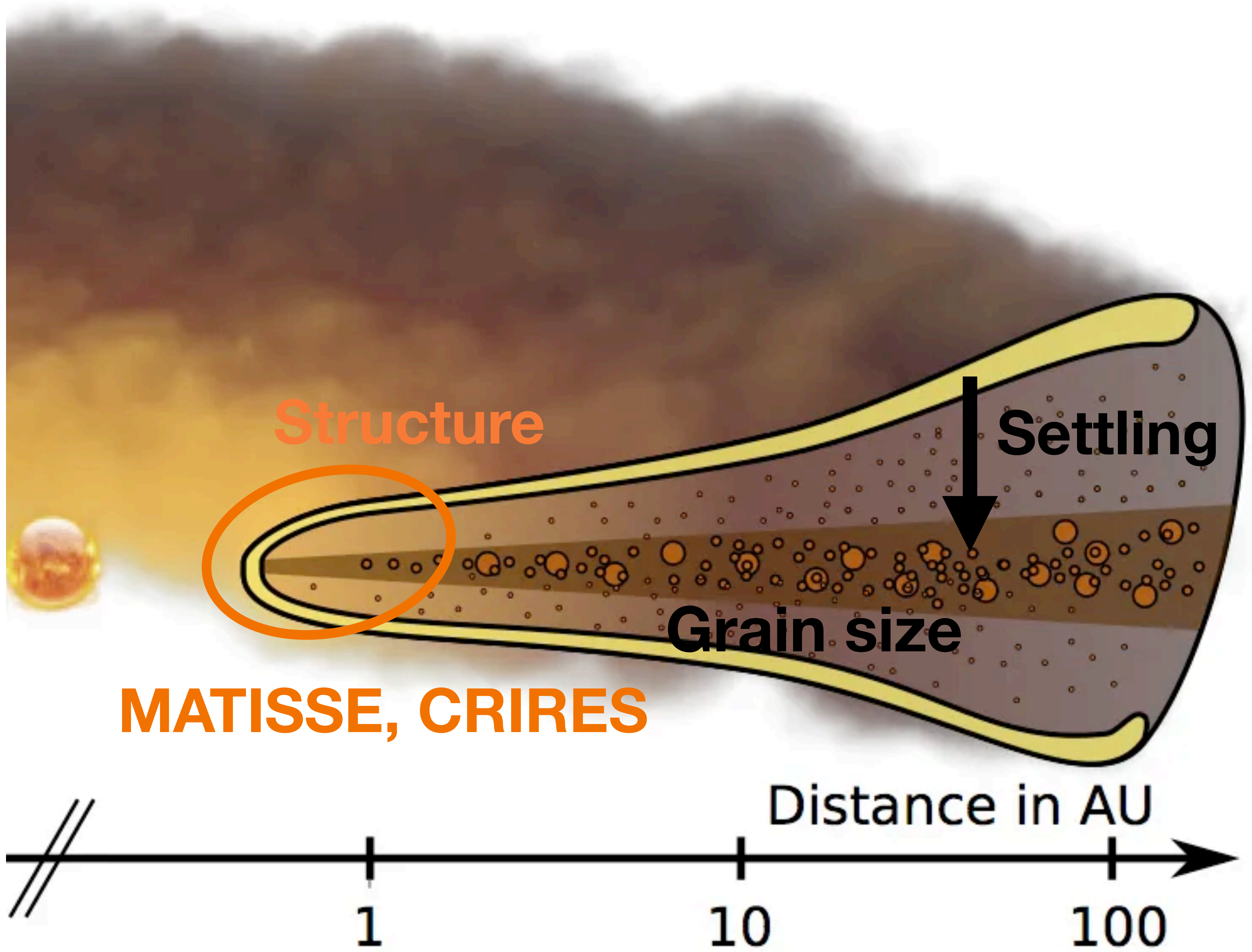
Next steps

→ Need additional constraints on **disk structure** to measure the C/O: VLTI/MATISSE, VLT/CRIRES …

→ Dust is important ! Refine **grain properties** in models: size, settling …

→ Go beyond C_2H_2/H_2O: HCN, CO_2, C_4H_2 ?





Context

→ This work is part of the GTO MIRI MINDS (P.Is: Th. Henning and I. Kamp)

→ ~ 30 collaborators

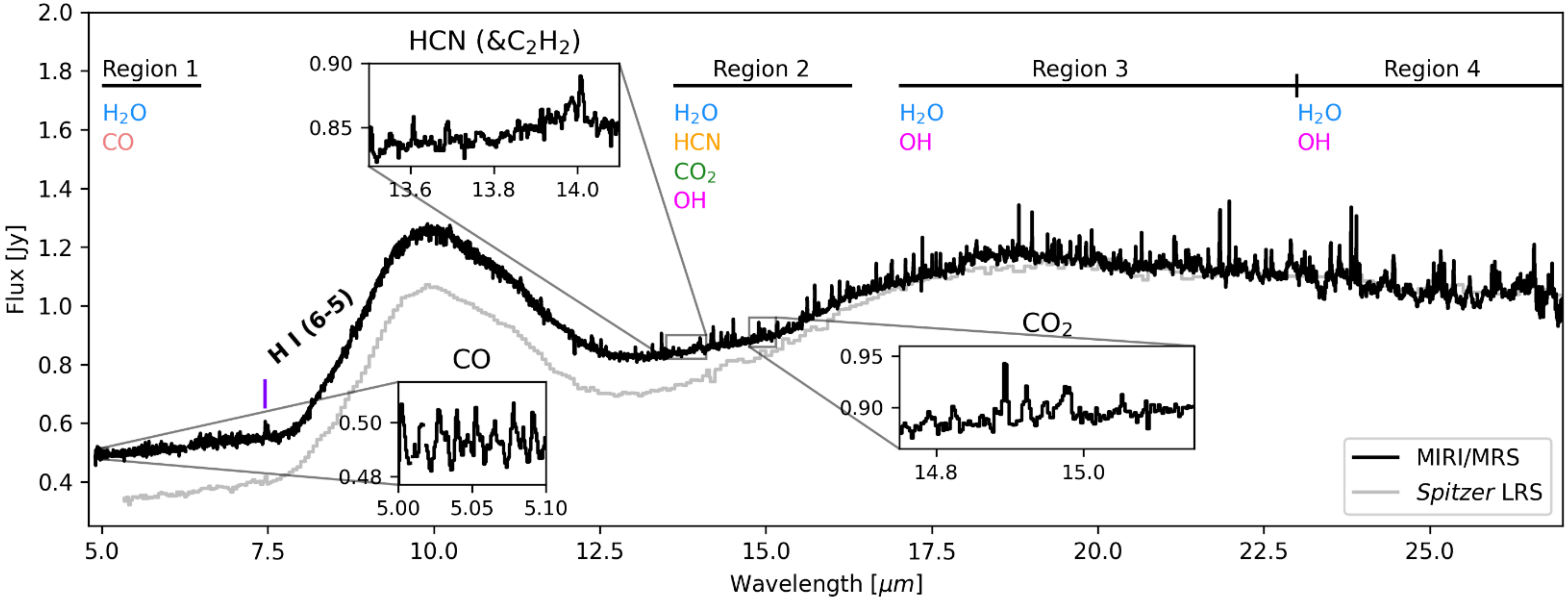
→ ~ 120h JWST observing time

→ 52 disks observed

- 65% TTauri ($0.3 < M < 2M_\odot$)
- 17% Very Low Mass Stars ($M < 0.2M_\odot$)

Context

→ Revolution with JWST: sensitivity and spectral resolution

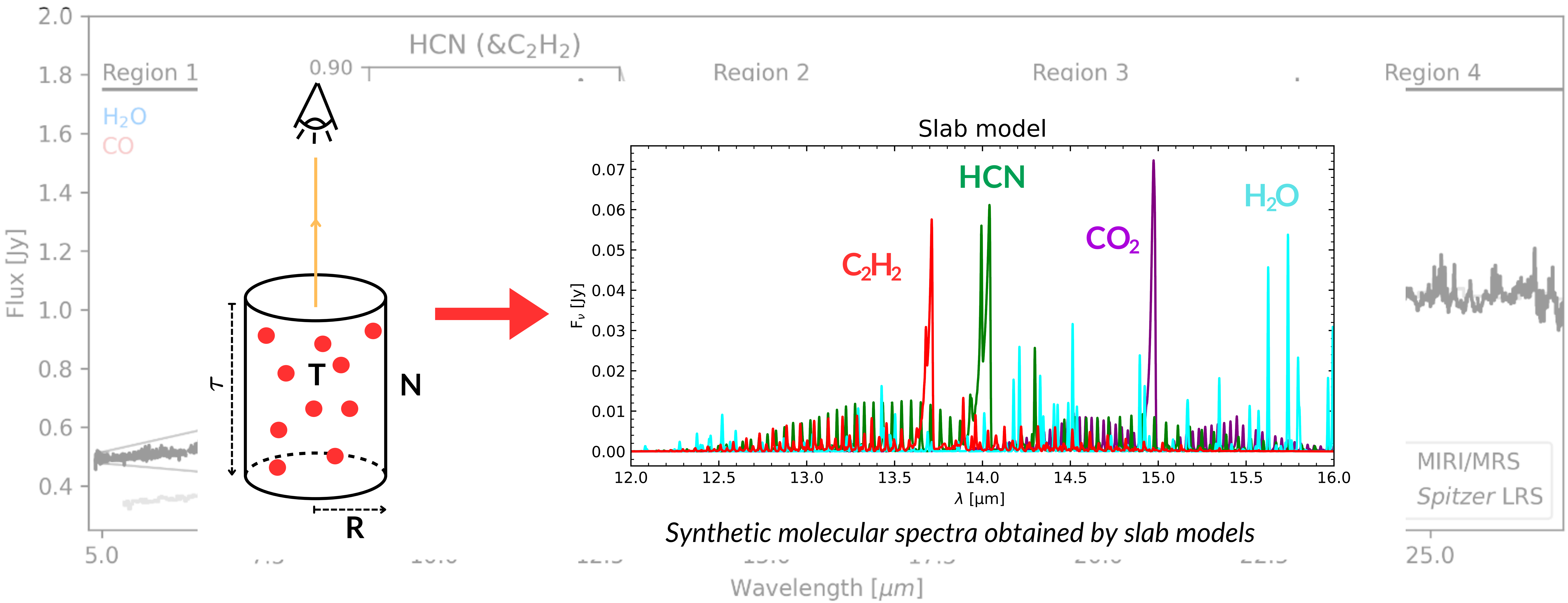


JWST/MIRI spectrum of Sz 98. From Gasman et al. 2023.

Context

→ Revolution with JWST: sensitivity and spectral resolution

→ Slab models retrieval: excitation of the main C, N and O carriers

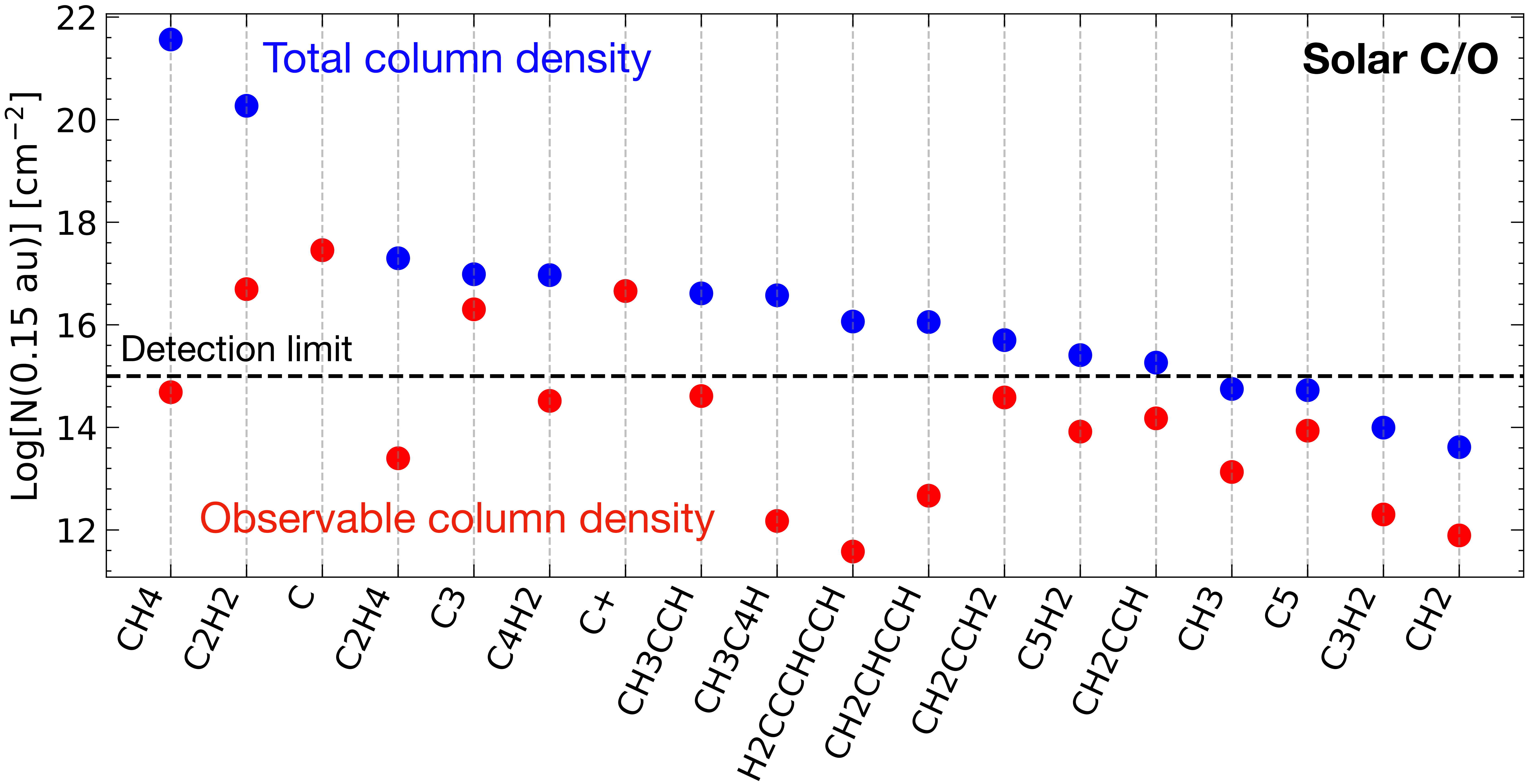


Synthetic molecular spectra obtained by slab models

JWST/MIRI spectrum of Sz 98. From Gasman et al. 2023.

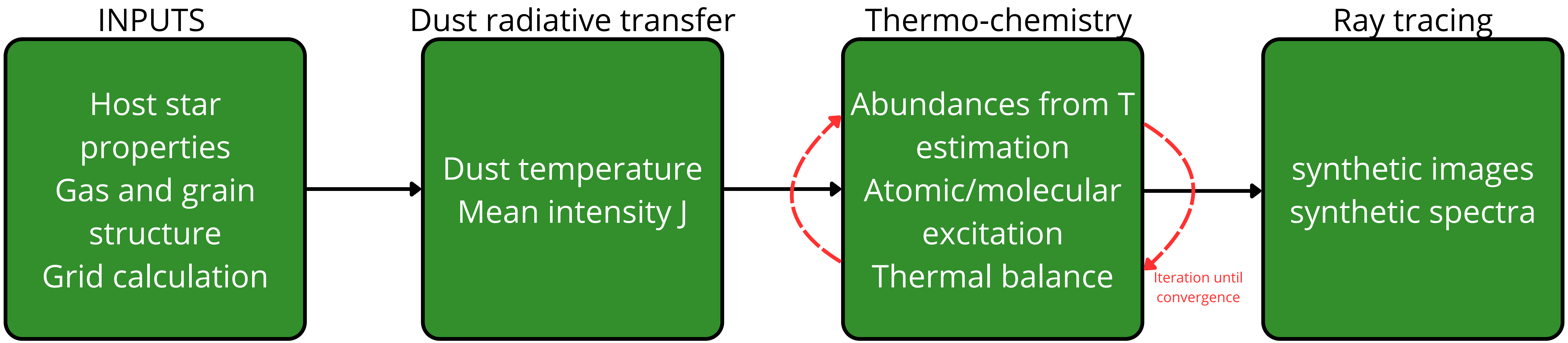
Distribution of hydrocarbons

→ The main hydrocarbon is CH_4 but the brightest is C_2H_2, consistent with JWST observations



DALI

- Using the thermo-chemical model DALI (**D**ust **A**nd **Li**nes) *(Bruderer+2012, Bruderer2013)*
- Self-consistent solution : T_{gas} ⟷ chemistry, according to a chemical network
- New processes added for inner disks: ro-vibrational cooling, line overlap, UV shielding; and new chemical network



New chemical networks : workflow

New chemical networks : workflow

New chemical networks : workflow

Network Miotello+2019 → Add all hydrocarbons with a given number of C → **UMIST database (*Millar+2024*)** → **Final network**

Missing reactions in UMIST !

$$C_2 + H_2 \rightarrow C_2H + H \qquad E_{barrier} = 1420\ \mathrm{K}$$

$$C_3 + H_2 \rightarrow C_3H + H \qquad E_{barrier} = 14200\ \mathrm{K}$$

$$C_3H + H_2 \rightarrow C_3H_2 + H \qquad E_{barrier} = 950\ \mathrm{K}$$

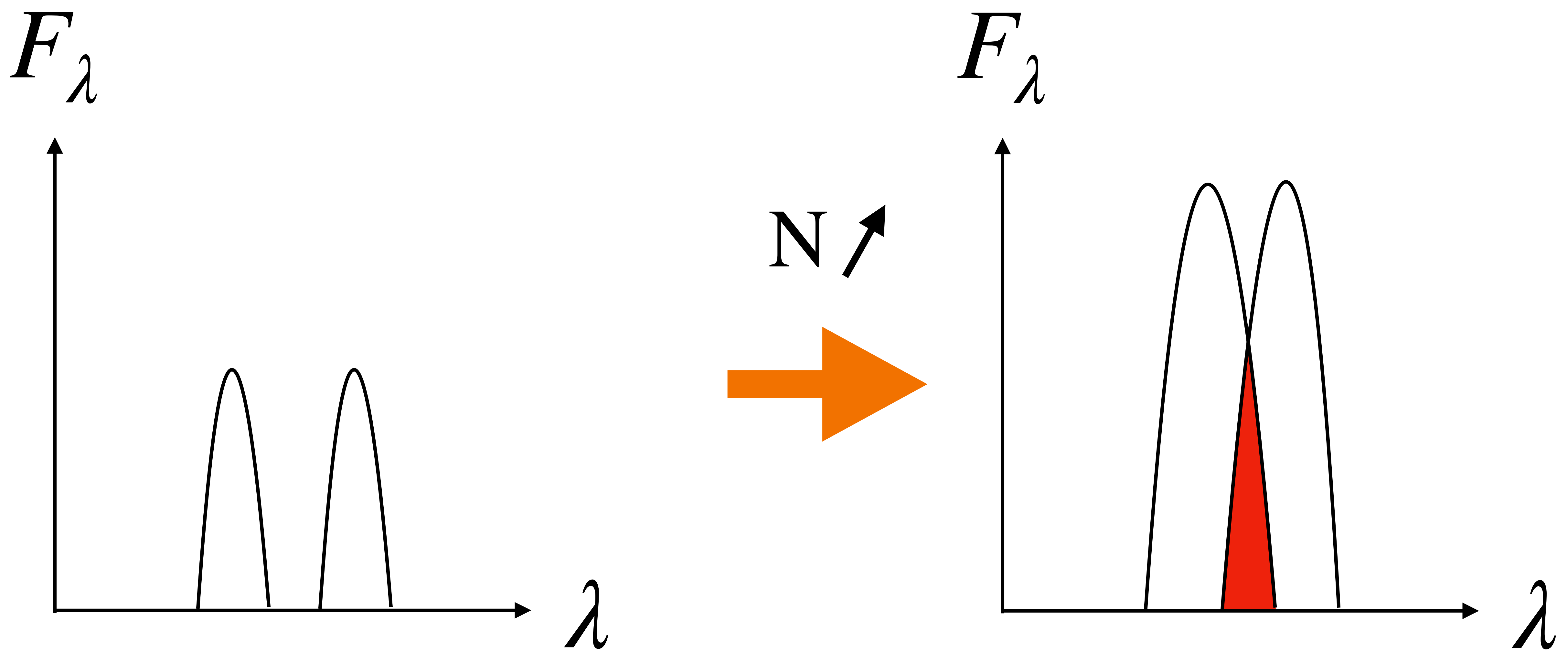
$$C_3H_2 + H_2 \rightarrow CH_2CCH + H \qquad E_{barrier} = 8760\ \mathrm{K}$$

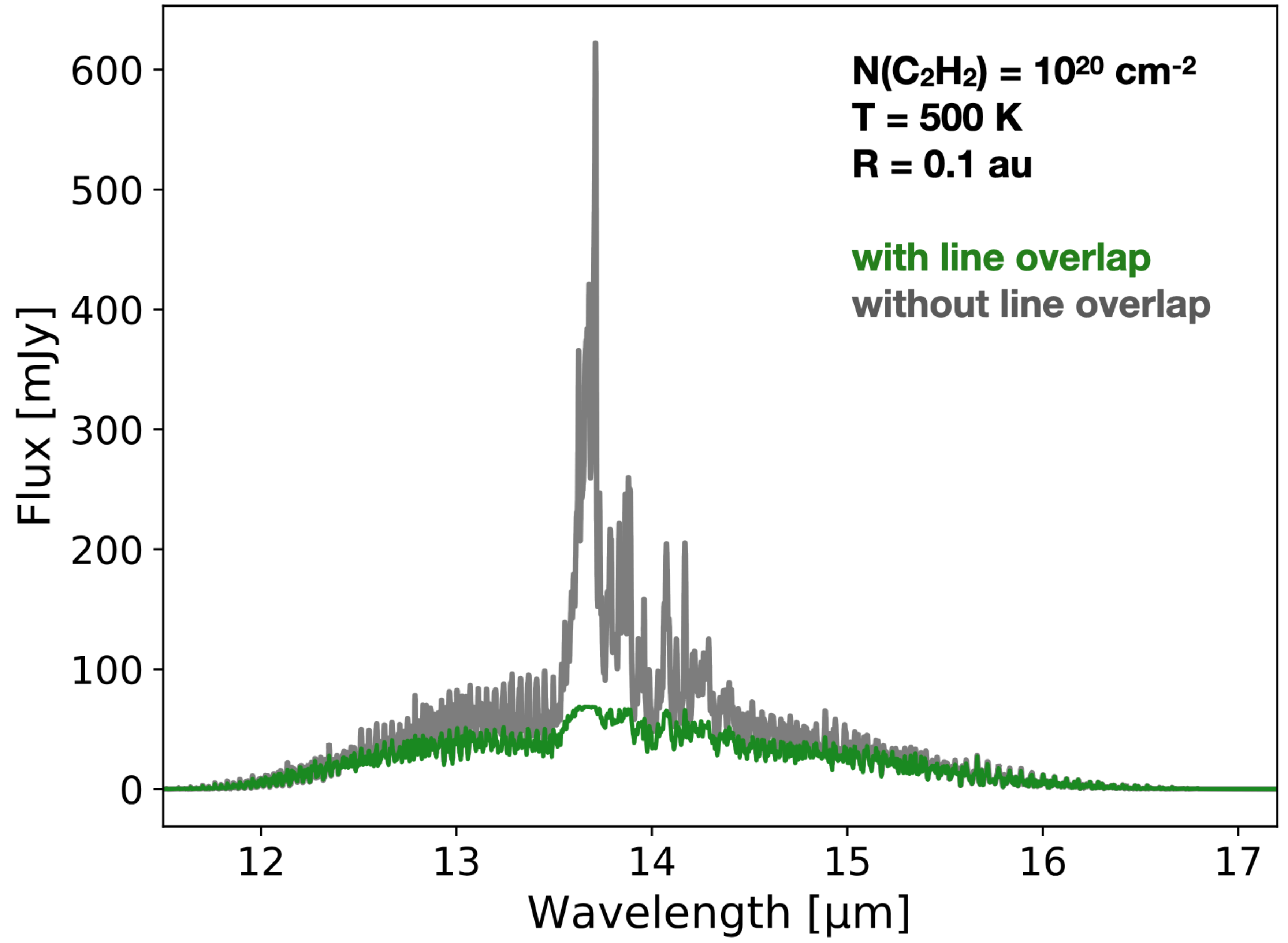
New chemical networks : workflow

Line overlap implementation

- Two separate lines close to each other can overlap when they are broaden by high column density

- The lines « shield » each other : line overlap

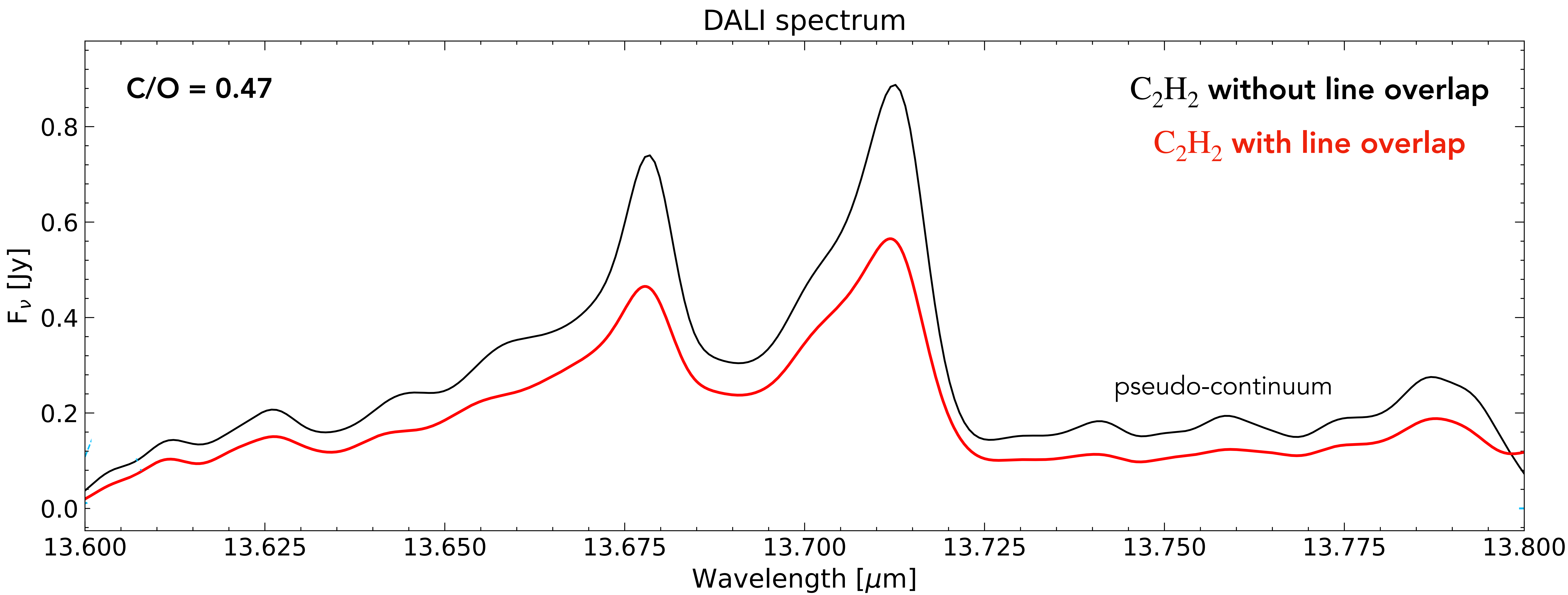




Effect of line overlap. From Tabone et al. 2023

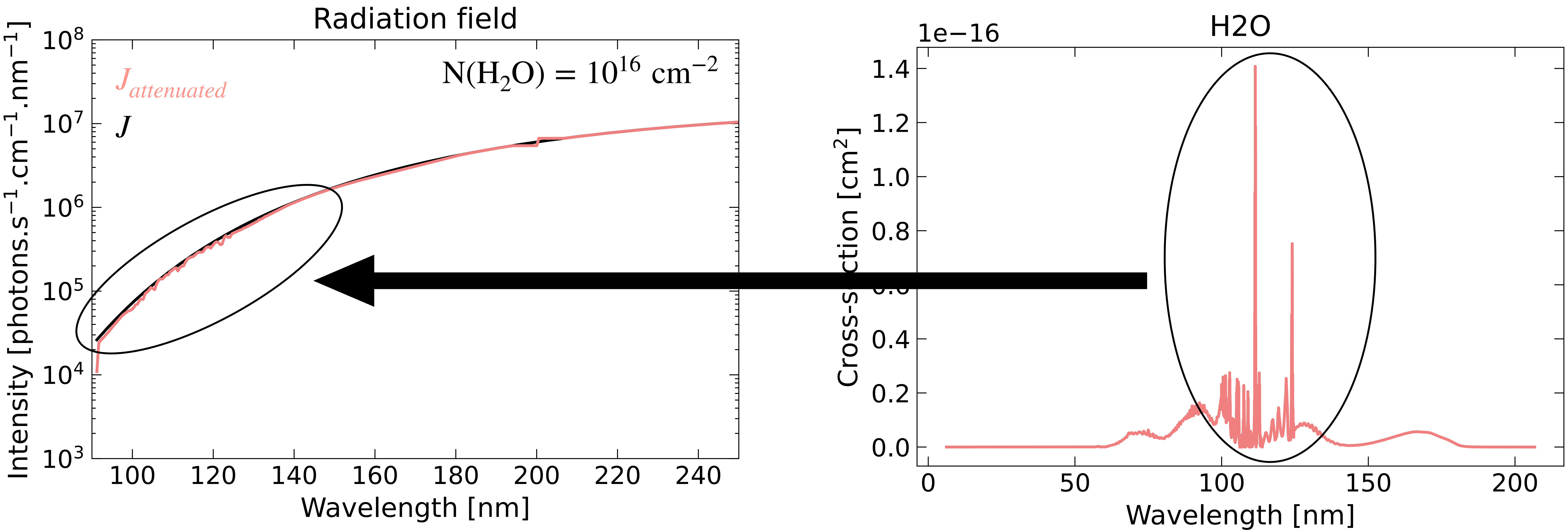
Line overlap implementation

→ Effect of the line overlap prominent in the main Q-branch feature of C_2H_2



UV shielding

→ Molecules can absorb UV photons and attenuate the UV field: $\sigma_\nu N_i$



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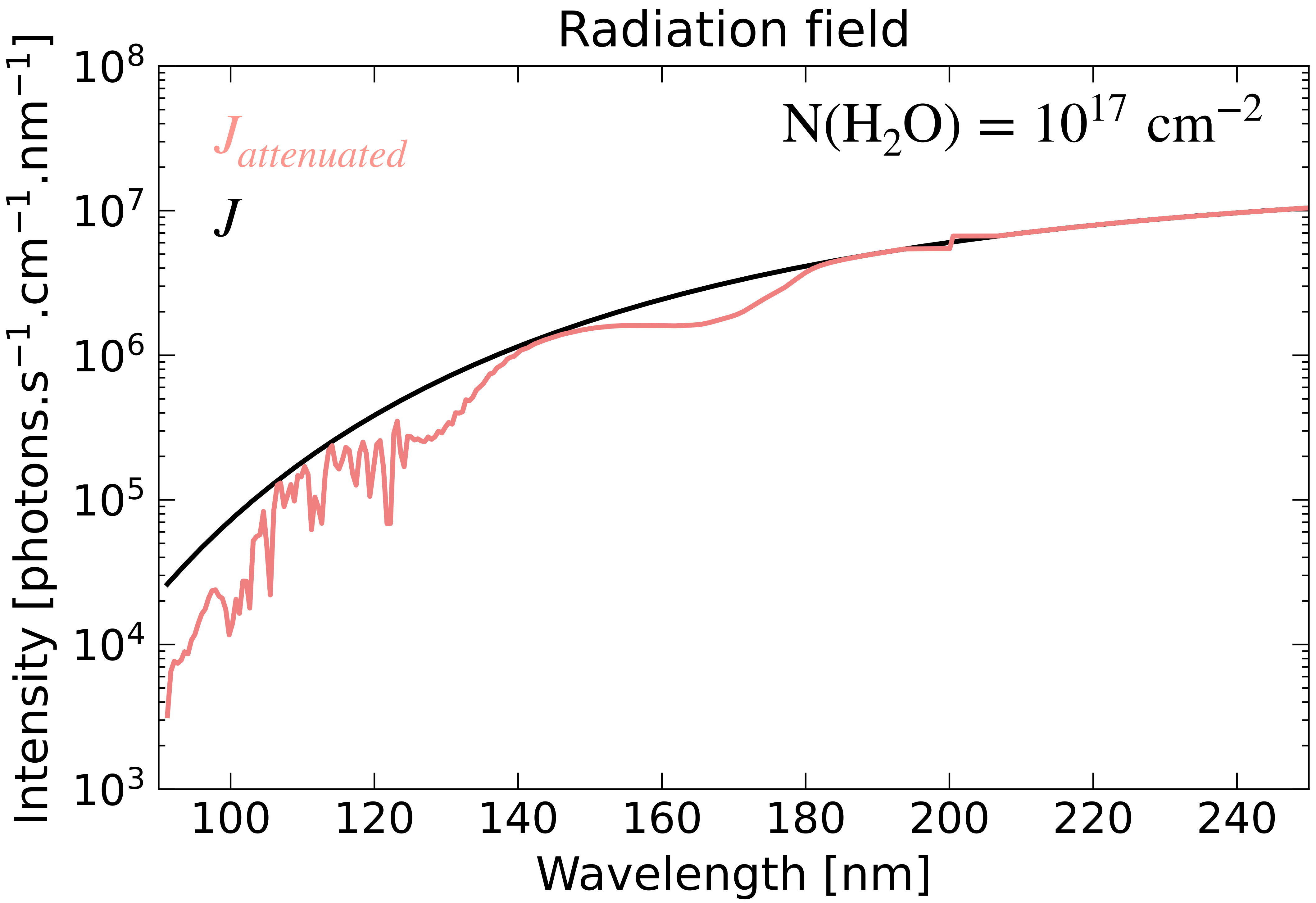

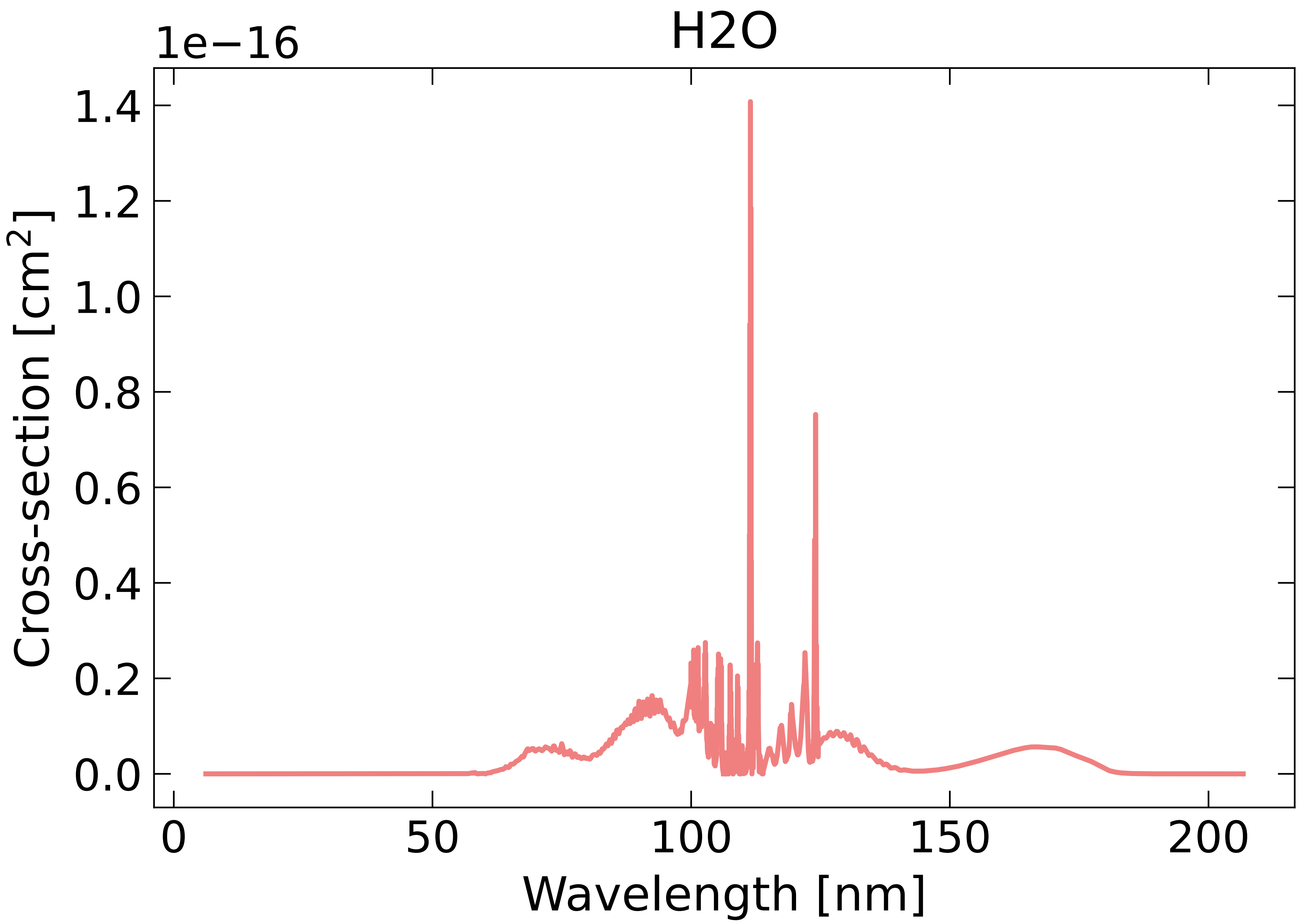

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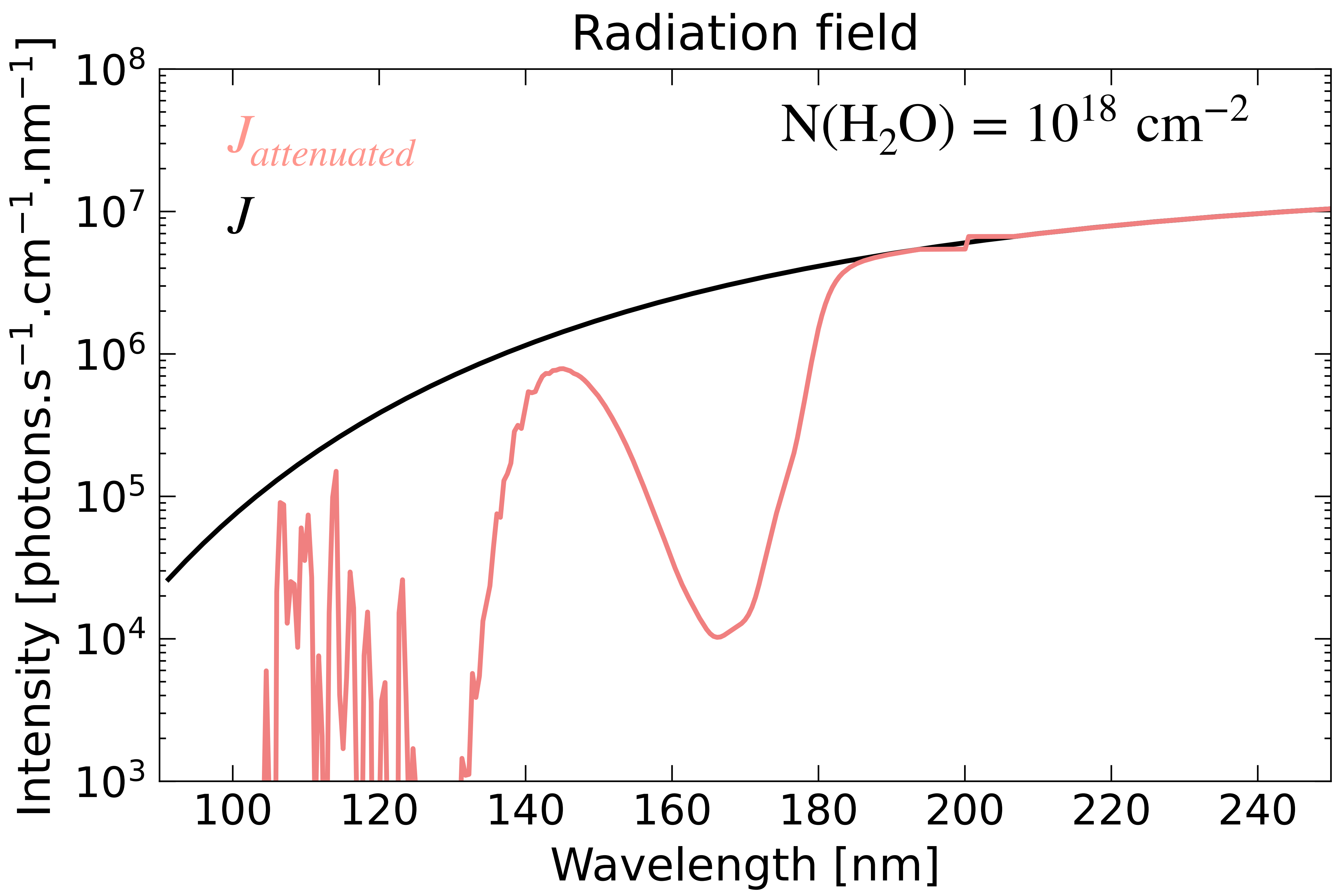
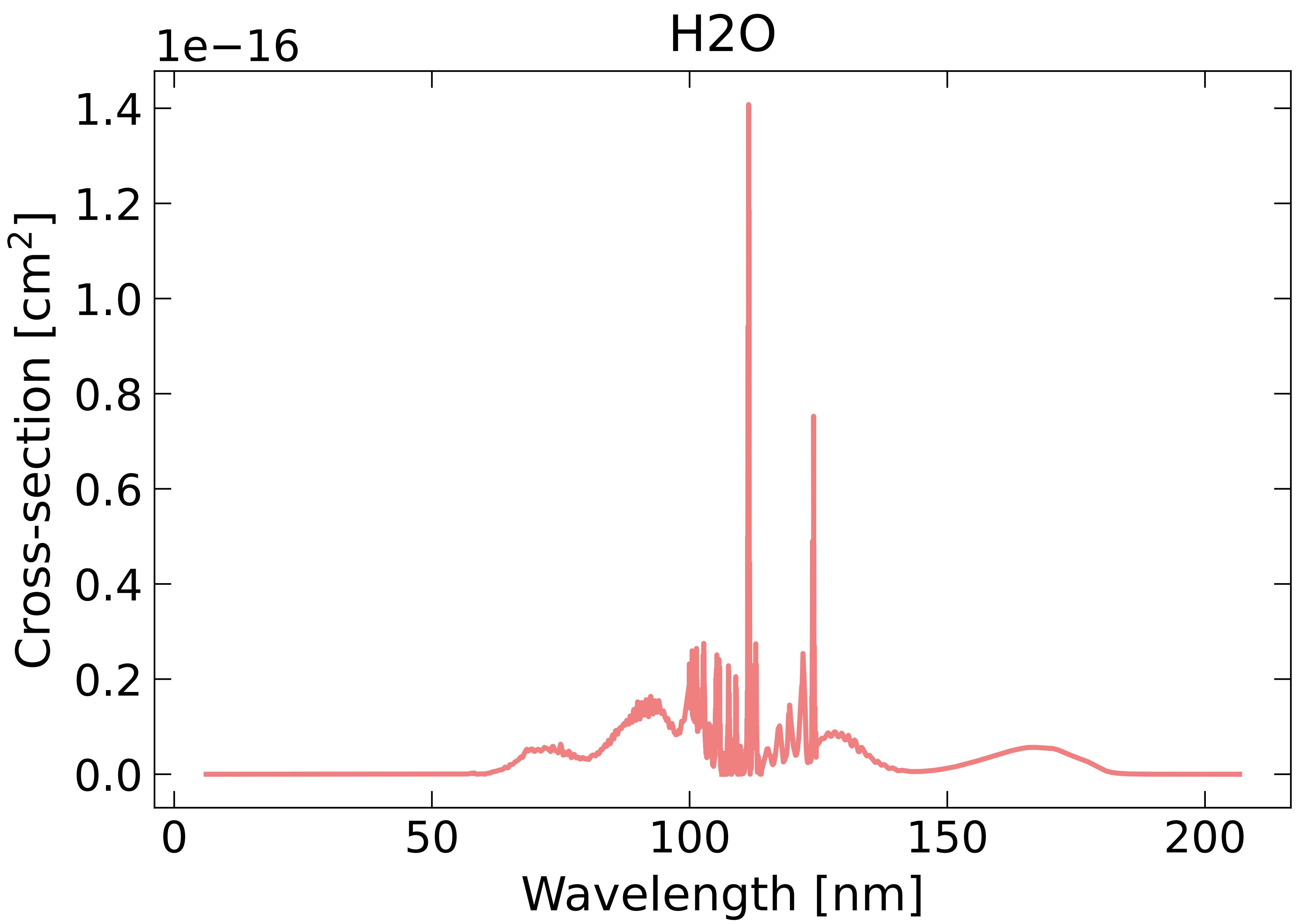
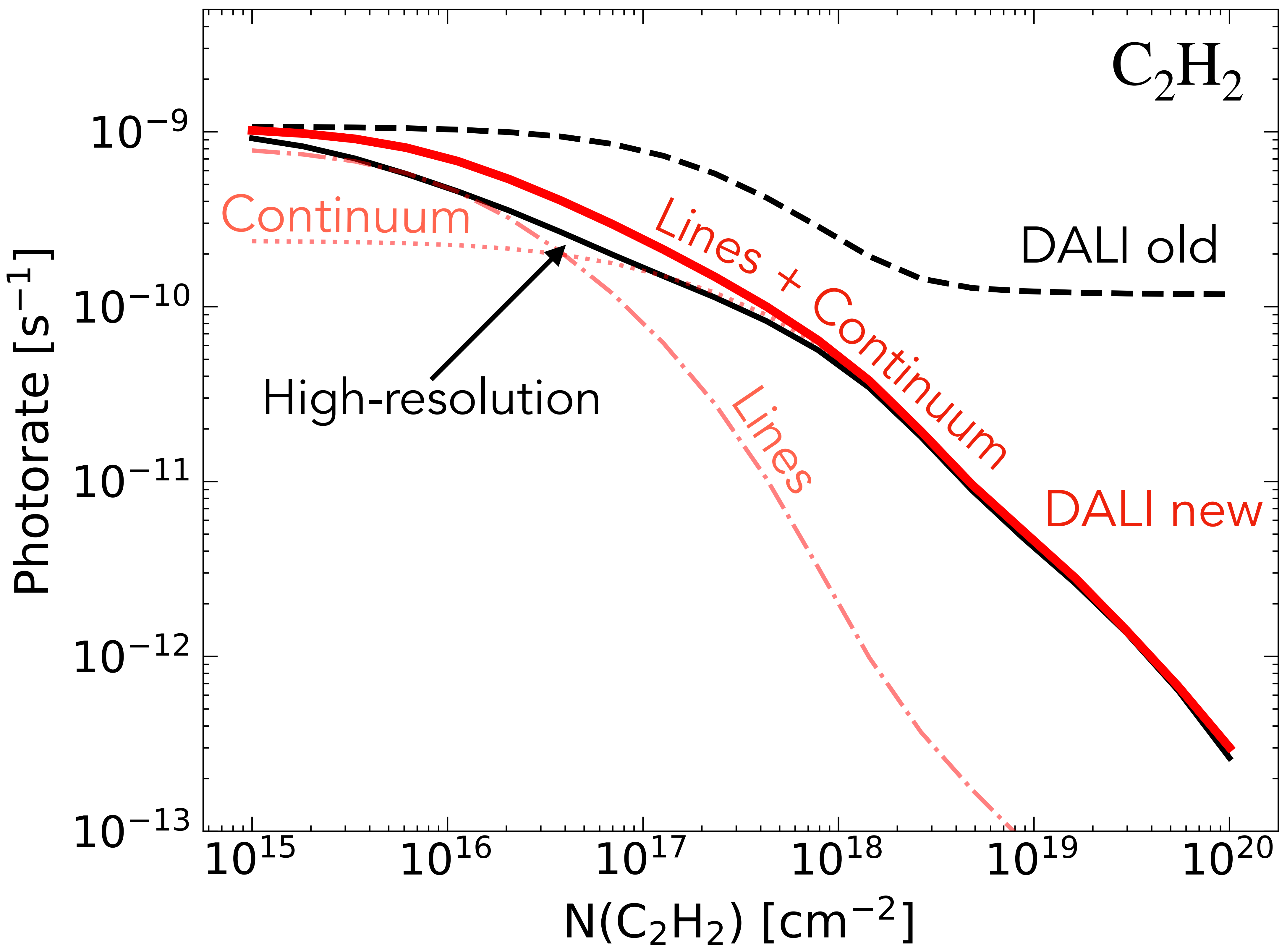




UV shielding

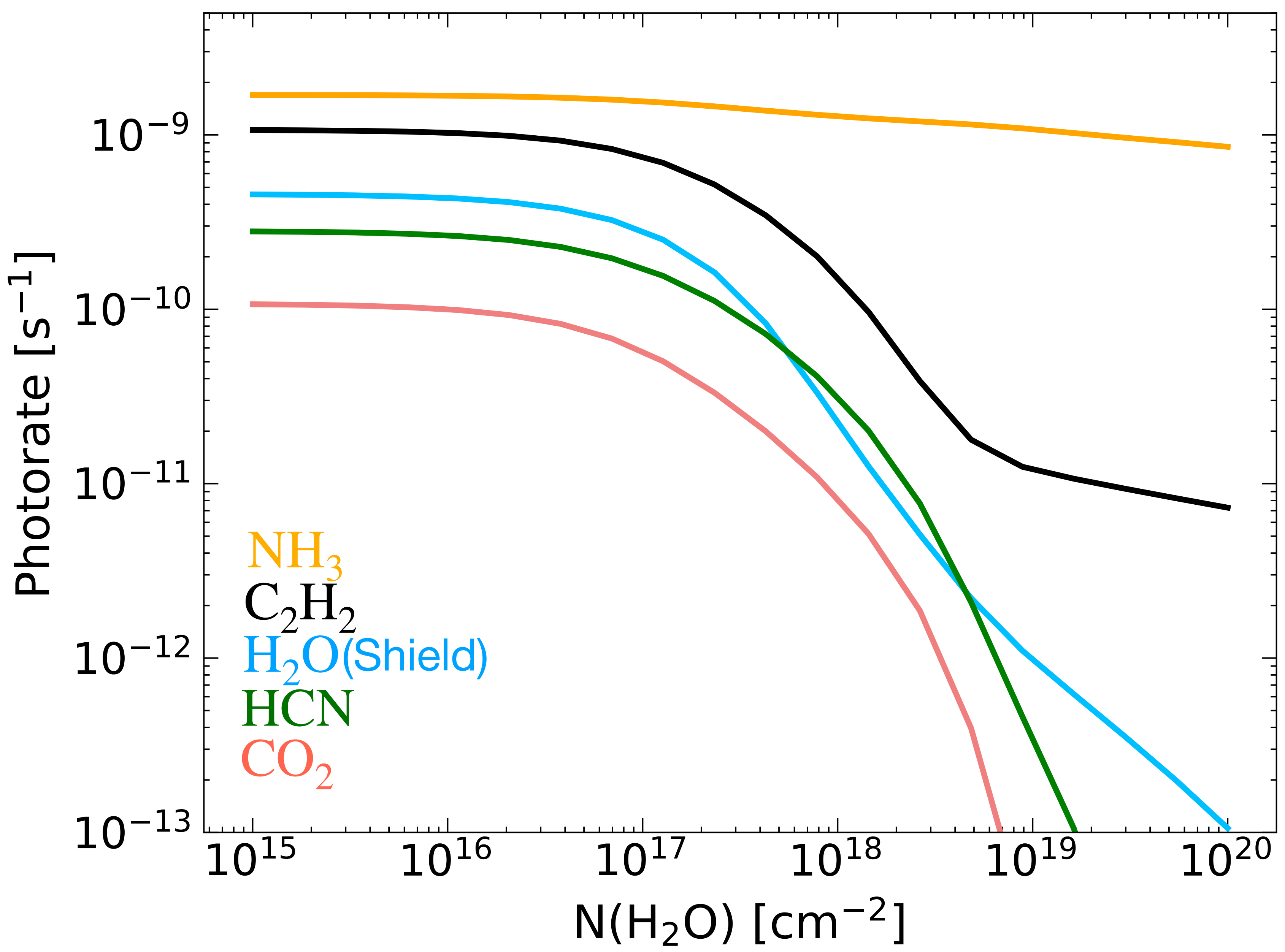
- Separation line/continuum reproduces very well the « real » self-shielding
- Crucial role of self-shielding at low column densities

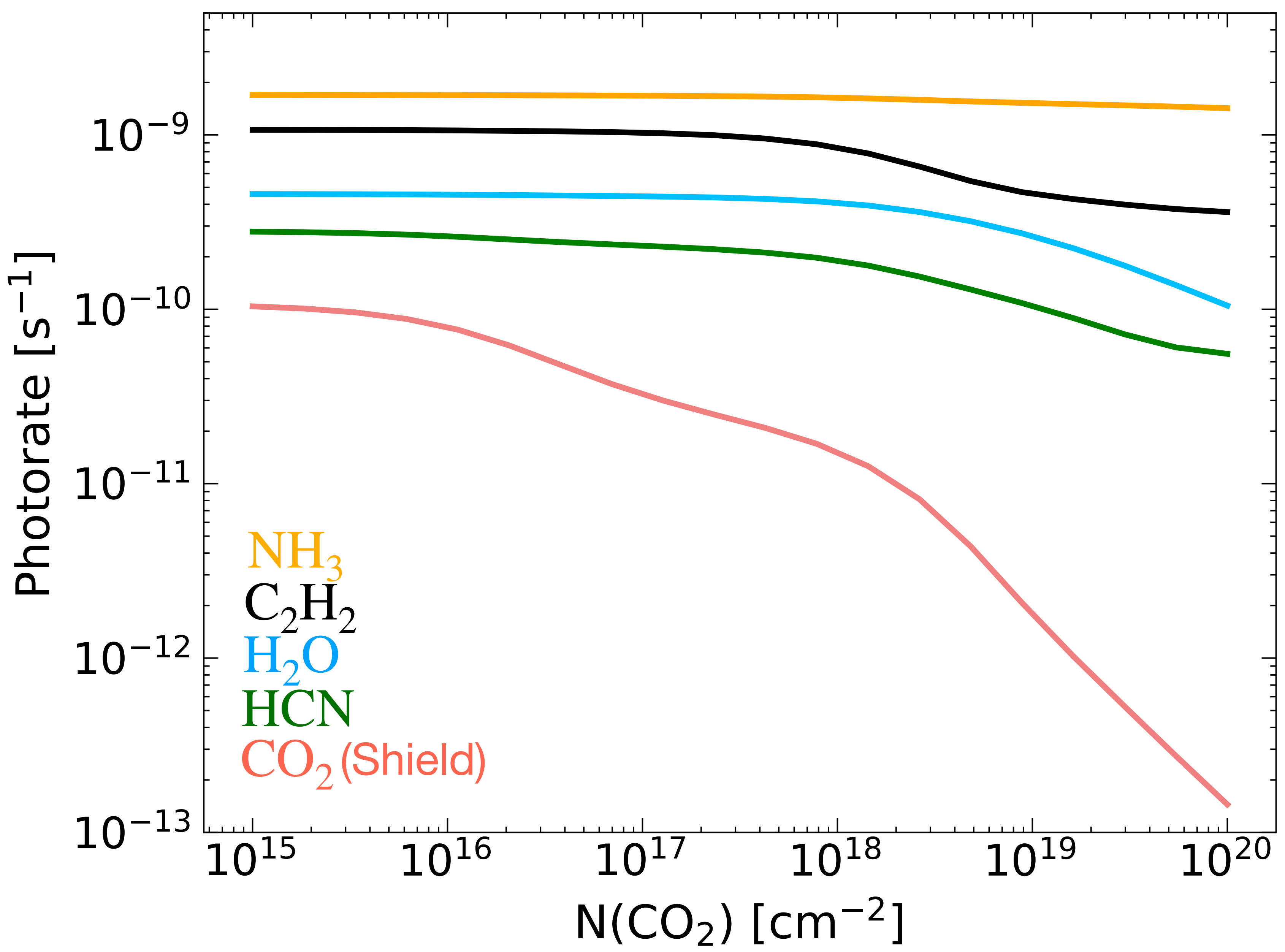


Photodissociation rate of C_2H_2 as a function of the column density (shielding)

UV shielding

- Mutual shielding as implemented in DALI (shielded by continuum only)
- Mutual shielding particularly efficient for: H_2O, C_2H_4, C_3, (C_2H_2)
- Mutual shielding not efficient for: CO_2, CH_4, NH_3, HCN

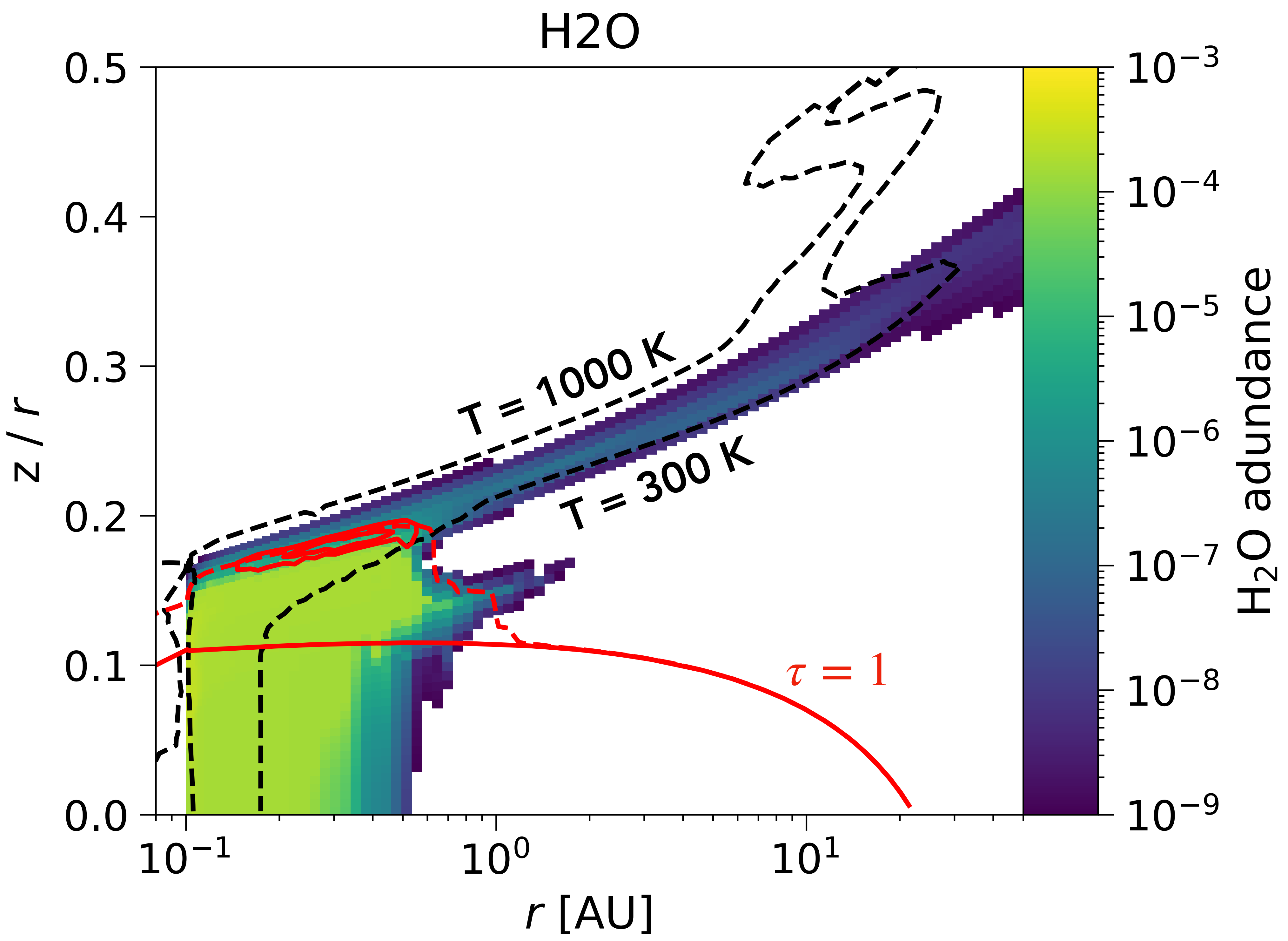




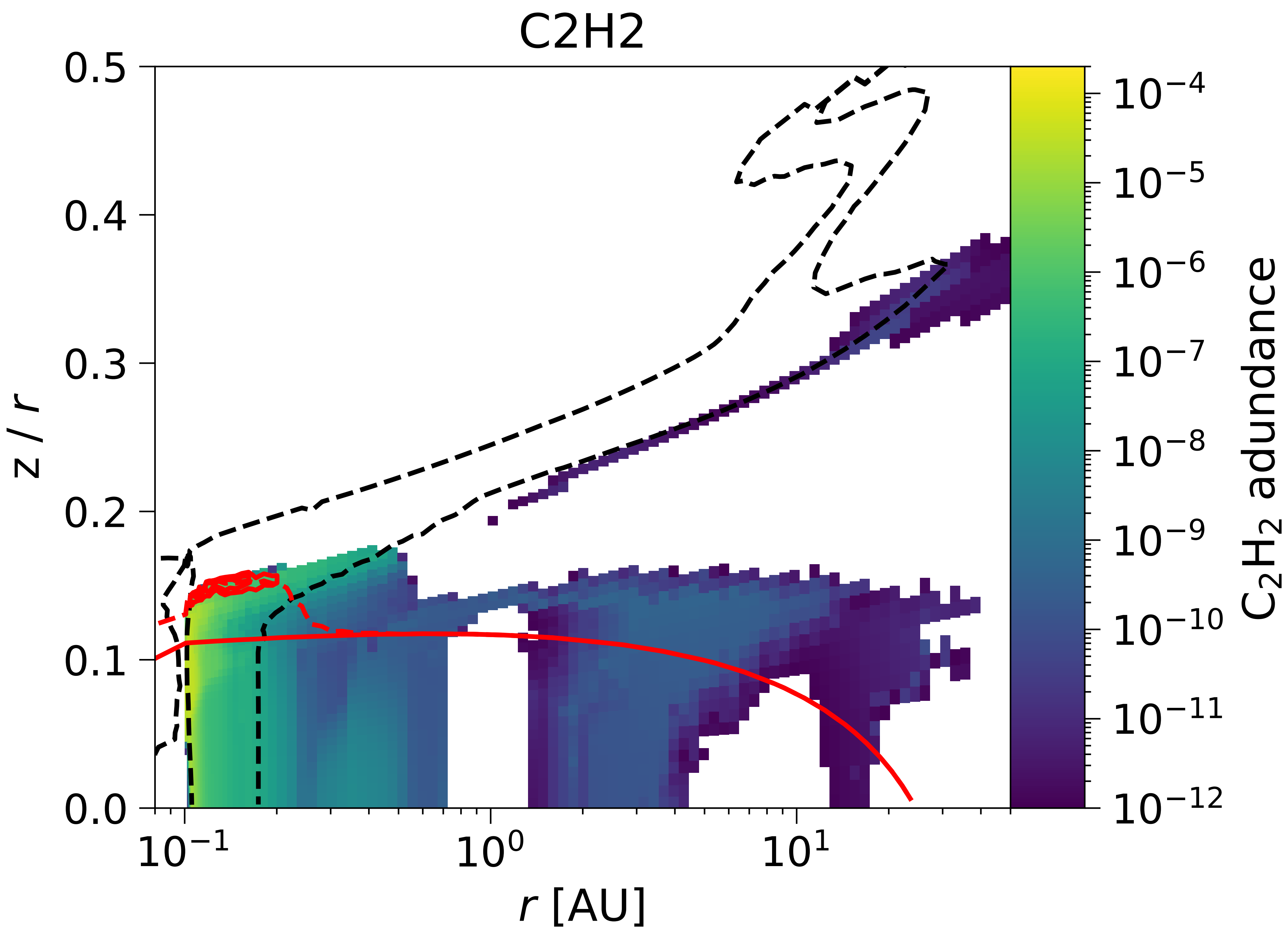
C_2H_2 and H_2O abundance map

→ H_2O abundant in the inner disk

→ C_2H_2 emitting region is slightly deeper and closer to the star



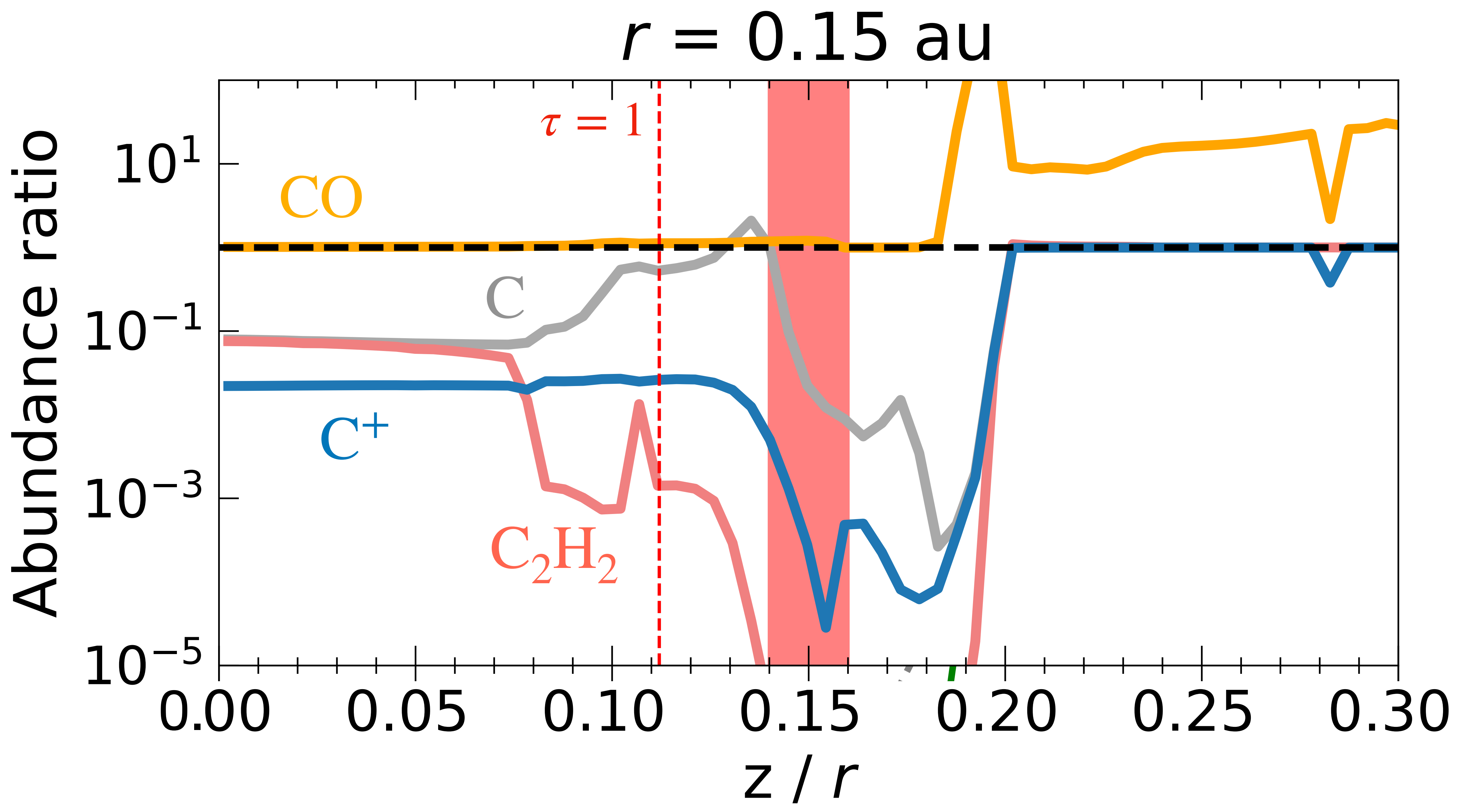
Abundance map of water



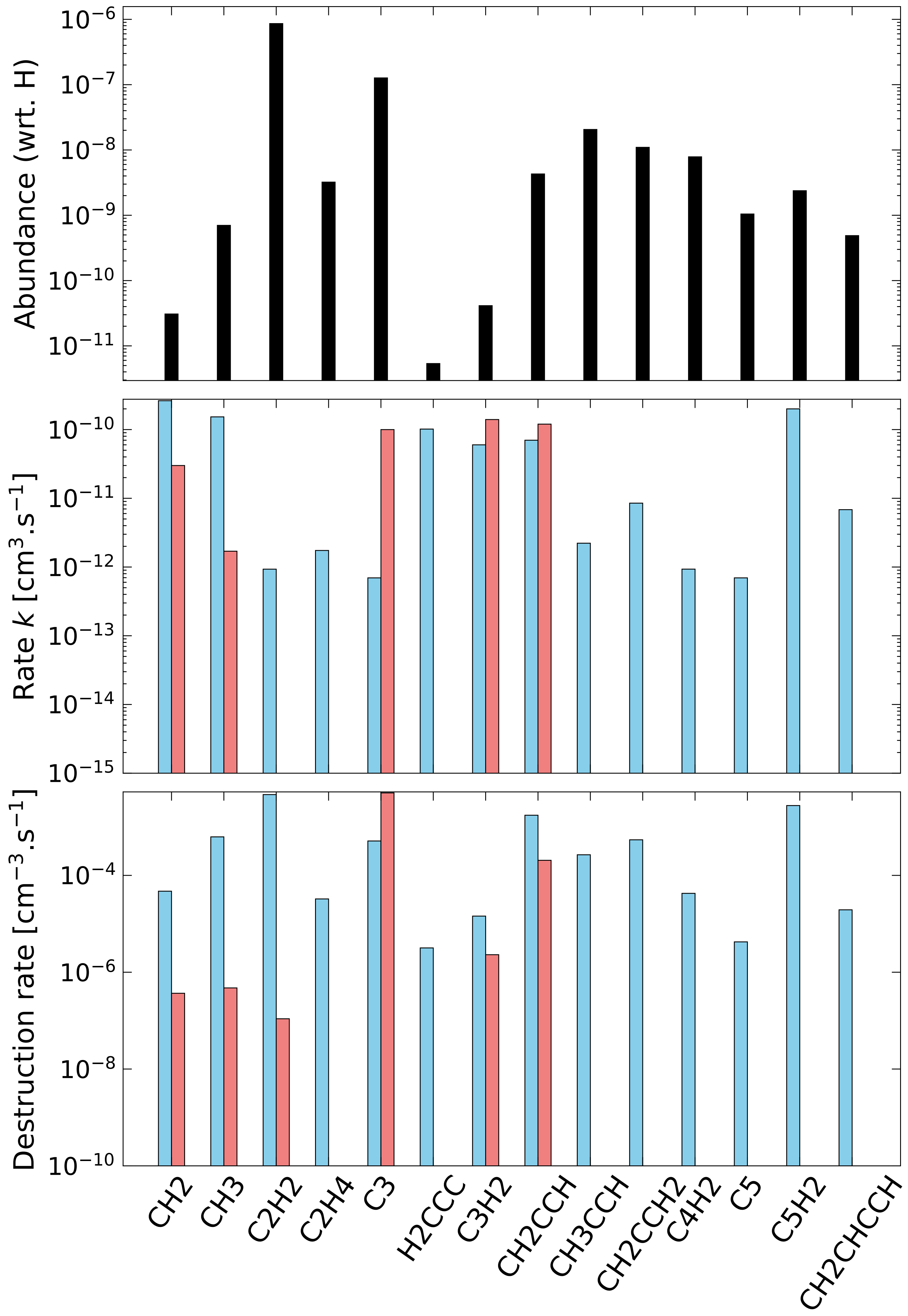
Abundance map of acetylene

Where does the carbon come from ?

→ Dissociation of CO releases free carbon avai



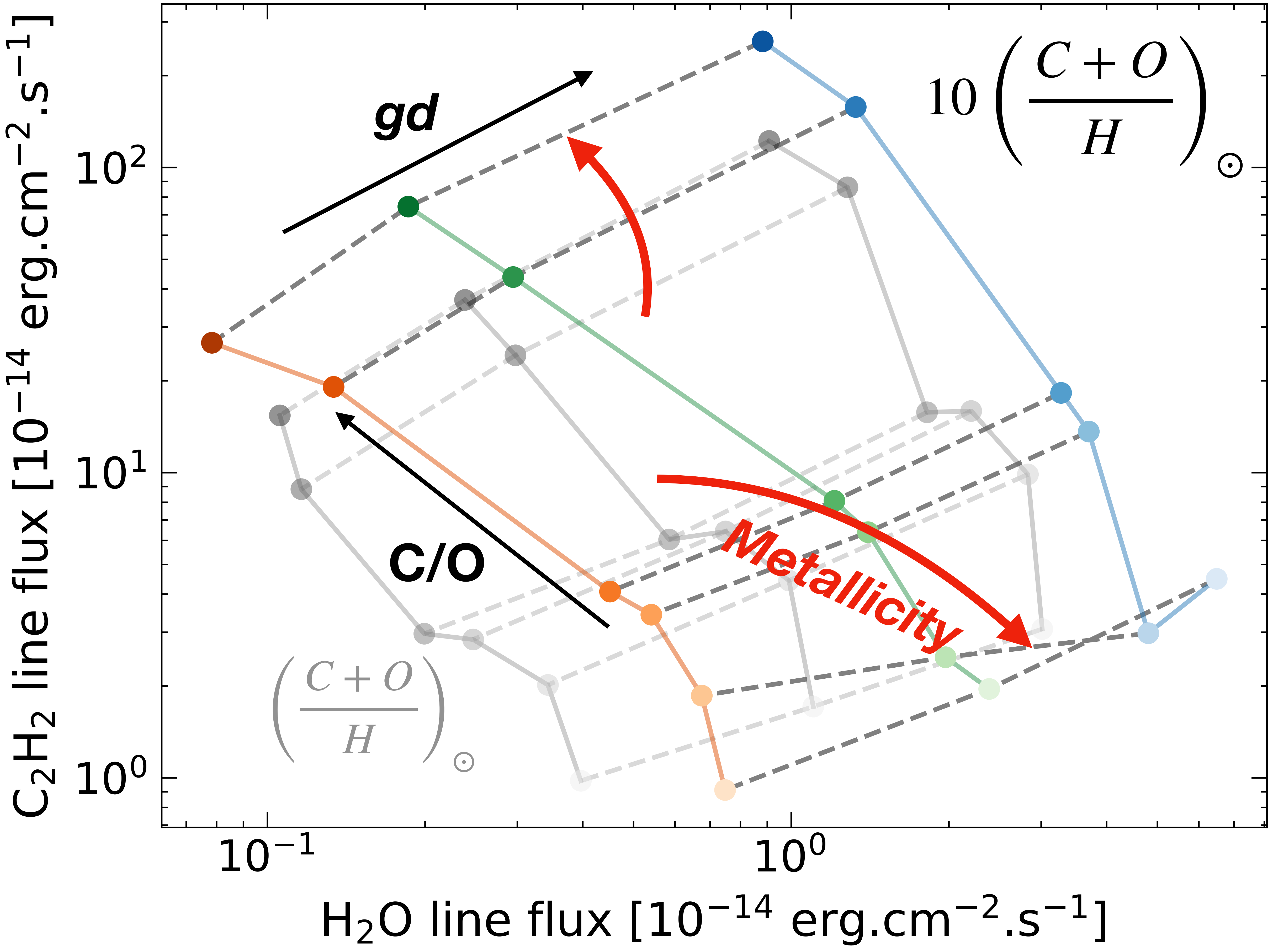
Abundance ratio between fiducial and fiducial without reactions (1) and (2). The red shaded area is the emitting layer of C_2H_2.



Metallicity

→ The grid seems shifted to the right : water is brighter when the metallicity is increased…

… but it is actually degenerated with the C/O ratio



- When C/O < 1:

  H_2O line flux increases while C_2H_2 decreases

  → O destroys carbon chains + C locked in CO

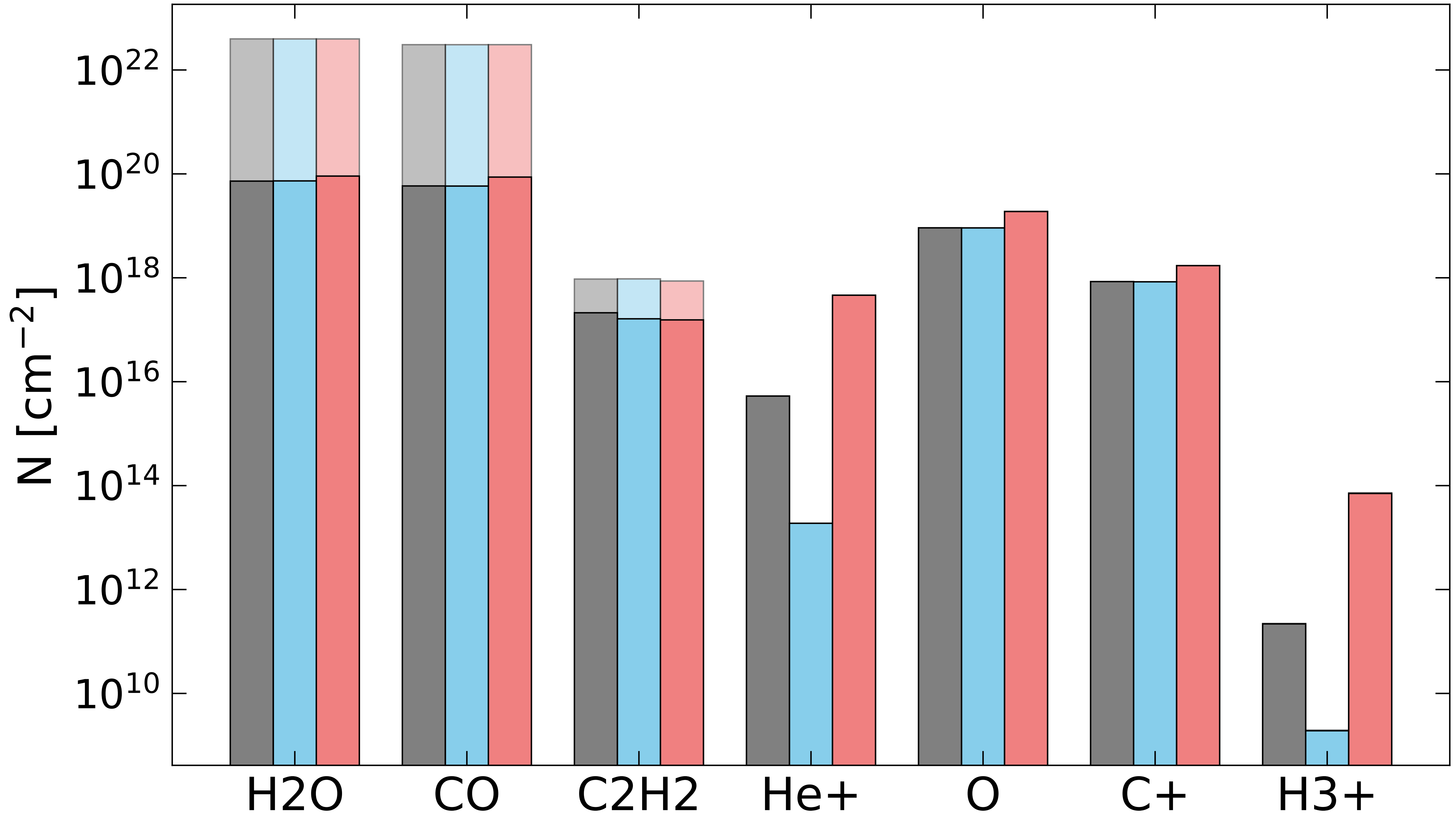
- When C/O > 1:

  H_2O line flux decreases while C_2H_2 increases

  → O locked in CO + more C available

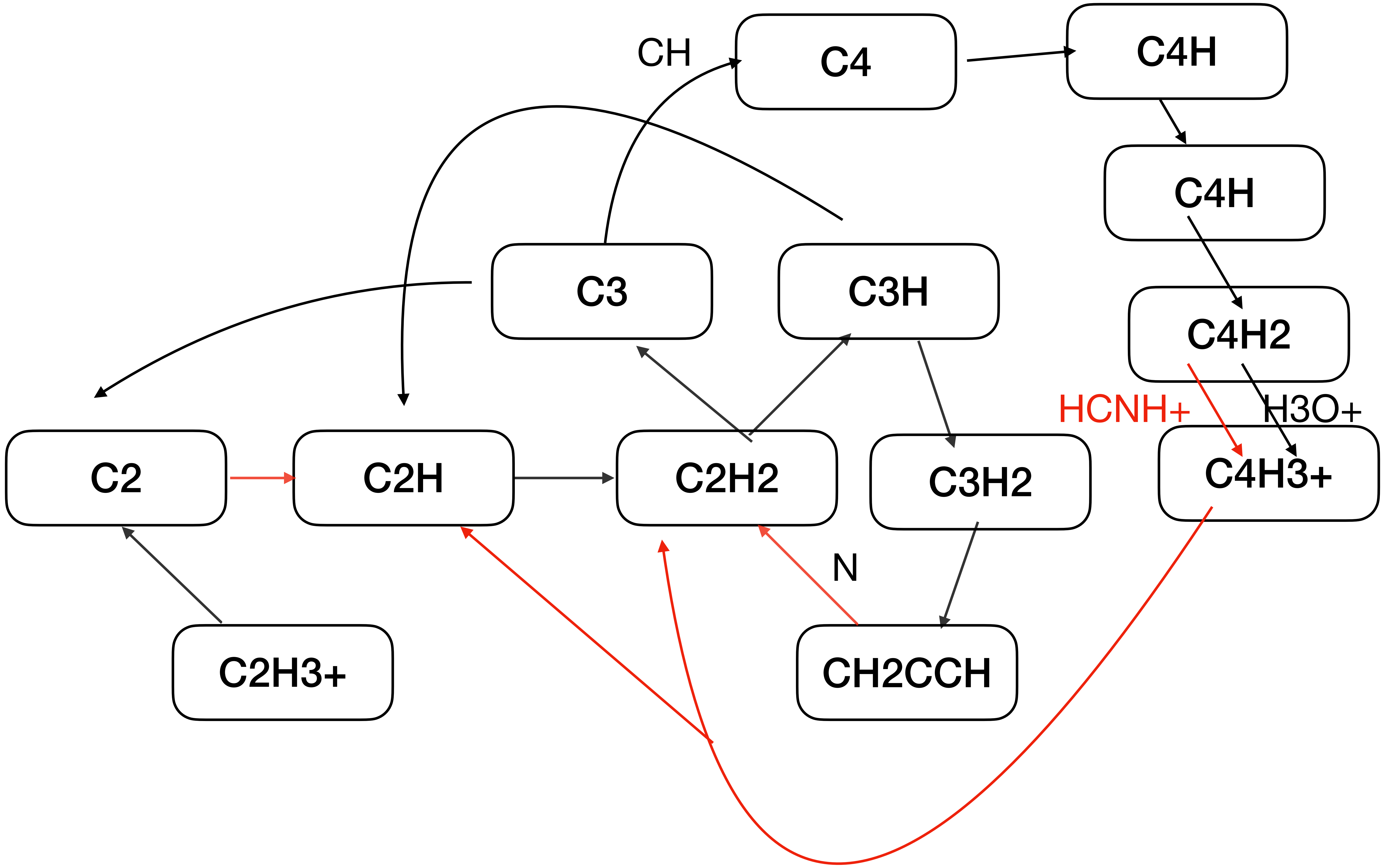
X-ray luminosity

→ X-ray luminosity does not impact H_2O and C_2H_2 emission: balance of formation and destruction



Column densities of different species as a function of the X-ray luminosity

Check the tau = 1 btw 10^27 and 10^33 because I don't raytrace it in my last models


CH
C4
C4H
C4H
C3
C3H
C4H2
HCNH+
H3O+
C2
C2H
C2H2
C3H2
C4H3+
N
C2H3+
CH2CCH