WATER FORMATION IN INTERSTELLAR ICES

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WATER IN THE UNIVERSE: FROM CLOUDS TO OCEANS

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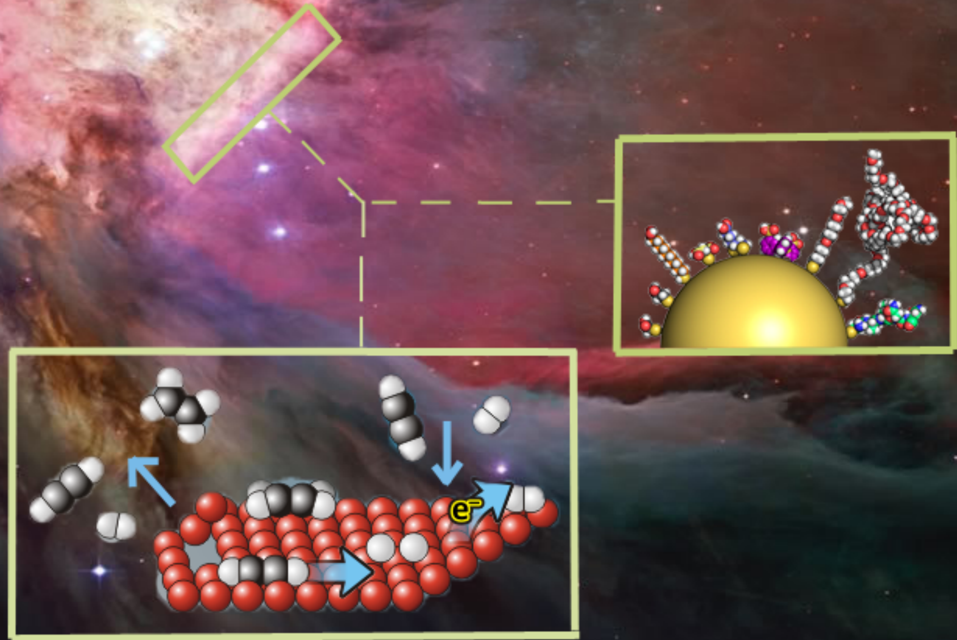

Aim:

Study of the different water formation routes through surface chemistry depending on the interstellar conditions

Why dust grains?

- Powerful interstellar catalysts
- Water is one of the most abundant ices on grains
- Adsorption is not enough to explain observations of H_2O ice abundances

⇩

Need of surface chemistry

Meijerink code

Before

(Meijerink & Spaans 2005)

Chemistry

- Gas chemistry (UMIST 99):
  4453 chemical reactions
- Dust chemistry: H_2 formation

Heating & Cooling

- Photo-electric effect on grains
- Carbon ionization
- H2 photo-dissociation
- H2 collisional (de-)excitation
- Gas-grain collisions
- UV & cosmic-ray ionization
- Fine-structure & metastable-lines
- Recombination
- Molecular cooling (H_2, CO, H_2O)

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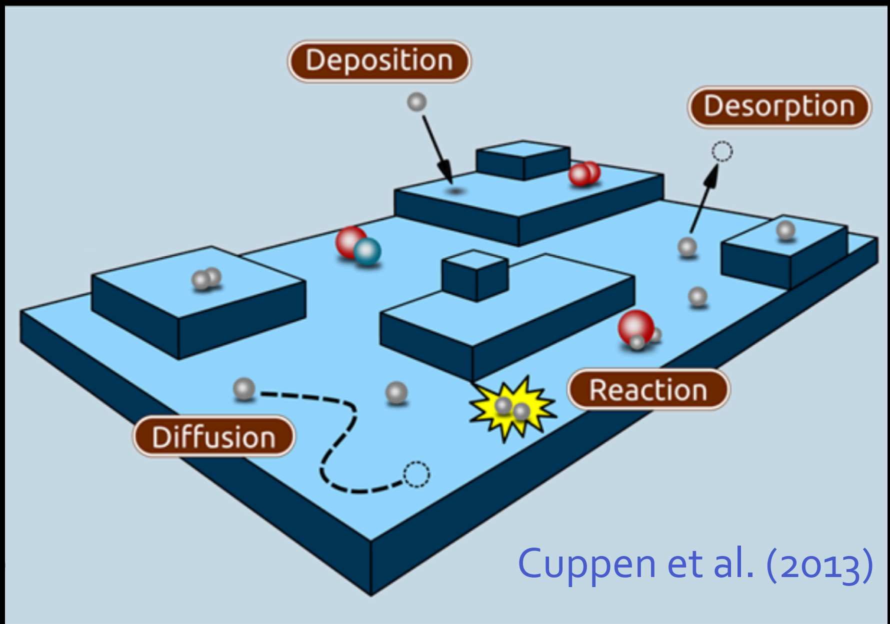


Now

(Esplugues et al. submitted to A&A)

Chemistry

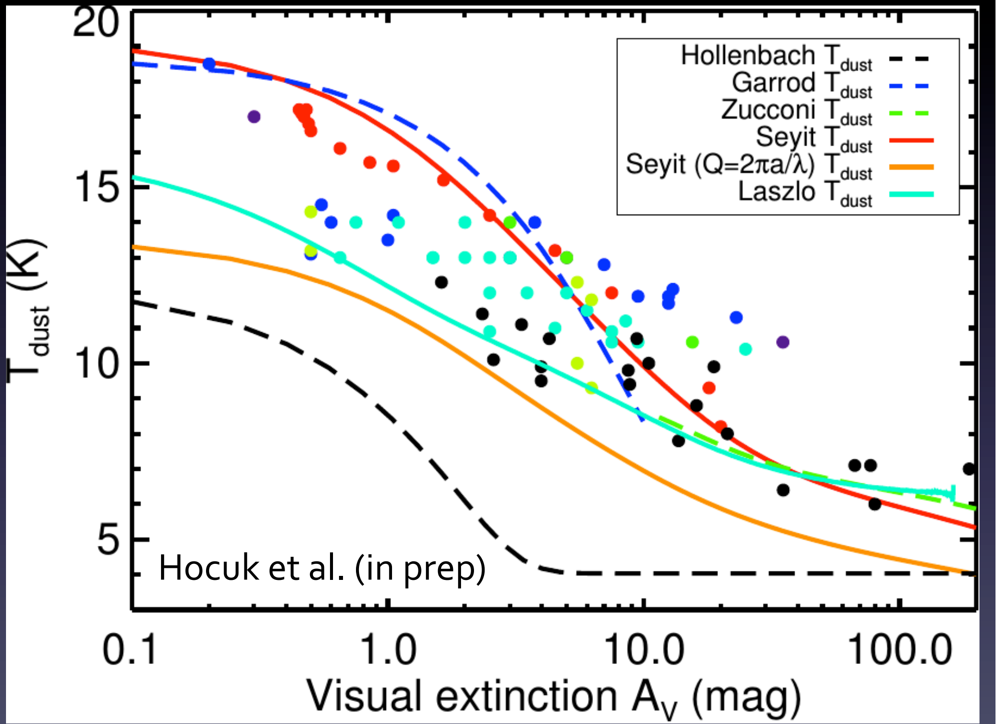
- Gas chemistry (KIDA 2014):
  7503 chemical reactions
- Dust chemistry (from laboratory experiments, e.g., Dulieu et al. 2013, Minissale et al. 2015, 2016):
  225 chemical reactions

  - Adsorption
  - Thermal & **chemical desorption**
  - Two-body reactions
  - Photo-processes
  - Cosmic-ray processes
- 22 solid species:
  H, H_2, O, O_2, OH, O_3, H_2O, HO_2, H_2O_2, CO, HCO, H_2CO, H_3CO, H_4CO, CO_2, N, N_2, C, CH, CH_2, CH_3, CH_4.

Meijerink code: dust treatment

- Icy grains and bare grains (different binding energies)

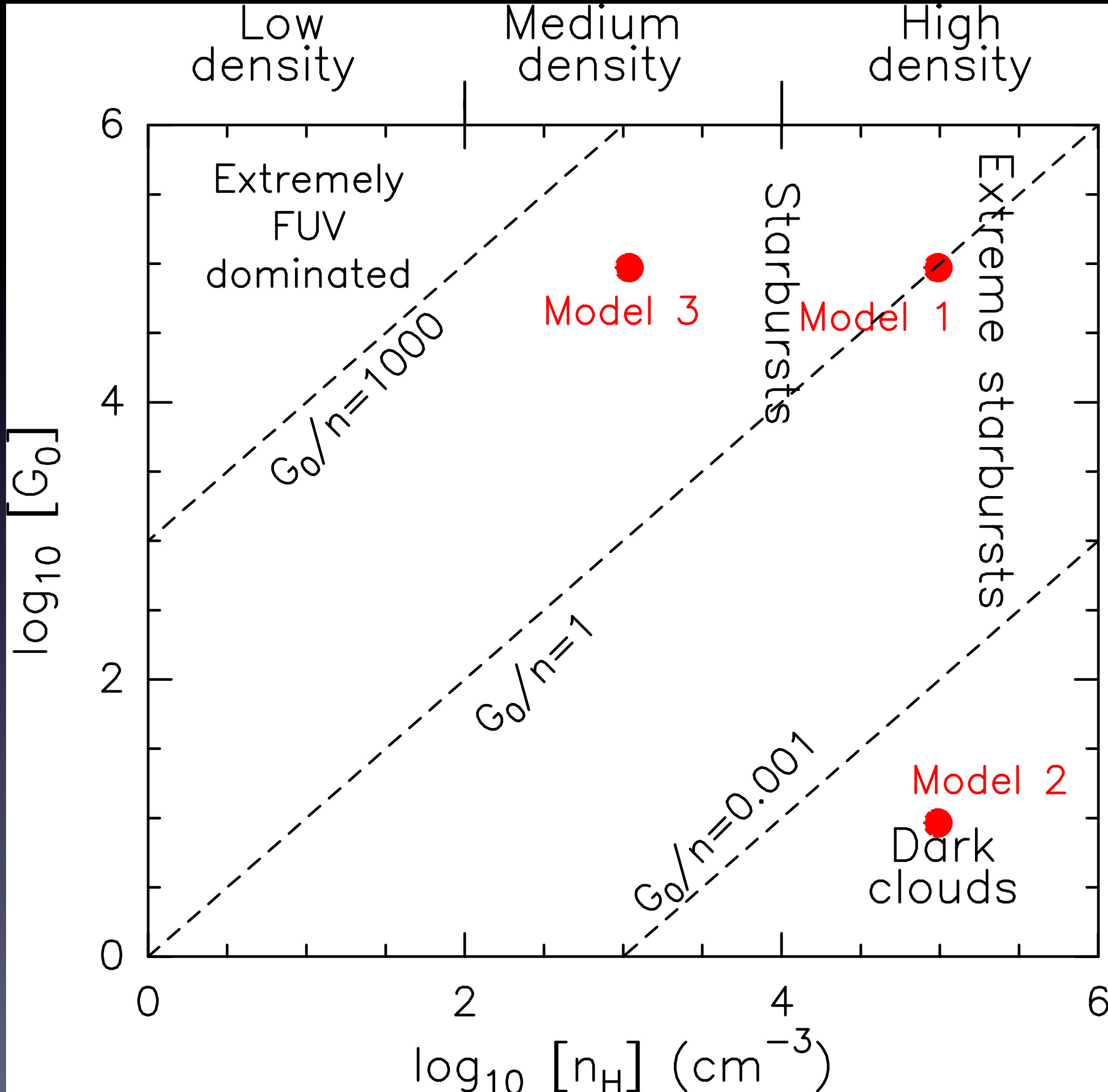
- Dust temperature (T_d):
  - Impact on gas temperature (T_g)
  - Variations in the reaction rates
  - Freeze out of gas species
  - Ice mantle formation



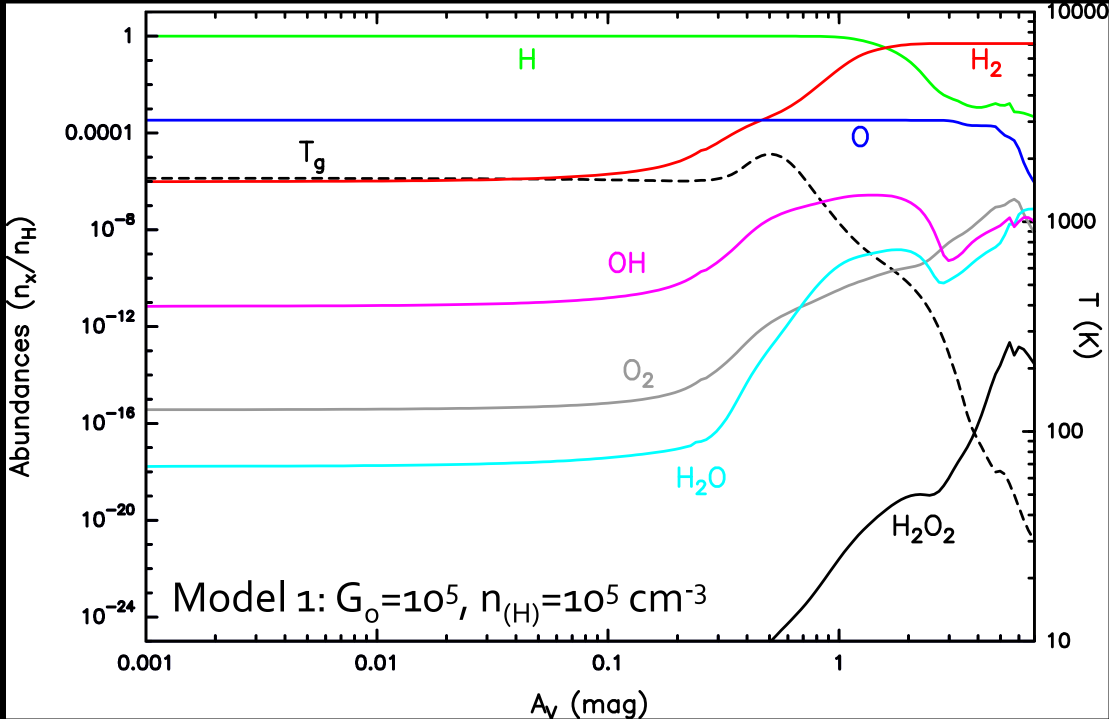
Garrod & Pauli (2011):

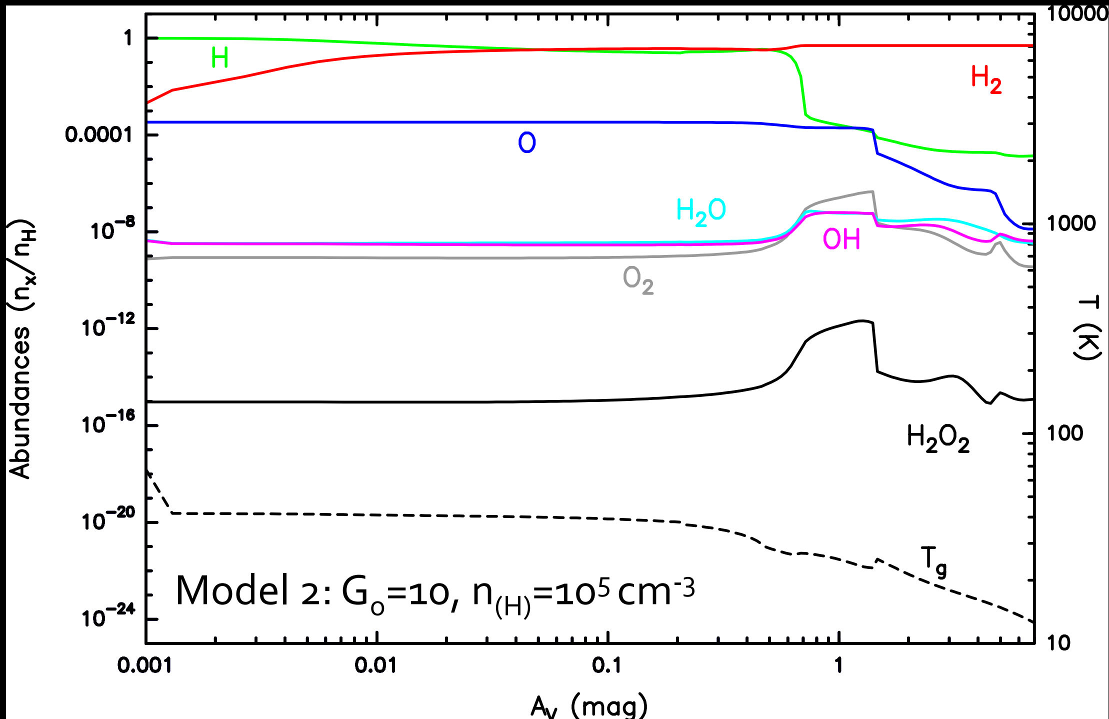
$$T_{dust} = 18.67 - 1.637\,[A_V - \log(G_0)] + 0.07518\,[A_V - \log(G_0)]^2 - 0.001492\,[A_V - \log(G_0)]^3$$

Water in different interstellar environments



G_o=1 corresponds to a flux of $1.6 \cdot 10^{-3}$ erg cm^{-2} s^{-1}

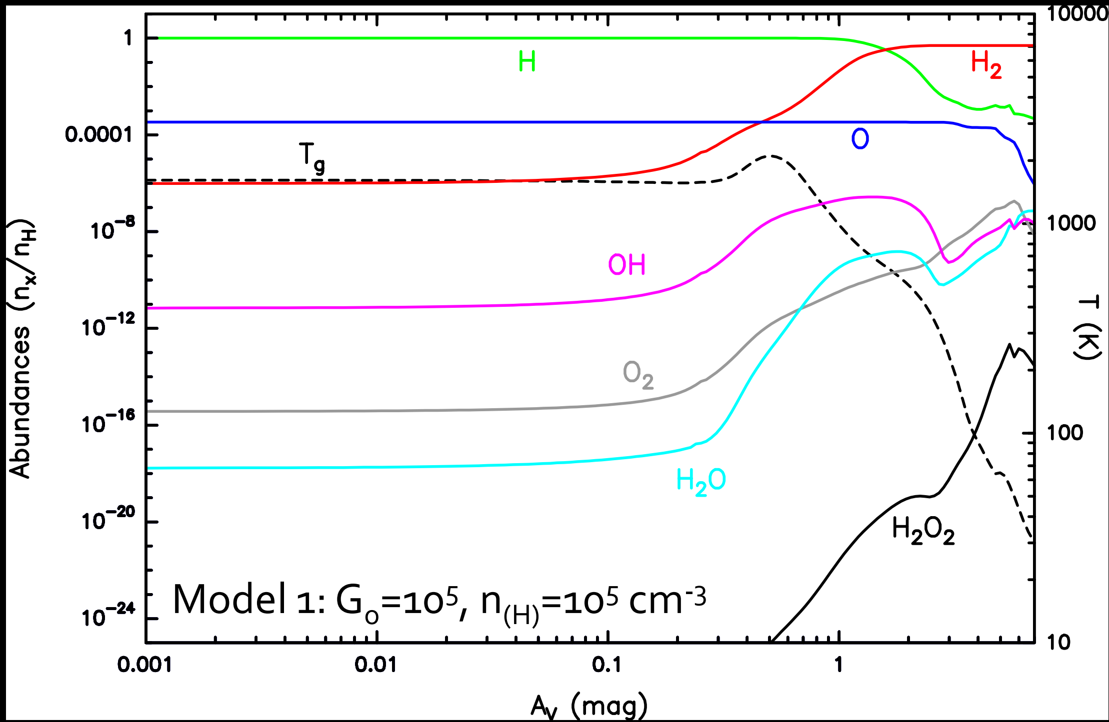


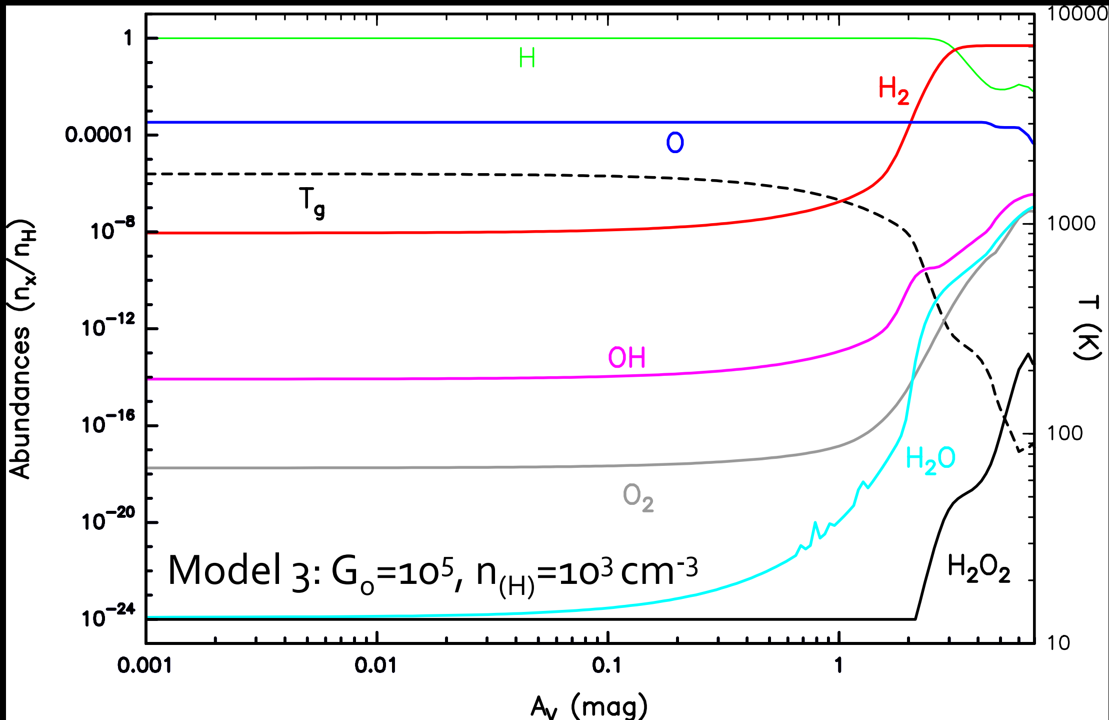


Gas-phase

Intensity of radiation (G_o)

- Large impact on the H_2O, H_2O_2, O_2 and H_2 abundances at Av<1 mag
- Low impact on the O and OH abundances
- Abundances drop at higher A_v for high *Go*, as ices become dominant





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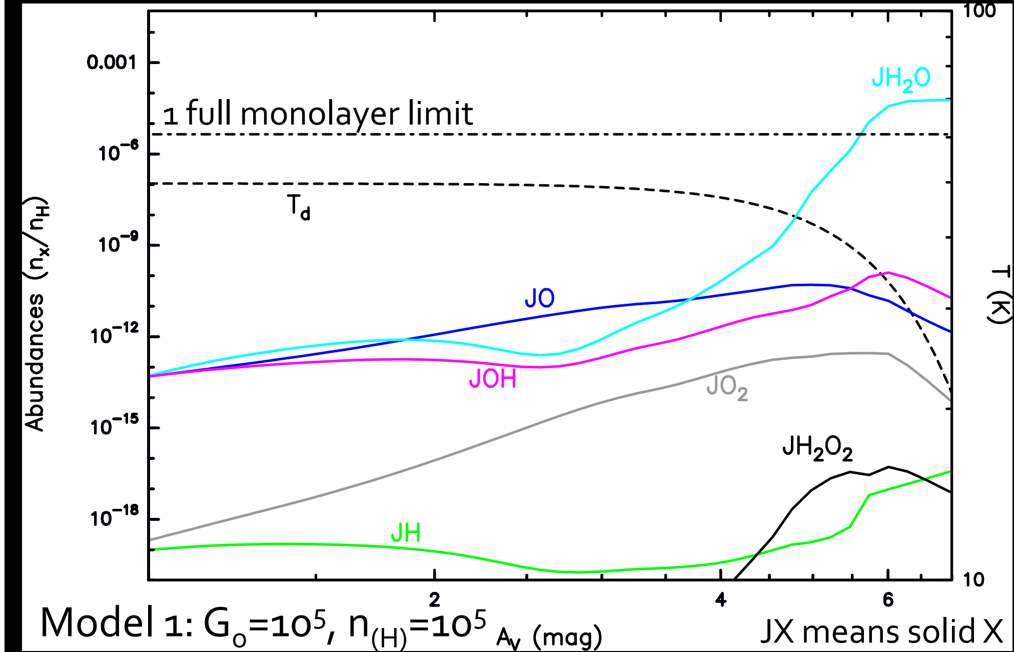
Density (*n*)

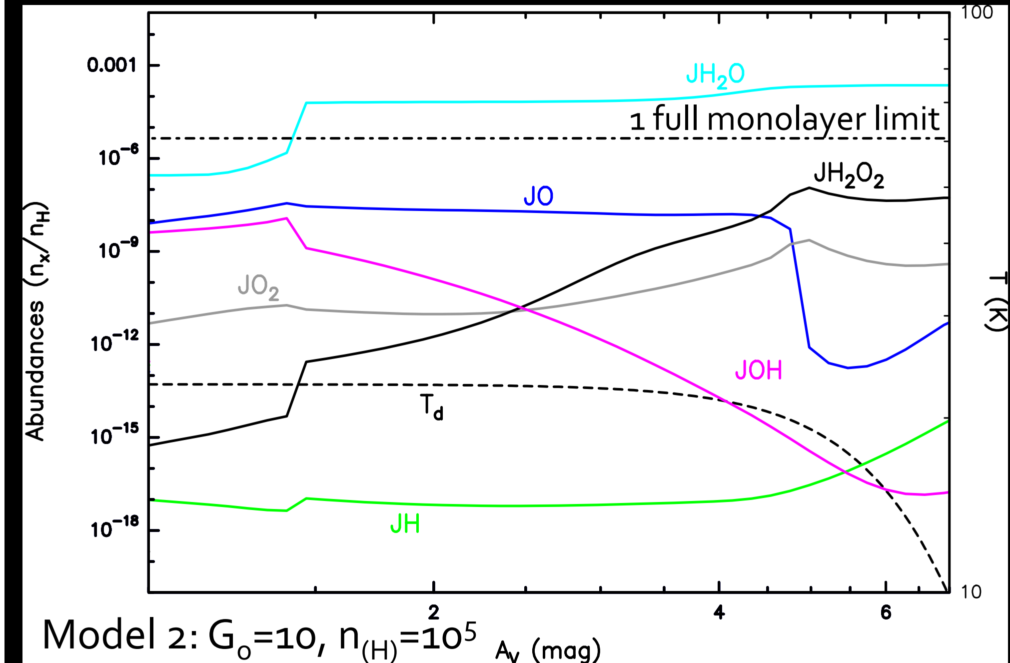
- The largest impact on the H_2O abundances at A_v<1 mag
- Abundances drop at higher A_v for low *n*

Dust-phase

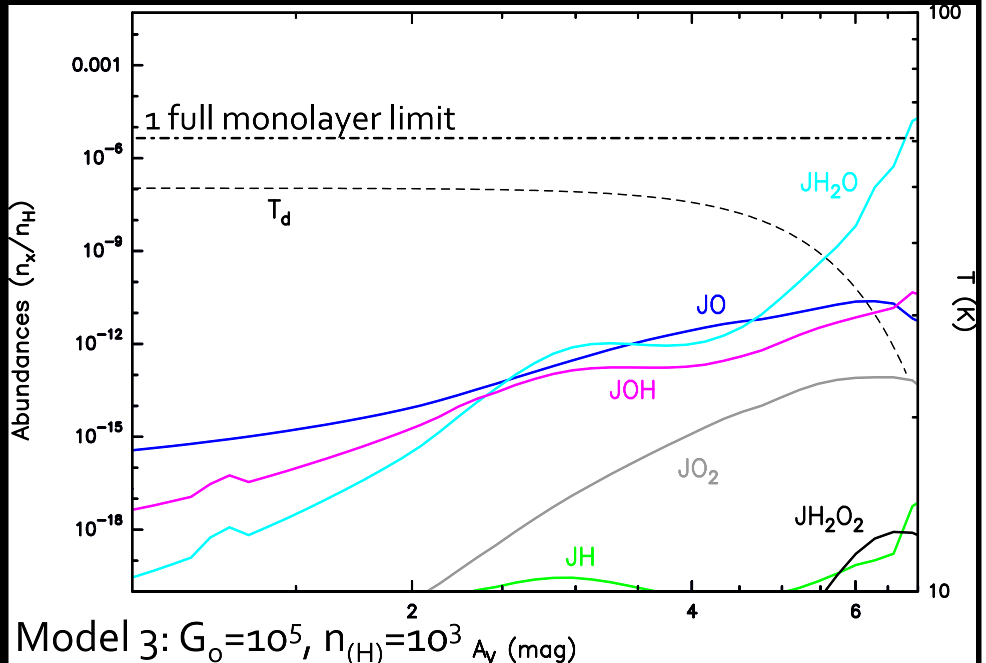


Model 1: $G_o=10^5$, $n_{(H)}=10^5$

- Large impact of G_o on the H_2O ice formation threshold
- Lower impact of *n* on the H_2O ice formation threshold
- Low G_o favours H_2O ice and H_2O_2 ice formation

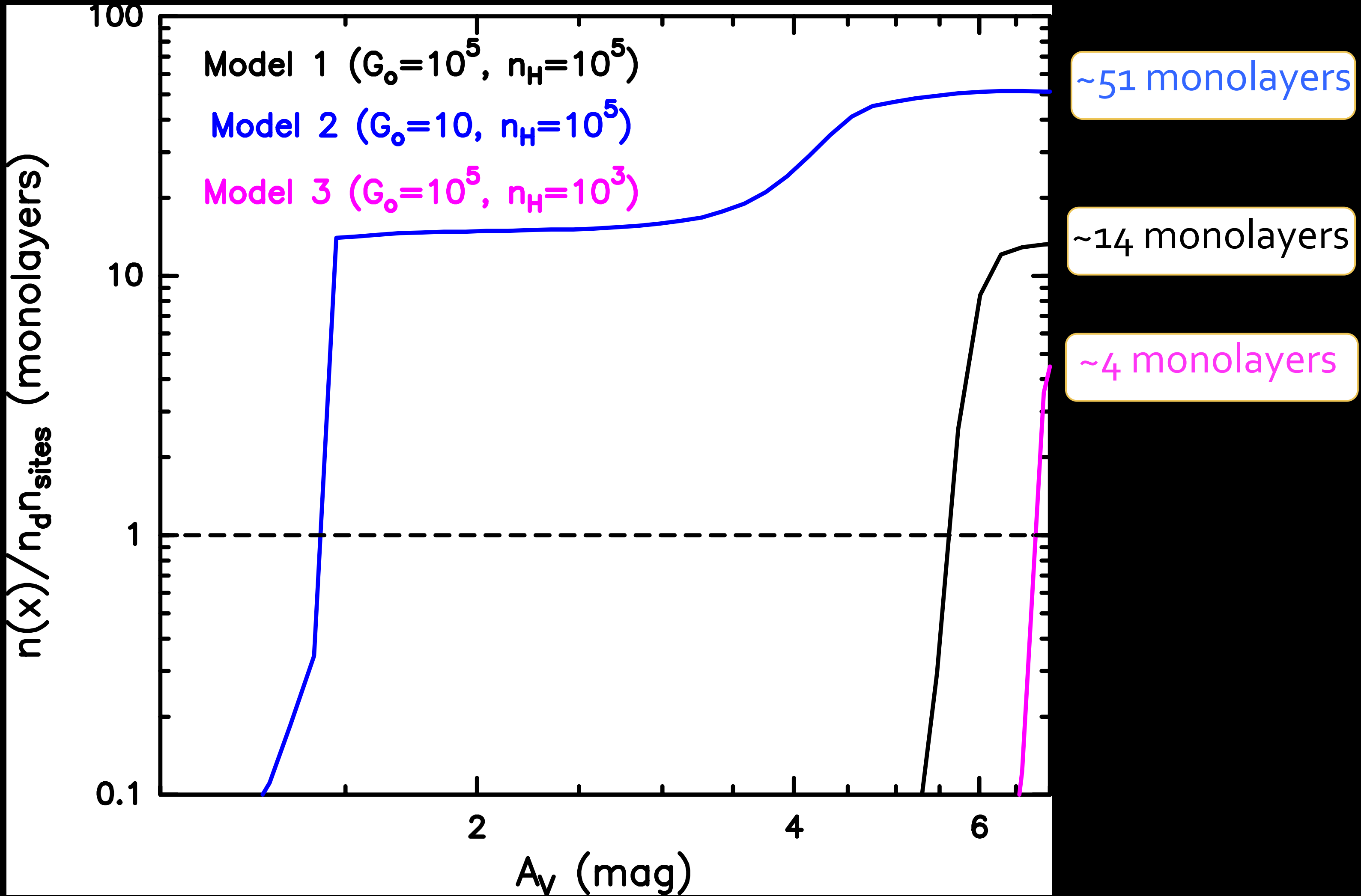


Model 2: $G_o=10$, $n_{(H)}=10^5$



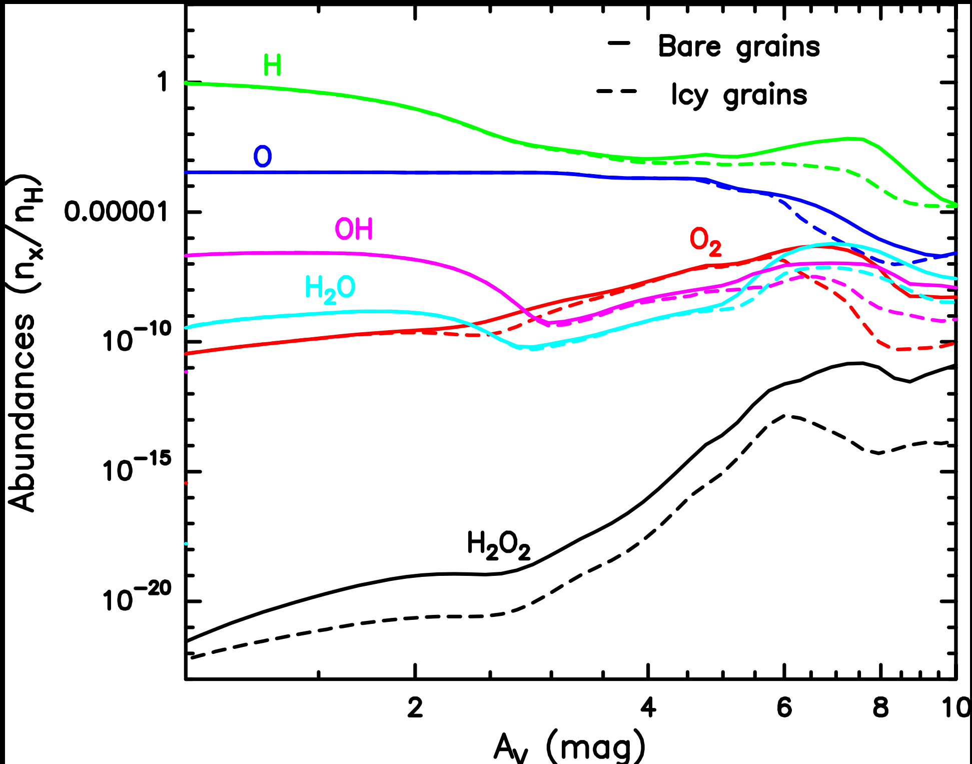
Model 3: $G_o=10^5$, $n_{(H)}=10^3$

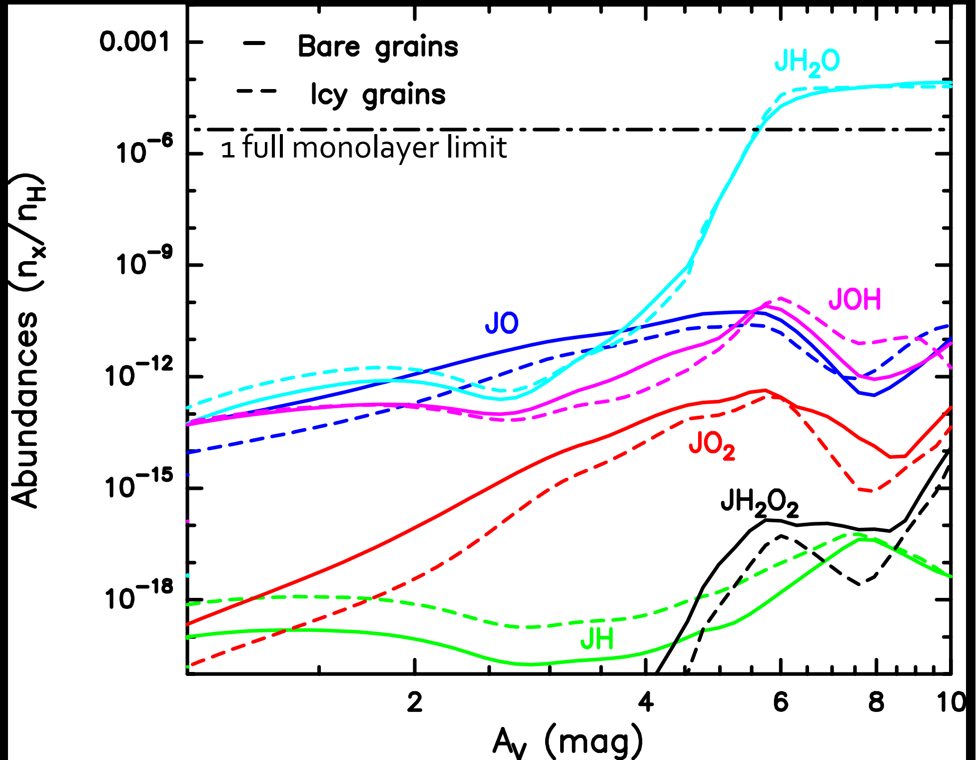
Dust-phase: H_2O ice monolayer formation



- High *n* and, especially, low G_o favour the formation of H_2O ice full monolayers

Water formation: Icy vs Bare grains



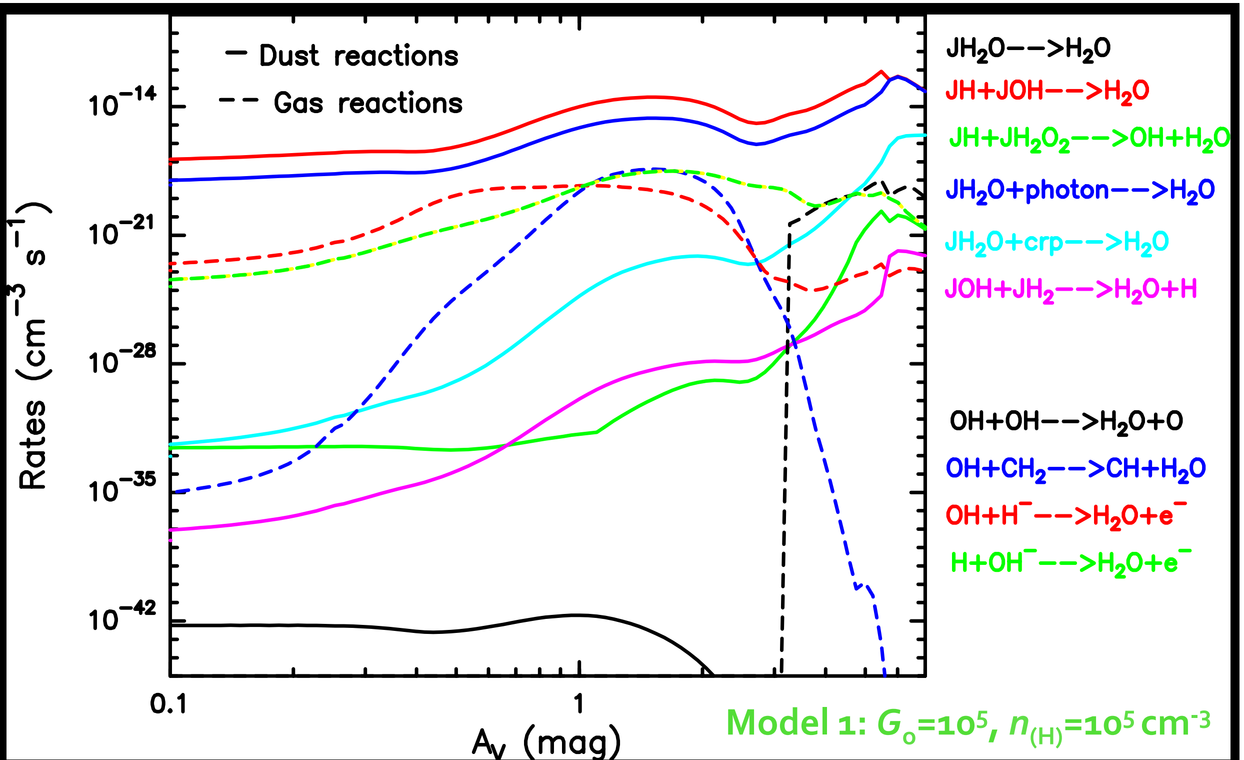


Model 1: $G_o=10^5$, $n_{(H)}=10^5$

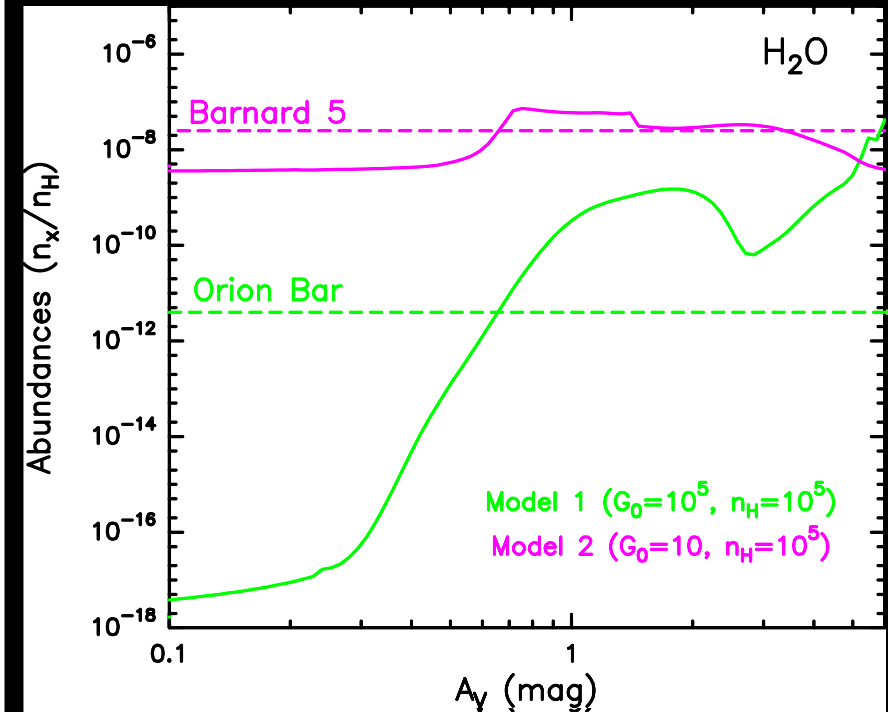
JX means solid X

- Solid H_2O: small differences between icy and bare grains.
- Gas H_2O: abundances ~1 order of magnitude higher with bare grains.
- Bare grains also favour the formation of solid and gas H_2O_2.

Comparison with observations



JX means solid X



Wirström et al. (2014)

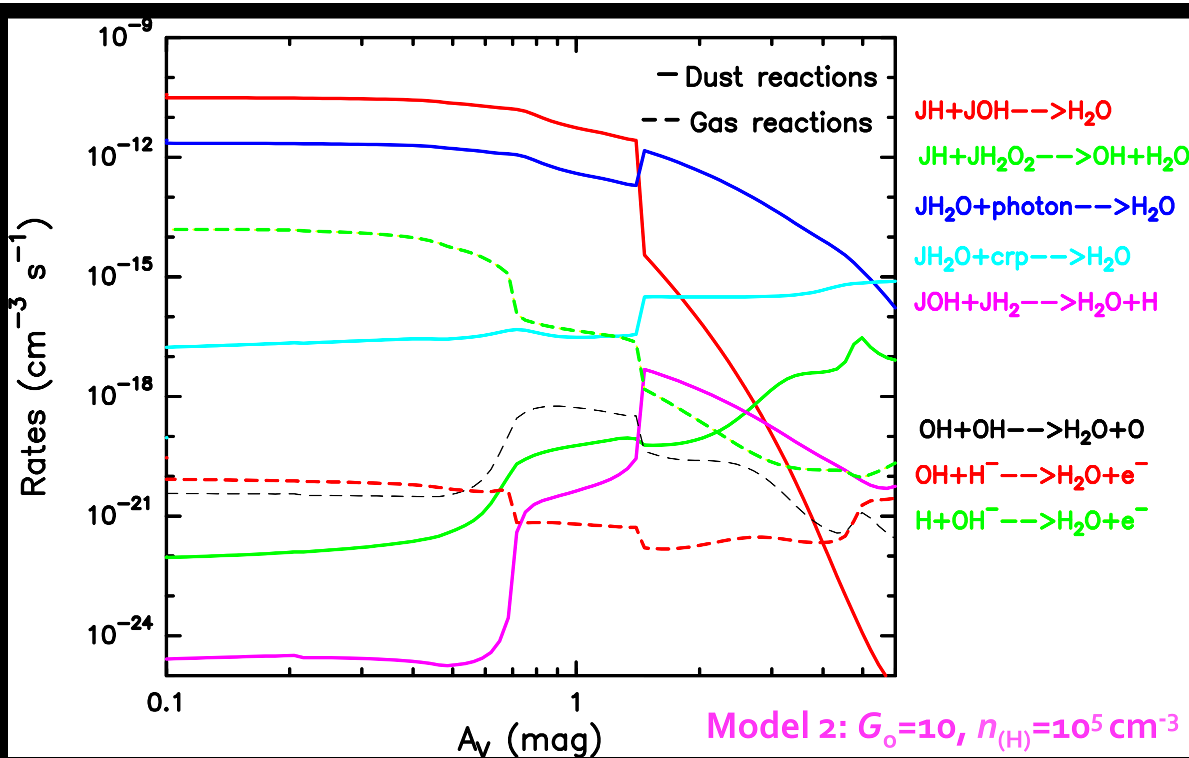
Choi et al. (2014)

-Low contribution from thermal desorption

- Low contribution from surface reactions with H_2O_2 and H_2

In extreme PDRs, gas-phase water formation is mainly dominated by chemical desorption at A_V≤5 mag

Comparison with observations



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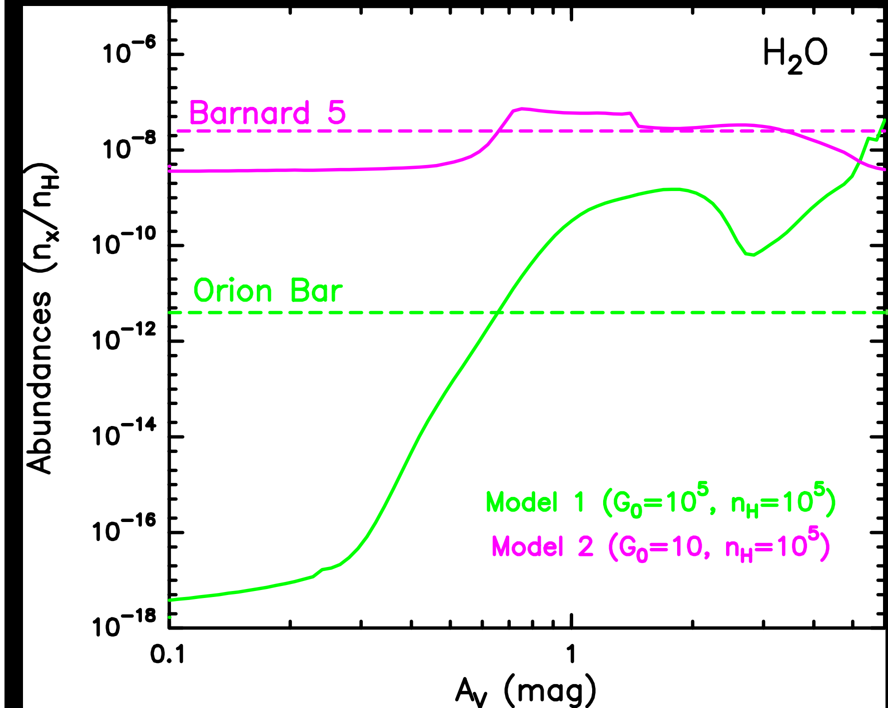

Wirström et al. (2014)

Choi et al. (2014)

In dark clouds, gas-phase water formation is dominated by chemical desorption at A_V<1.5 mag and by photo-desorption at 1.5≤A_V≤5 mag

Conclusions

➡ Chemical desorption and icy-bare dust (different binding energies)

➡ Type of grain substrate:

- Solid water: small abundance differences between bare and icy grains
- Gas water: bare grains favour its formation

➡ Gas water formation precursors (at $A_v \leq 5$ mag):

- Solid H and solid OH

➡ Surface processes forming gas water:

- PDRs: chemical desorption ($A_v \leq 5$ mag)
- Dark clouds: chemical desorption ($A_v < 1.5$ mag) & photo-desorption ($1.5 \leq A_v \leq 5$ mag)