Water trail: from molecular clouds to protoplanetary disks

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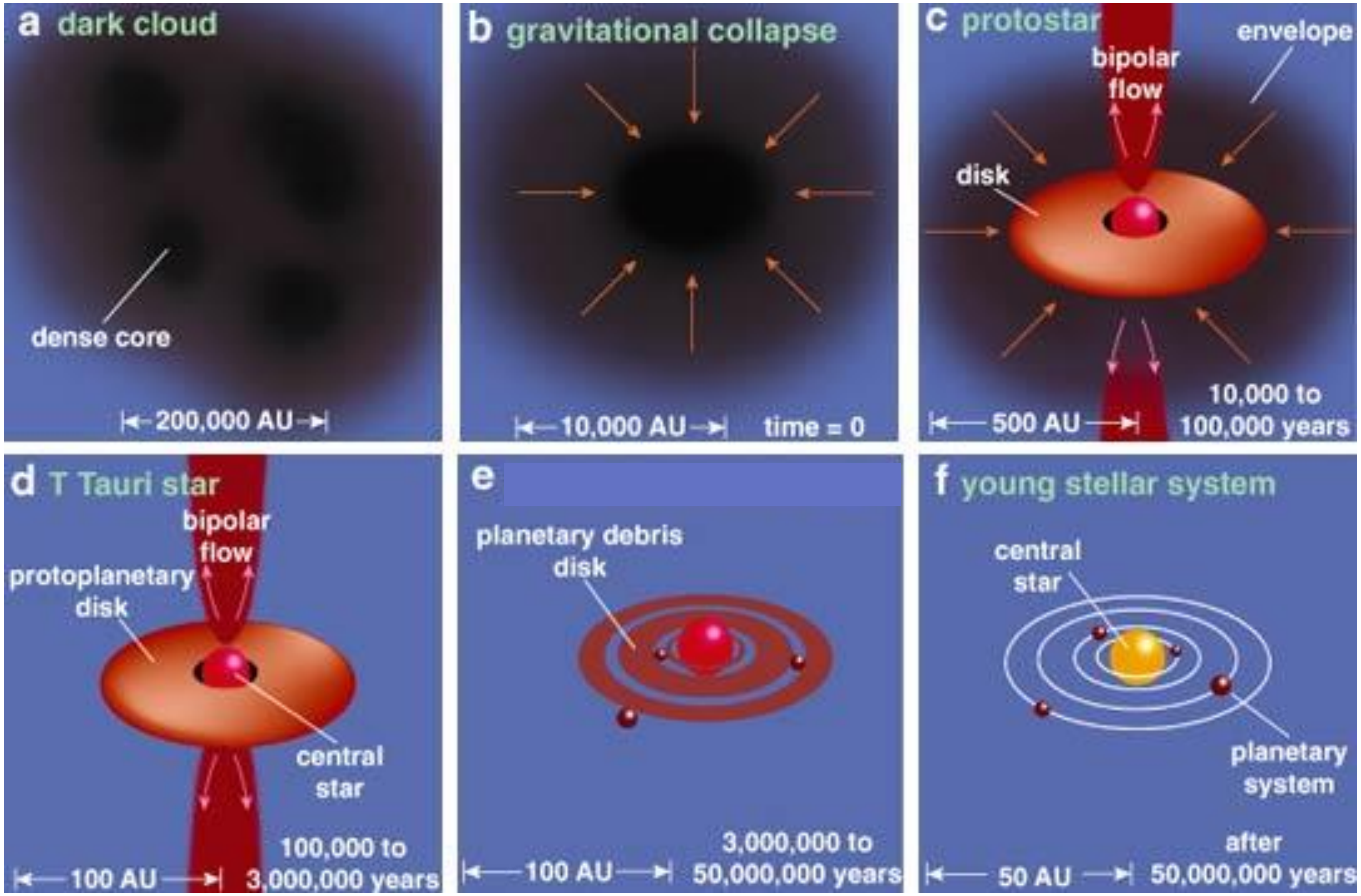
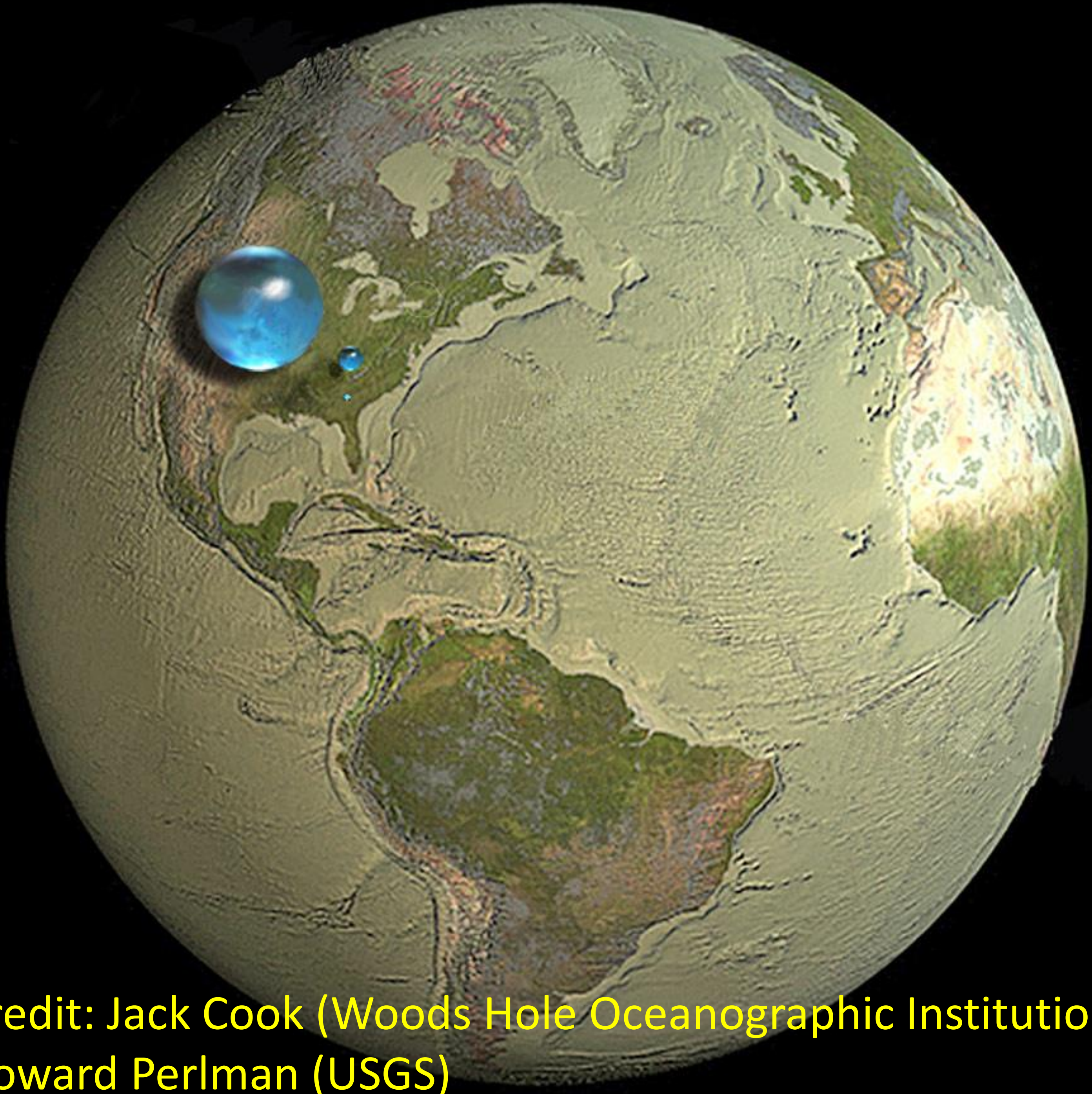
Follow the water trail



(Greene 2001)

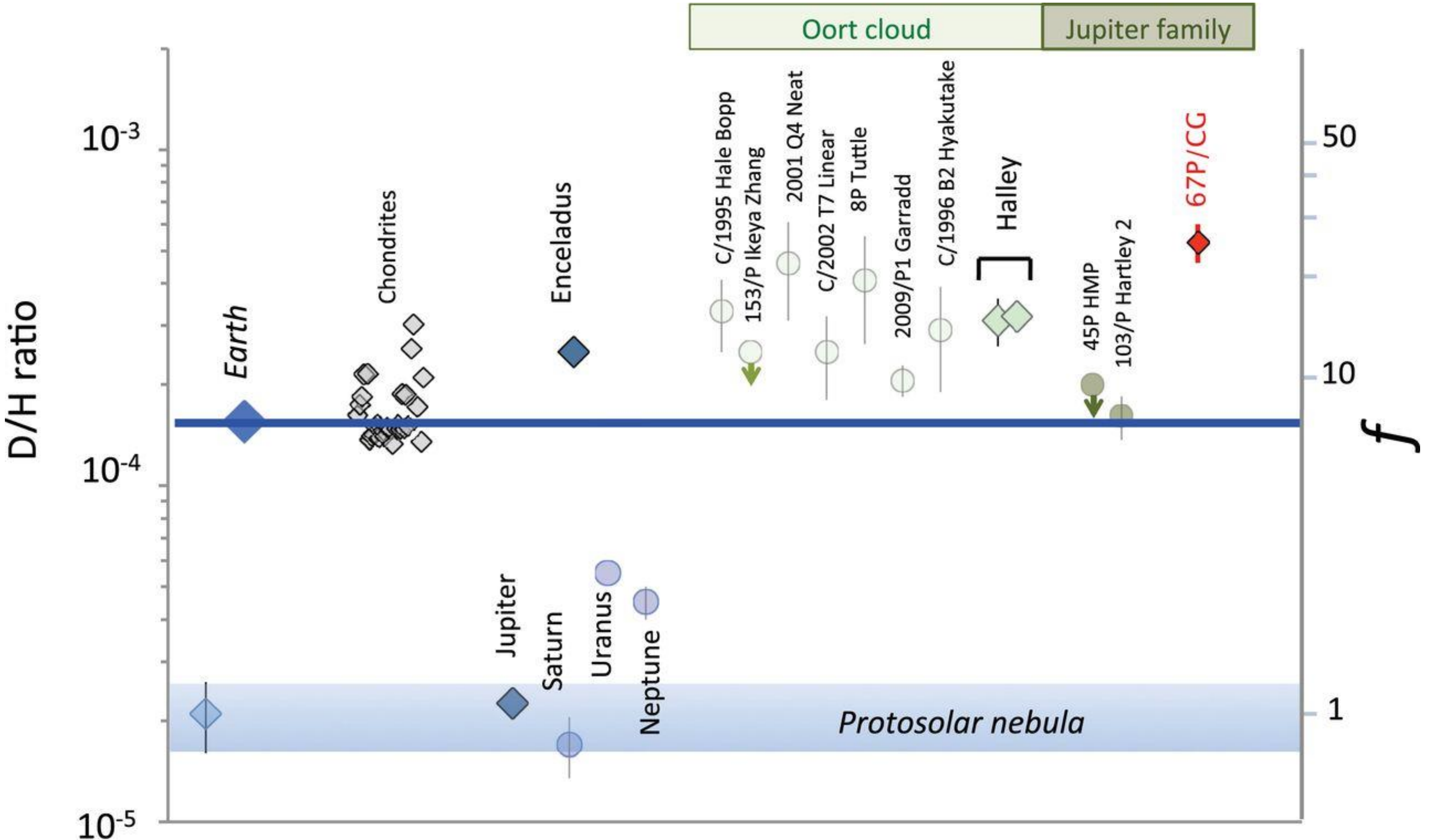
Where did our water come from?

Credit: Jack Cook (Woods Hole Oceanographic Institution) & Howard Perlman (USGS)



Credit: Jack Cook (Woods Hole Oceanographic Institution) & Howard Perlman (USGS)

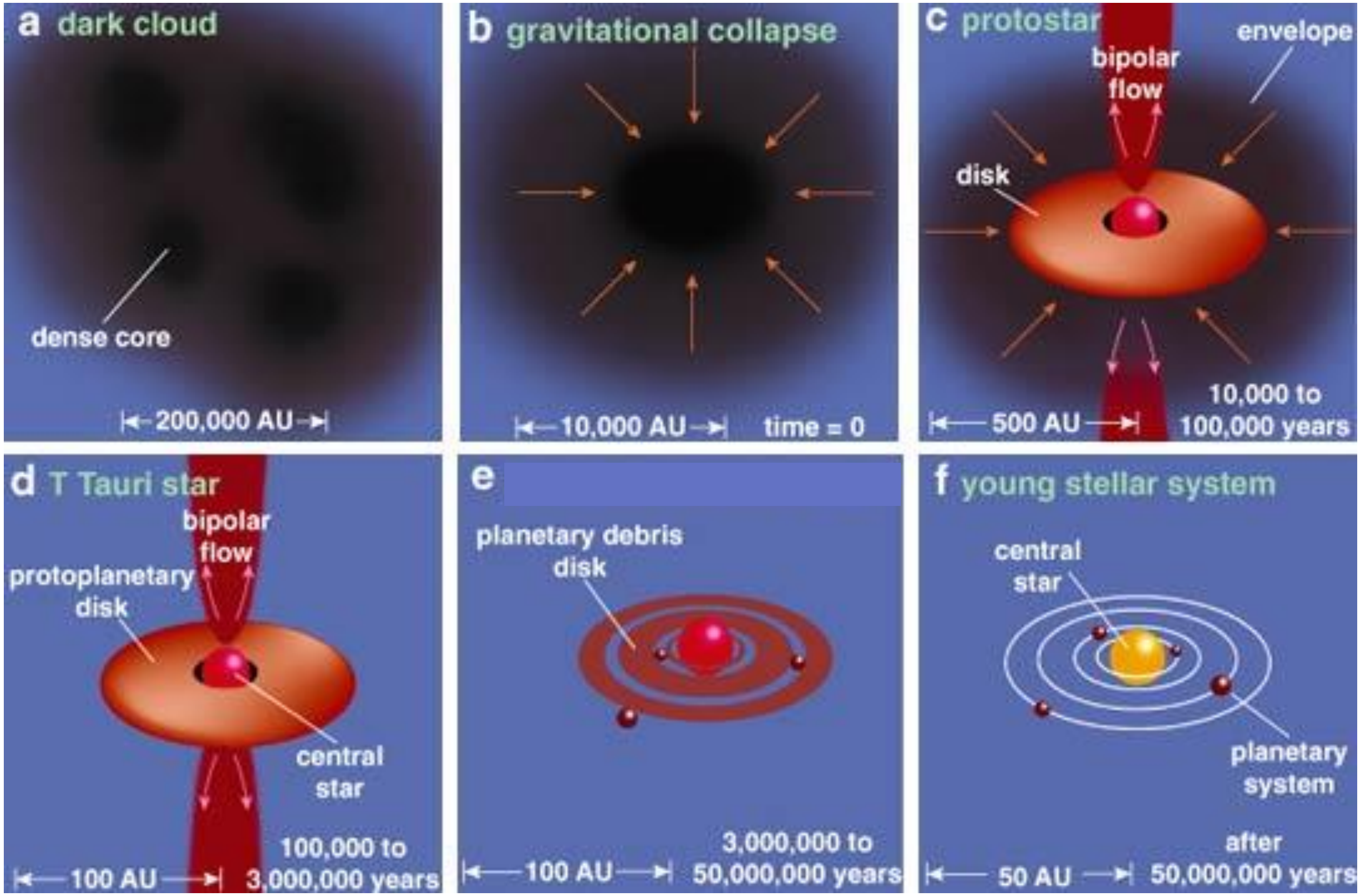
Origin of Earth’s ocean



(Altwegg+2015)

Potential sources of Earth’s ocean: asteroids and comets

Follow the water trail



(Greene 2001)

Where did our water come from?

Contents

- Water chemistry in star-forming regions
- (Water) ice formation in molecular clouds and cores
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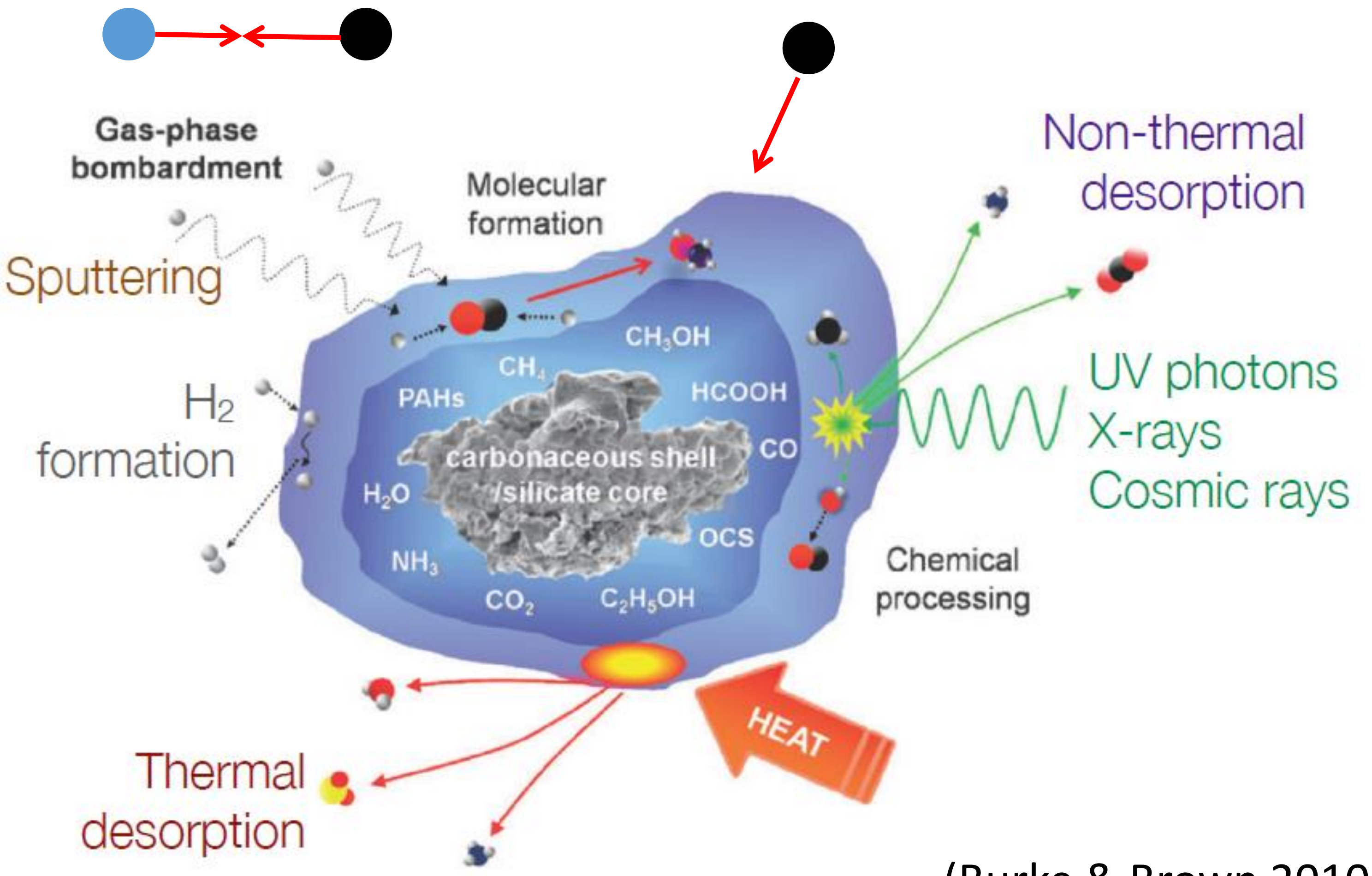
Chemical processes in star-forming regions

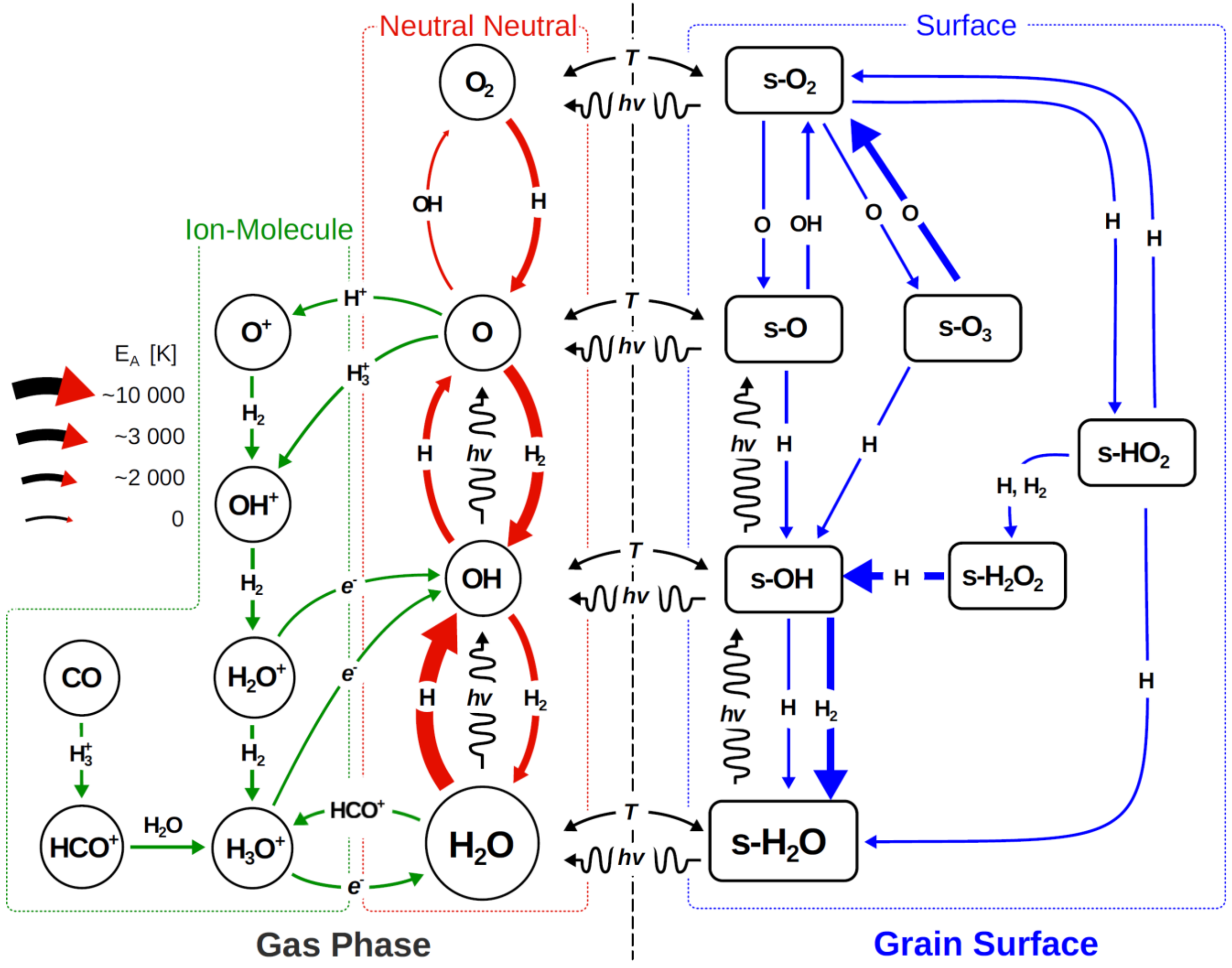
Gas phase reaction

Accretion onto dust grains



(Burke & Brown 2010)

Water chemistry: well studied



(van Dishoeck et al. 2013)

(Original ref. Jensen+2000; Miyauchi+2008; Ioppolo+2008; Oba+2012 and many others)

The formation of water on interstellar dust particles

prof. Ewine F. van Dishoeck, PhD, A.L.M. “Thanja” Lamberts, MSc

Universiteit
Leiden
The Netherlands

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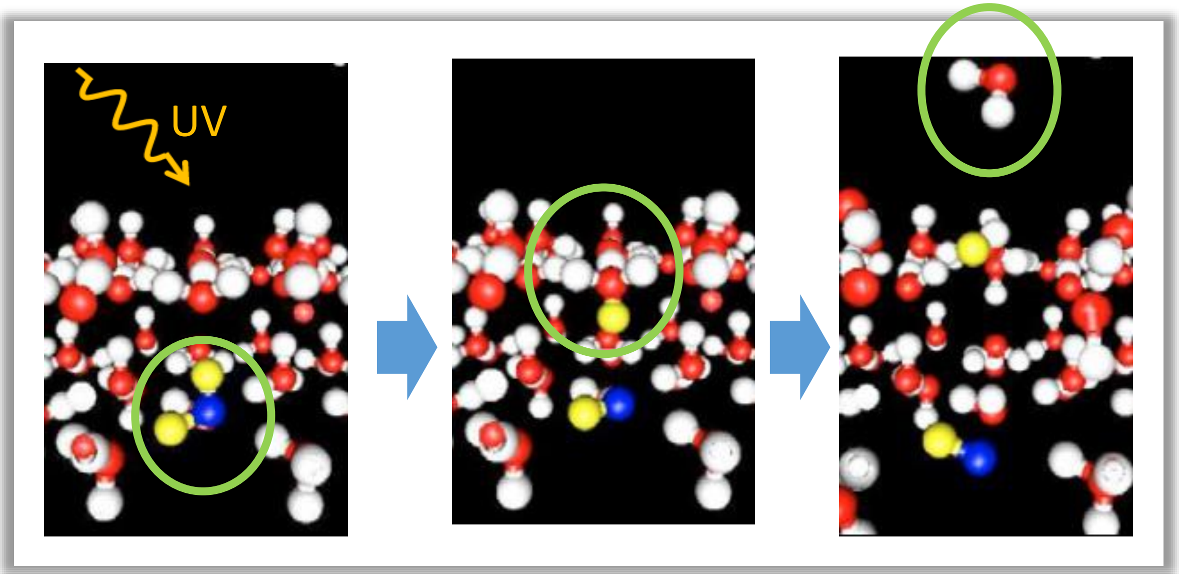
光脱離

- Kick-out

$H_2O(\mathrm{ice}) + h\nu \rightarrow H^* + OH,$

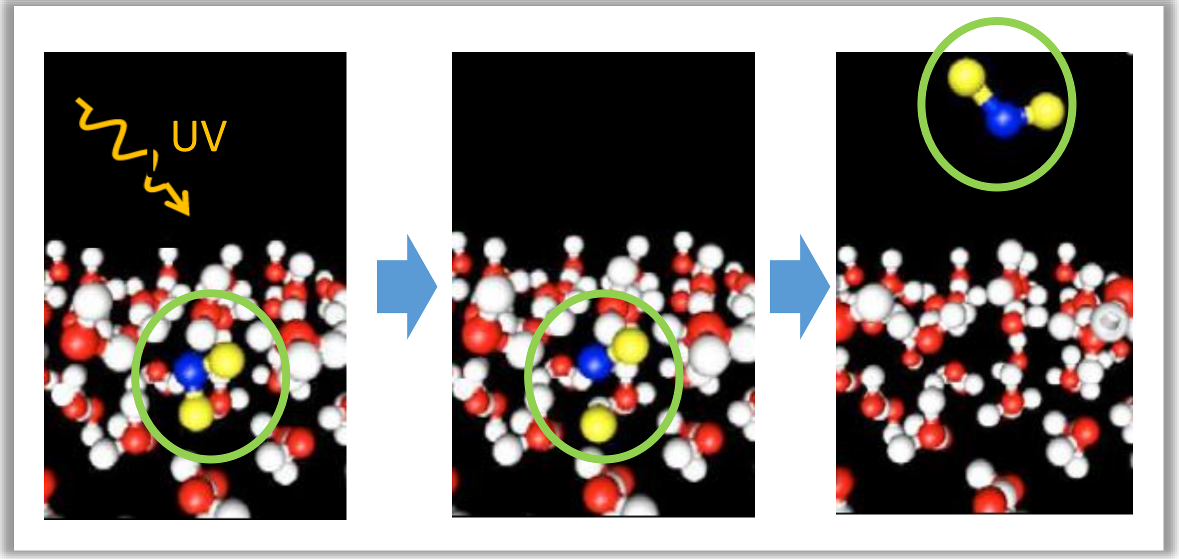
$H^* + H_2O(\mathrm{ice}) \rightarrow H + H_2O(\mathrm{gas}).$



- Recombination

$H_2O(\mathrm{ice}) + h\nu \rightarrow H^* + OH,$

$H + OH \rightarrow H_2O(\mathrm{gas})$



氷表面でのみ

MD計算; Andersson & van Dishoeck (2008)

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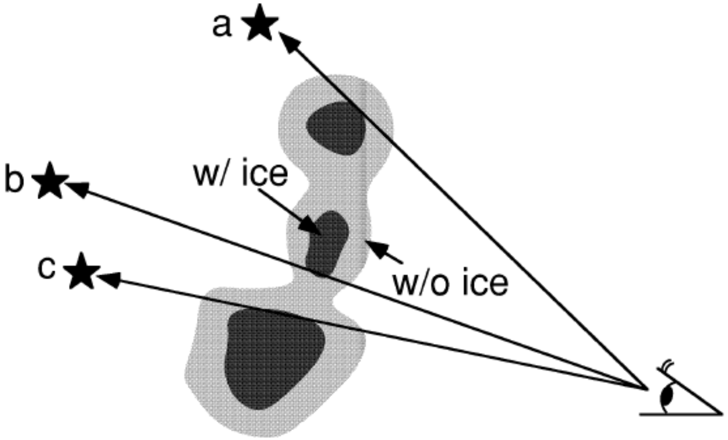
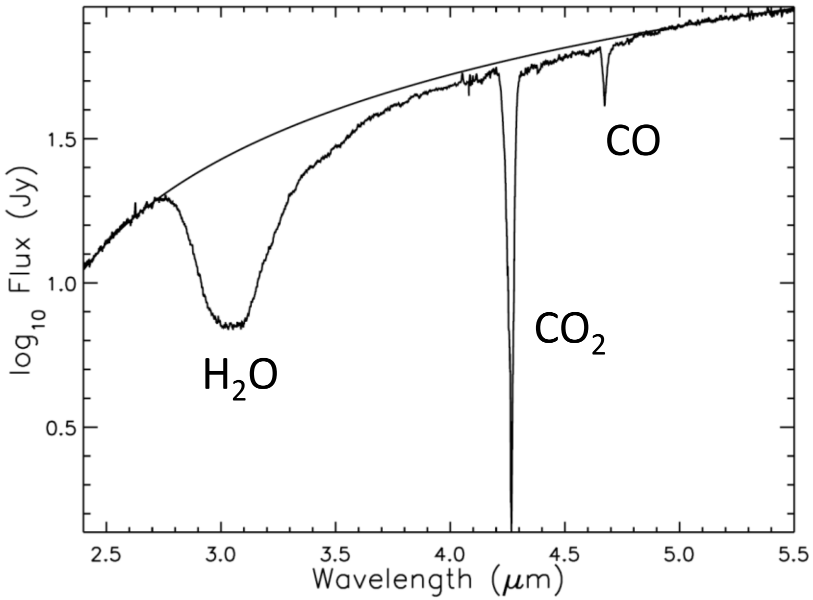
Water in prestellar stages

- 分子雲に既にダストを覆う氷として豊富に存在 (Whittet+1983)
  （1 M_{sun}の分子雲コア → ~1000 M_{earth}の水）
- 酸素の主要な形態 (~40 % of volatile oxygen, Whittet 2007)





(Gibb+ 2004)

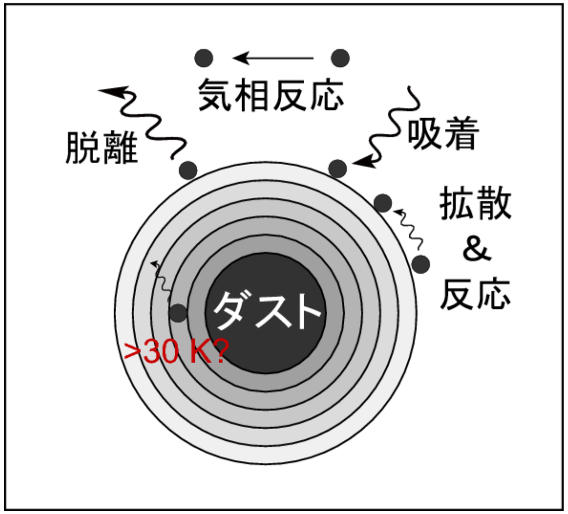
反応ネットワークモデル

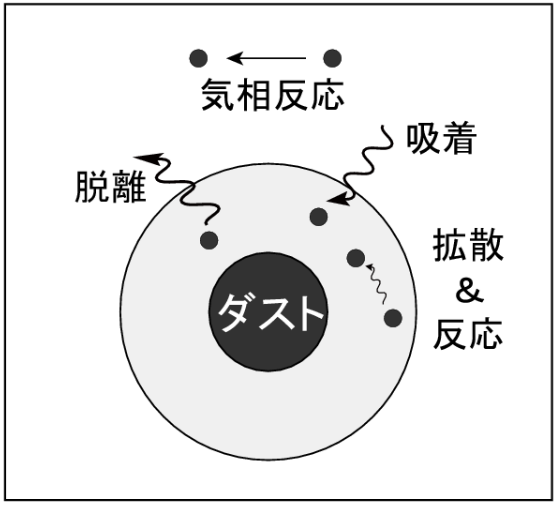
- 基礎方程式

$$\dot{n}_i^{(x)} = \underbrace{P_i^{(x)} - L_i^{(x)}}_{\text{化学反応}}$$

n_i ：化学種 i の数密度

x : 気相、氷表面、氷マントル





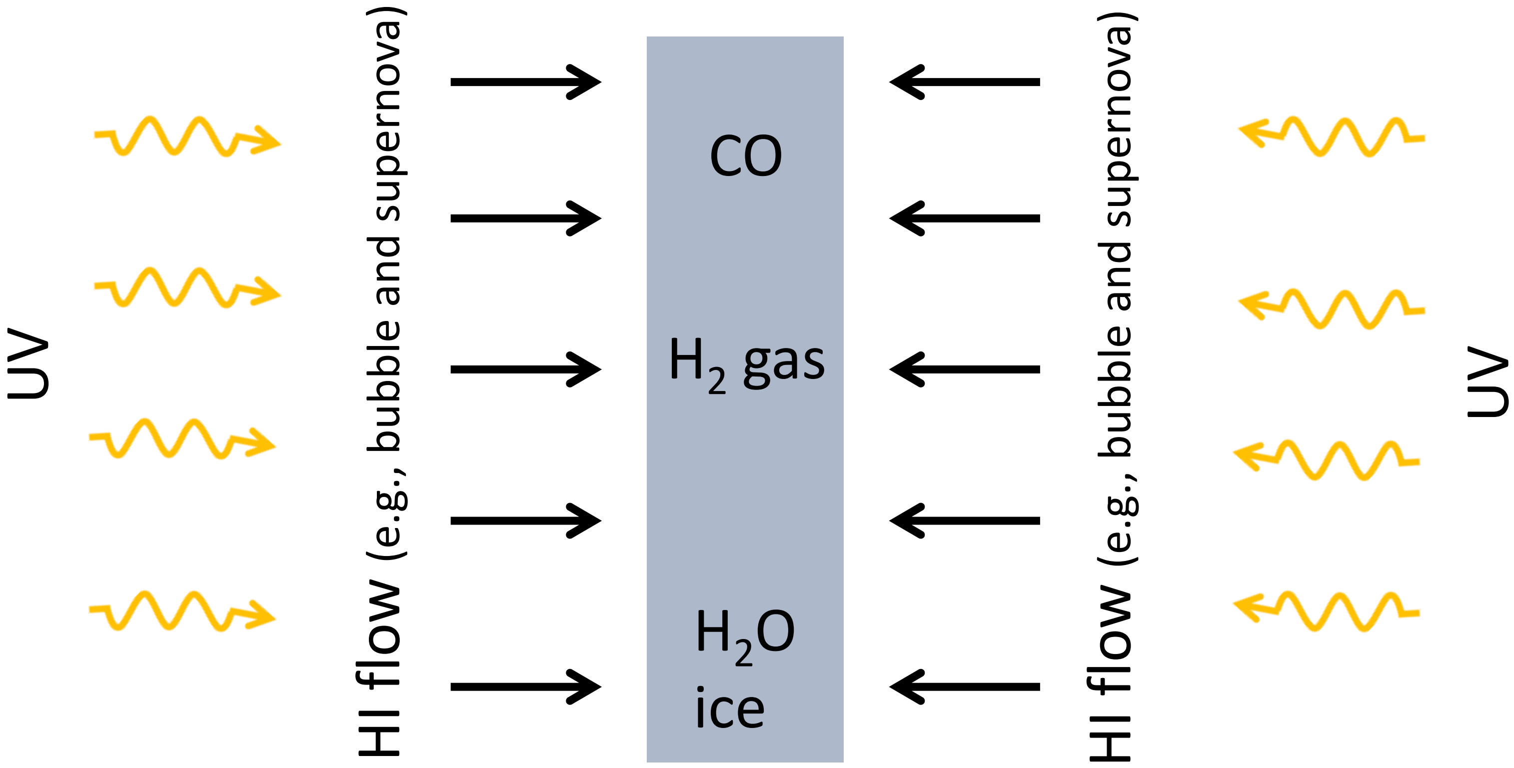
- 多層モデル(e.g., Taquet+2012)
  - 気相
  - 氷表面
  - 非一様な氷マントル

  相互作用

- 単層モデル(Hasegawa & Herbst 1992)
  - 気相
  - 一様な氷マントル

  相互作用

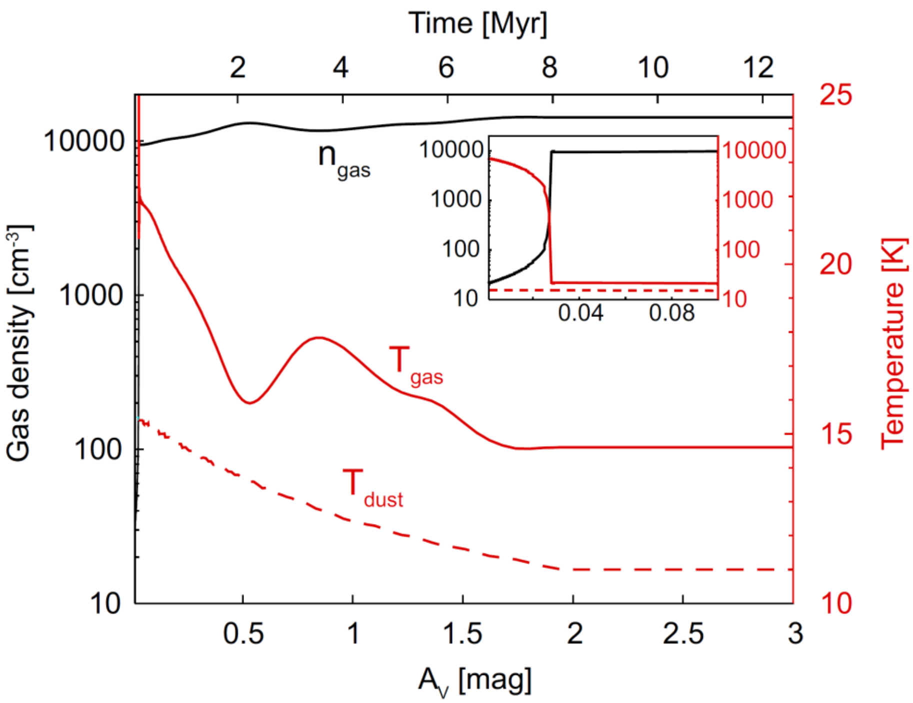
Molecular cloud formation

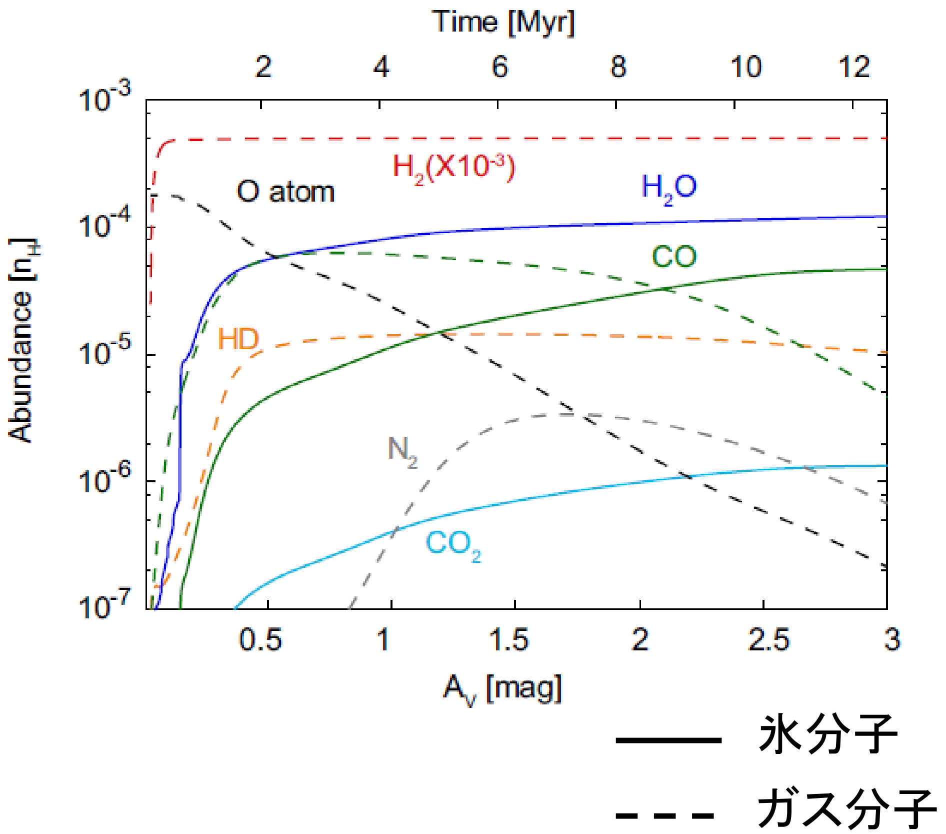


Accumulation of HI gas by accretion flows
→ molecular cloud formation

(e.g., Hartmann+2001; Inoue&inutsuka 2012)

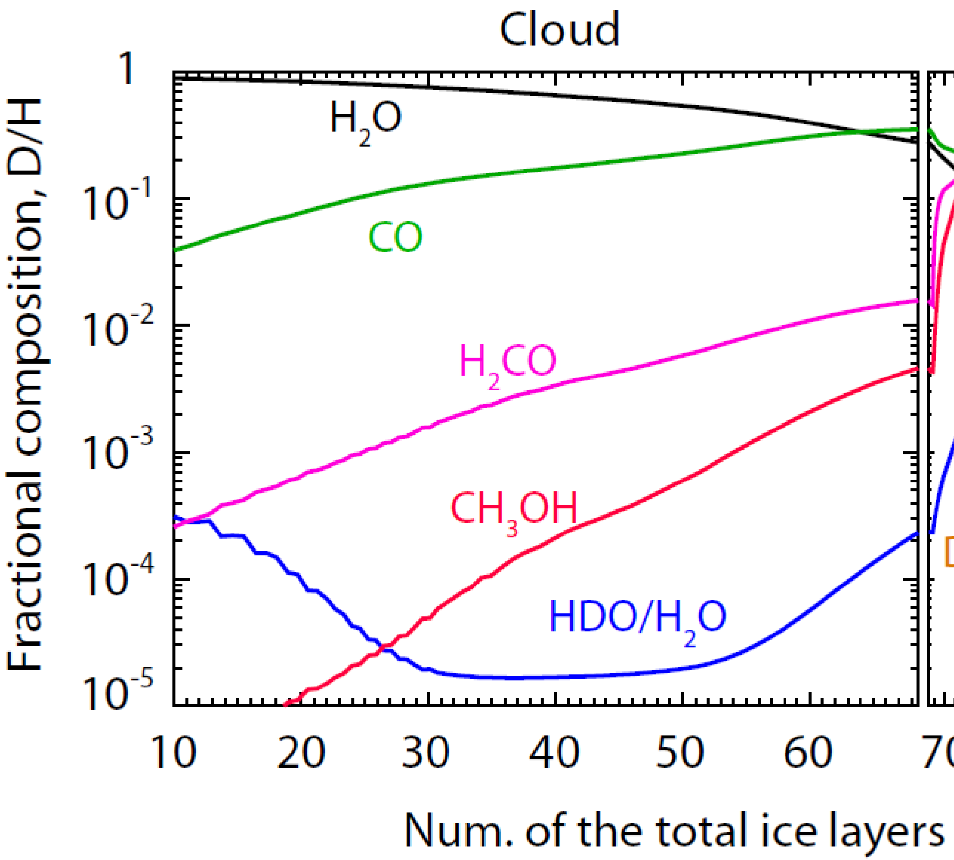
Atomic-to-molecular transitions





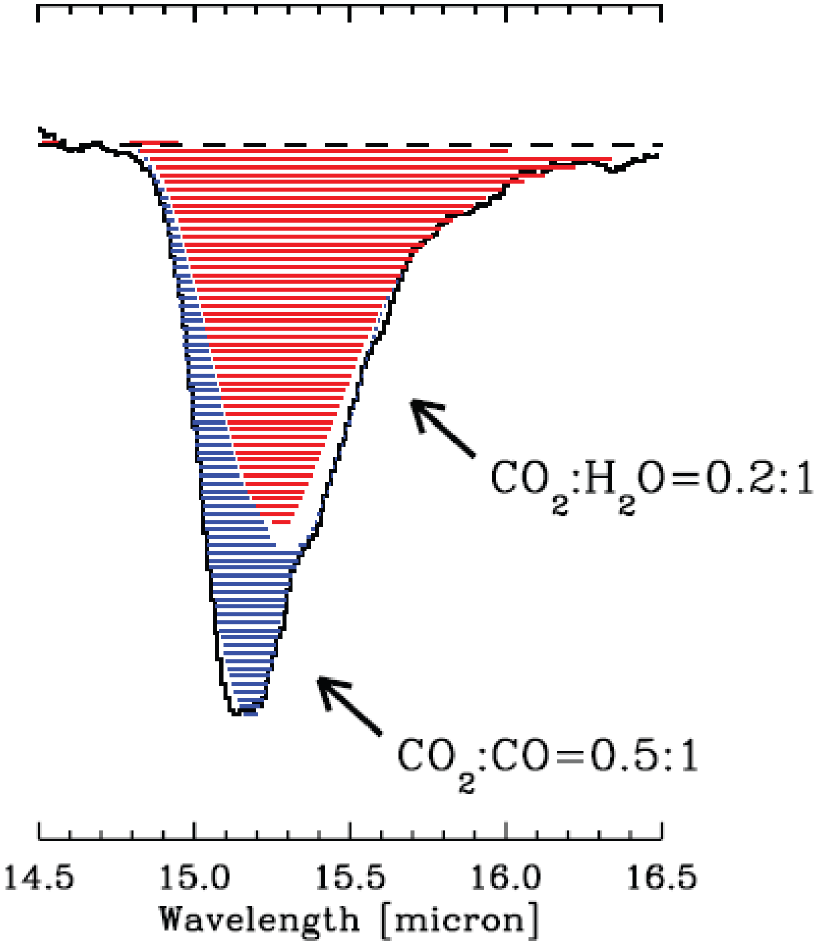
- 1D流体 + heating/cooling + gas-phase chemistry (Bergin+04)
- Post-processing gas-ice chemistry
- 柱密度増加→ 星間紫外線の遮蔽 → 原子から分子へ

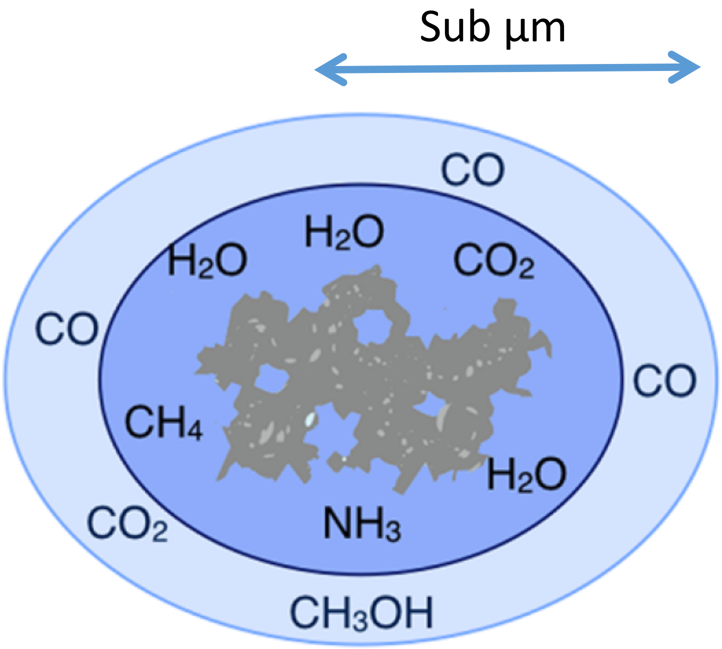
Ice layered structure



(Furuya+2015,2016)

Layered ice structure in the ISM ice

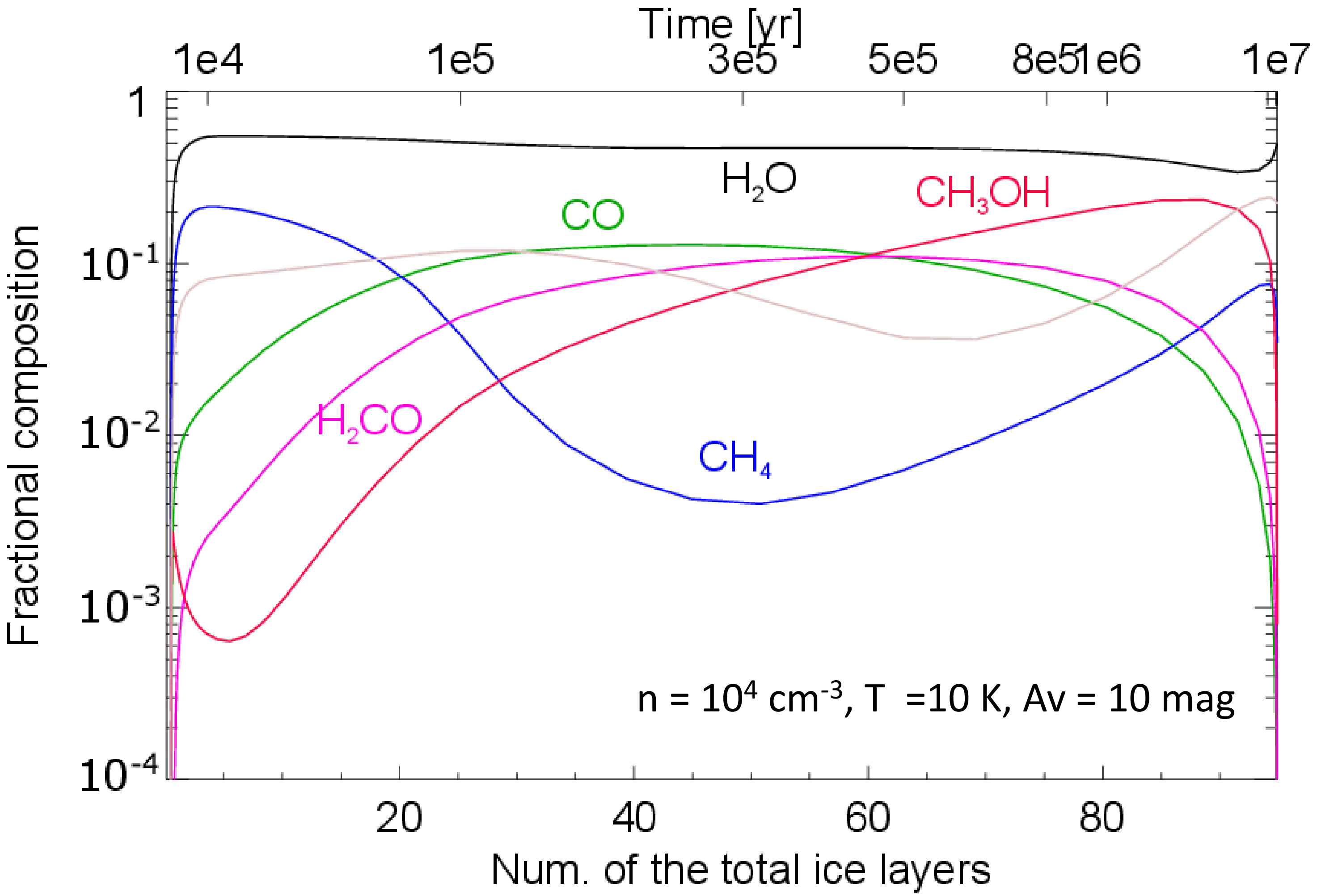




(Pontoppidan+ 2008; Ehrenfreund+1997)

(Oberg 2016; Pontoppidan 2006)

Pseudo-time dependent model of dense clouds

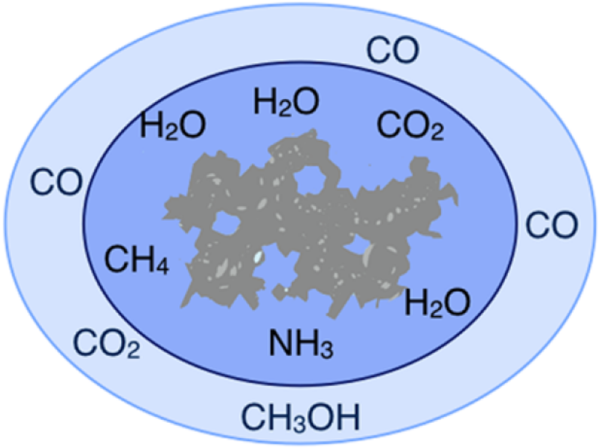


(see e.g., Garrod & Pauly 2011)

Intermediate summary

- Water is formed before the stellar birth as ice
- Chemical (and Isotopic) compositions in the ISM ice are inhomogeneous

  → preserves memory of the physical and chemical evolution



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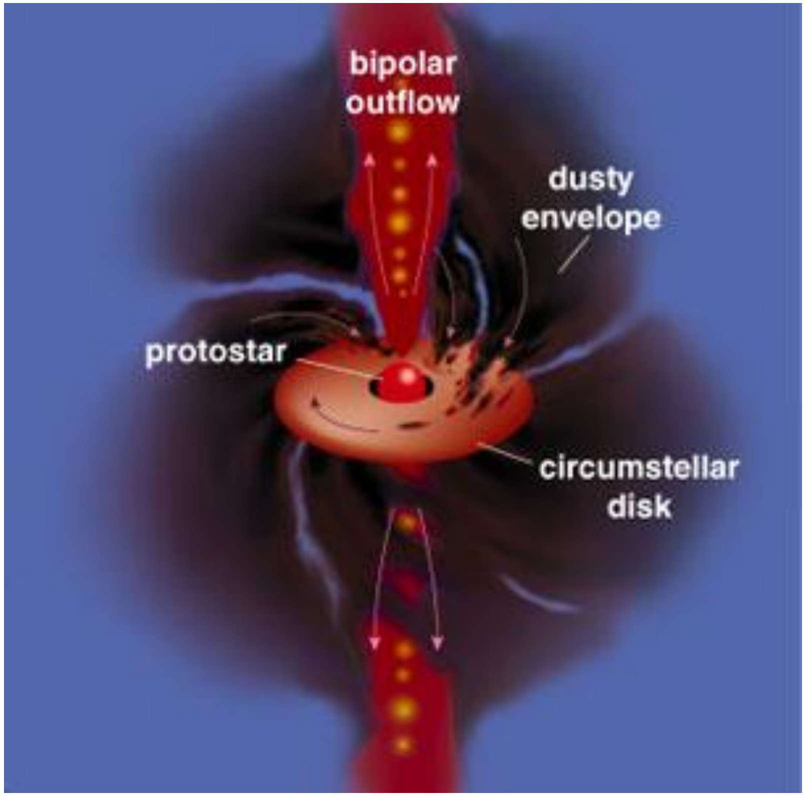
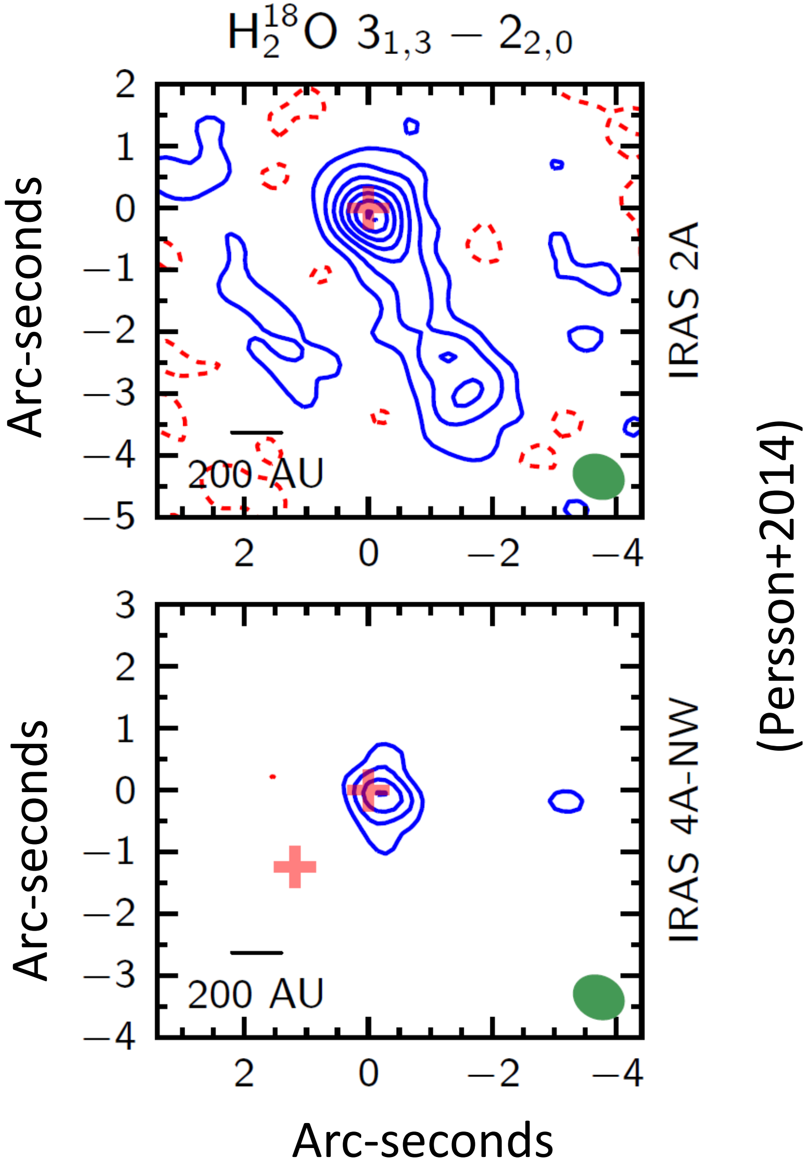
Hot water near protostars



(Greene 2001)



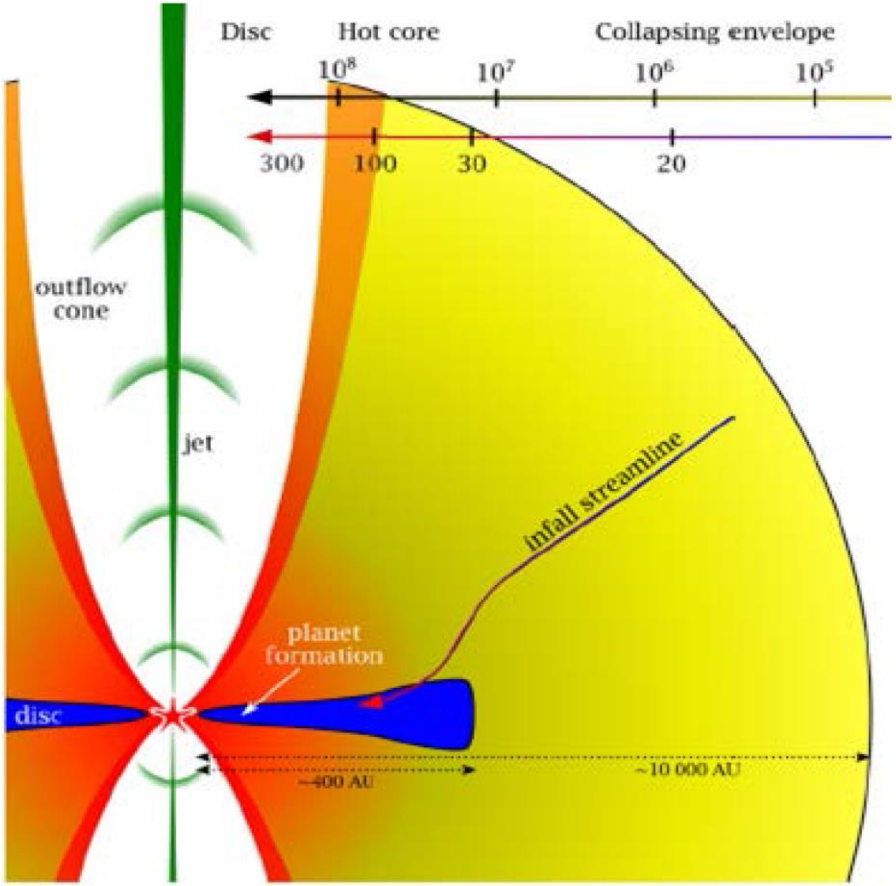
(Persson+2014)

Open question:

Where do the water emissions originate from?

Envelope, disk, or both?

Ice delivery from cores to disks



(Herbst & van Dishoeck 2009)

2-D collapsing core model to the disk formation

(Visser+2009, 2011)

- Density & velocity
  -semi analytical models
  (Terebey+1984; Cassen&Moosman 1981; α-disk model)
- Temperature & UV field
  - radiative transfer
  (RADMC-3D; Dullemond&Dominik 2004)
- Chemistry is solved along trajectories of in-falling materials

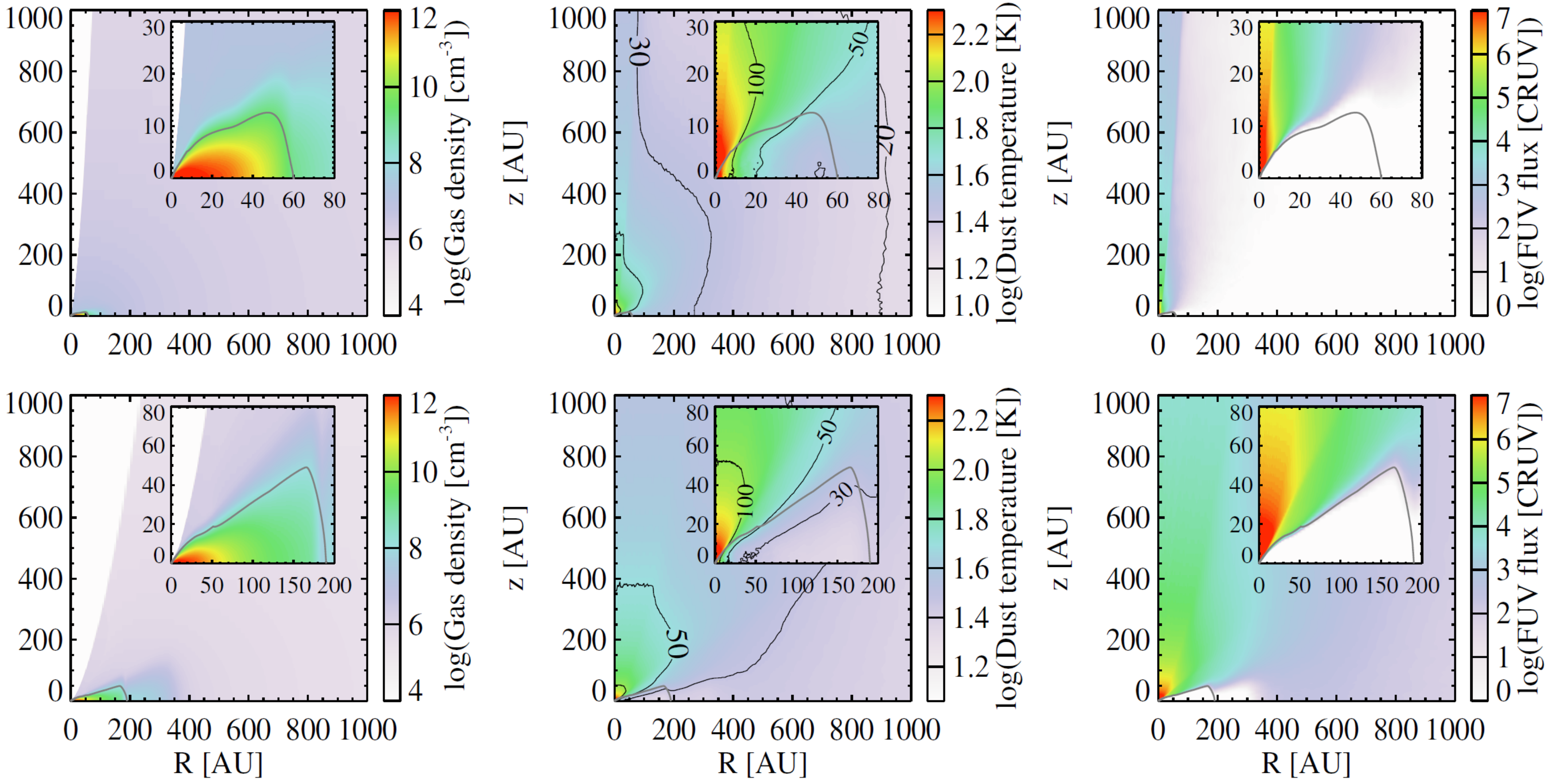
Physical evolution

密度

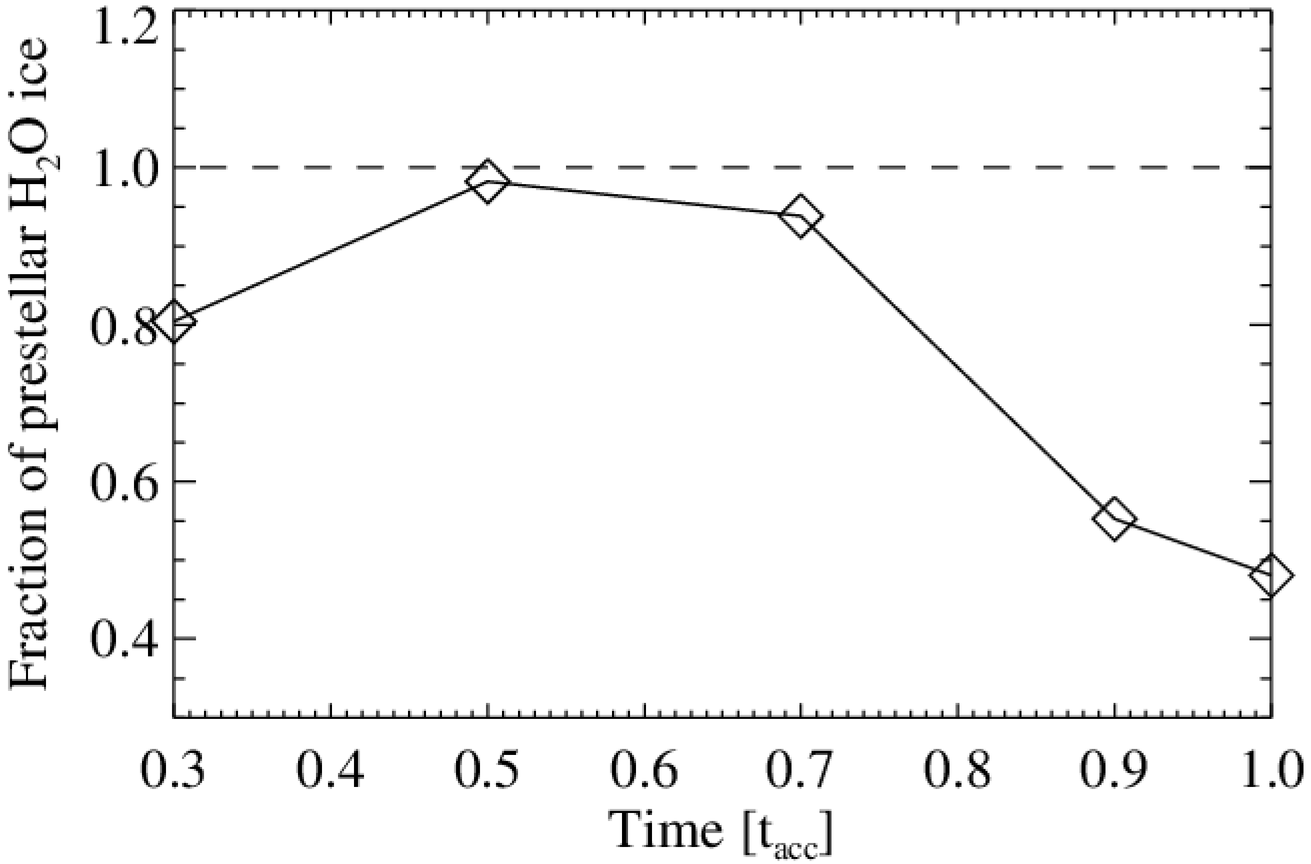
温度

FUV field

time



Bulk-disk averaged H_2O ice abundance



0.01 M_{sun} disk → several M_{earth} water ice, being inherited from the prestellar stages

Intermediate summary

- Forming disks contain lots of interstellar H_2O ice

→ favorable for the formation of icy planetesimals (and planets)

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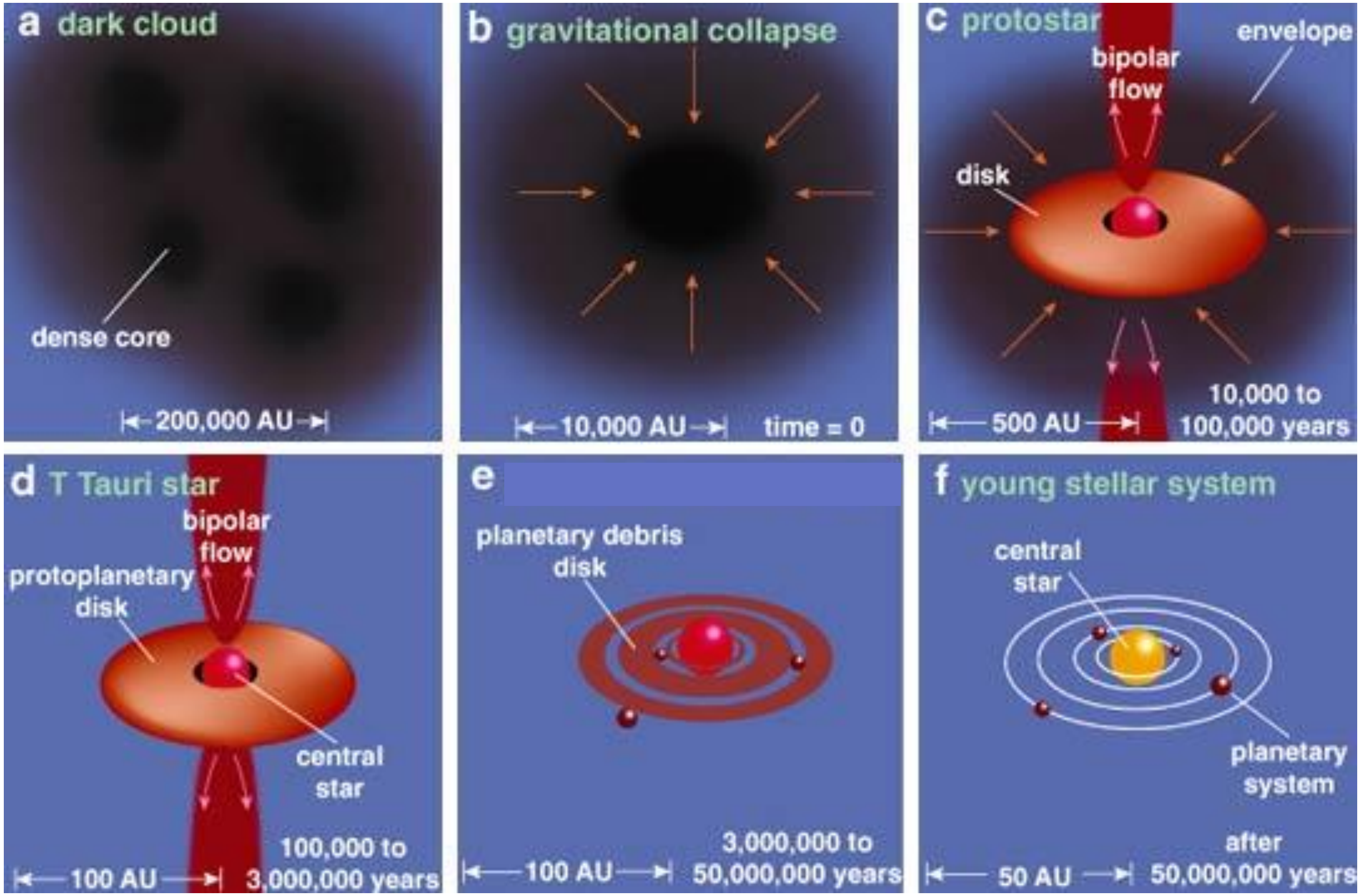


(Greene 2001)

Where did our water come from?

Deuterium fractionation

➡ Probe of the formation environments of molecules

- The [D/H] elemental ratio in the local ISM ~ 10^{-5} (Linsky 2003)
- Molecules formed at low temperatures, XD/XH >> 10^{-5}

(e.g., Watson+1976; Tielens 1983)

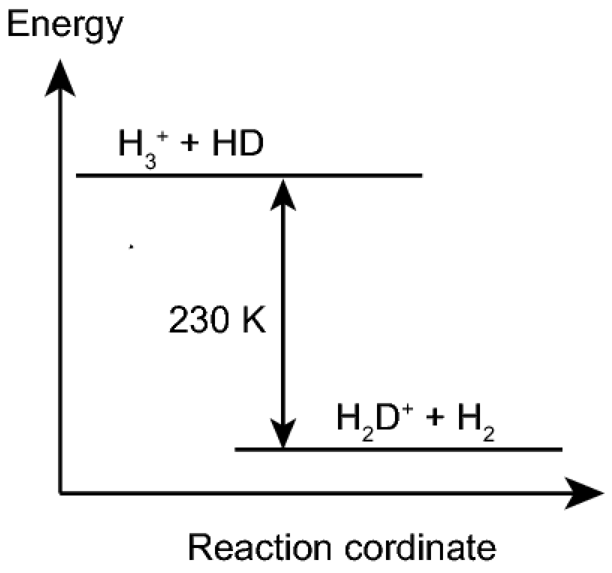
$H_3^+ + HD \overset{\longrightarrow}{\cancel{\longleftarrow}} H_2D^+ + H_2 + 230\ \text{K}$

➡ $H_2D^+/H_3^+ >> 10^{-5}$

$H_2D^+ + e \rightarrow D + H_2$

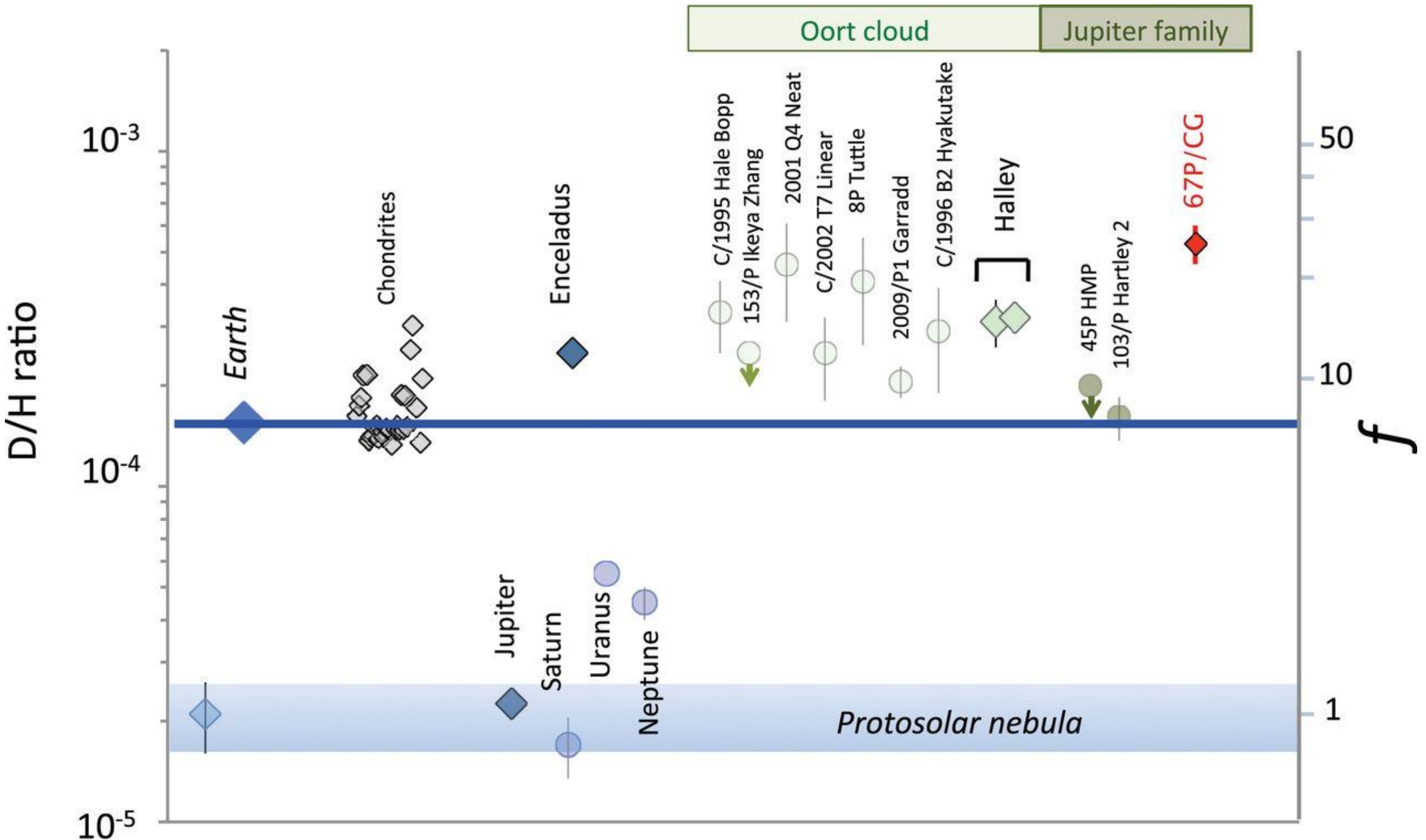
➡ High atomic D/H

➡ High D/H in Icy molecules



- CO freeze-out, higher density, lower H_2 o/p
  → enhanced deuterium fractionation

HDO/H_2O measurements



(Altwegg+2015)

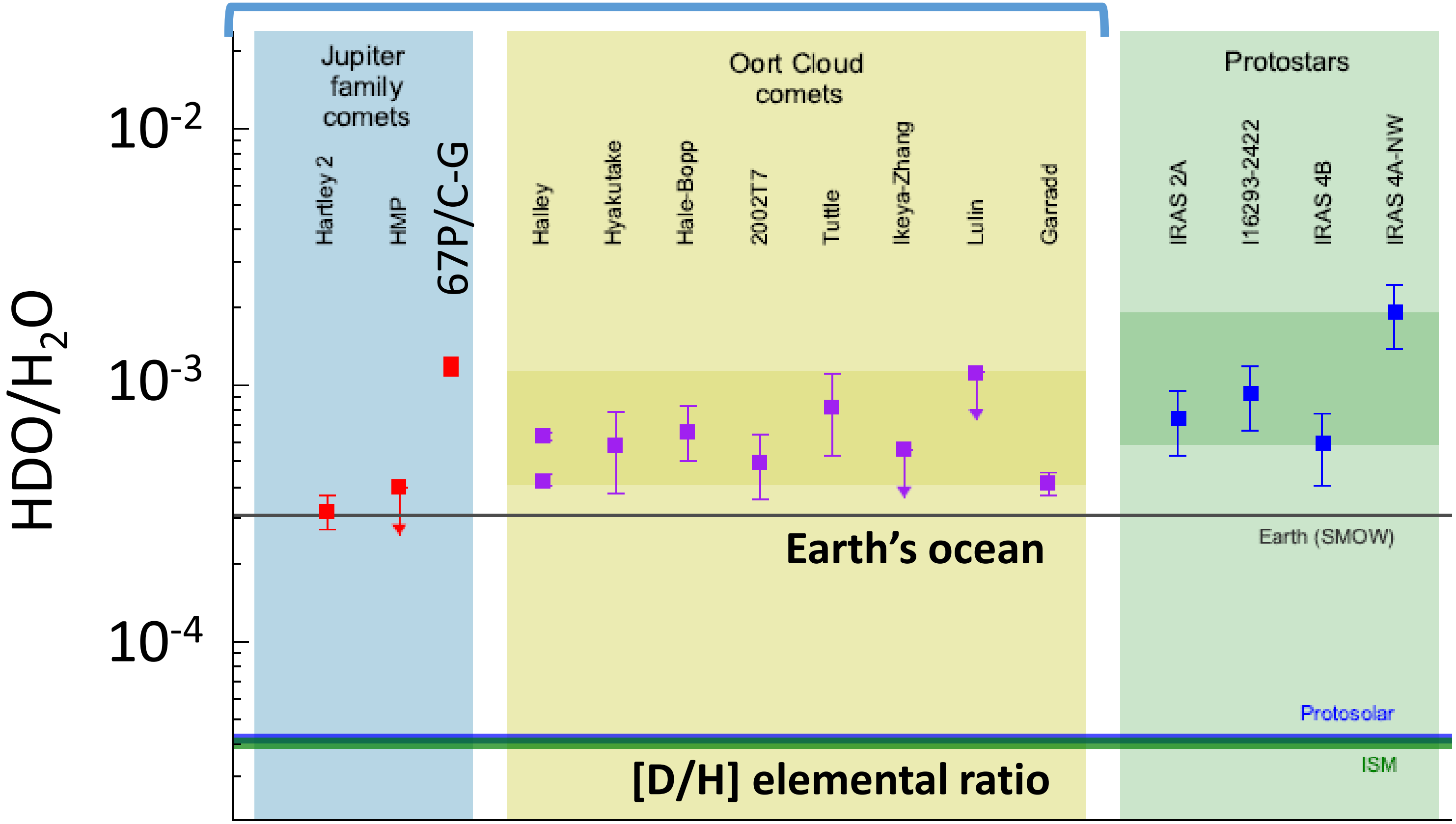
Water is enriched in deuterium → formed at low temperatures

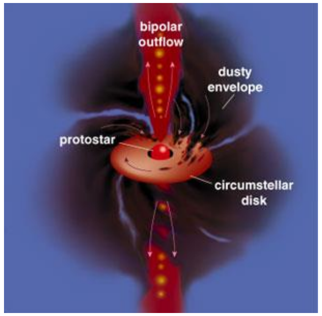
→ In molecular clouds? Or in disks?

HDO/H_2O measurements

Cometary coma
(~ice in the protosolar disk)

Hot gas (>100 K) around
protostars (~ISM ice)





(Mumma & Charnley 2011; Altwegg+2015; Persson+ 2014)

- The ISM and cometary water have the similar HDO/H_2O
  → prestellar inheritance? BUT…

Prestellar inheritance of water?

BUT

- Variations of HDO/H_2O in pristine materials in the solar system -> how?

- In-situ formation in disks can also explain the cometary HDO/H_2O ratios

(e.g., Furuya+2013; Albertsson+2014)

Yet inconclusive

(e.g., Geiss & Reeves 1981; Aikawa & Herbst 1999)

Heavy water (D_2O)

- In the hot inner regions around a protostar

  → $D_2O/HDO = 7*HDO/H_2O$ (Coutens+ 2014)

- The ratio of D_2O/HDO to HDO/H_2O reflects the ice layered structure (i.e., preserves memory of the physical and chemical evolution) (Furuya+ 2016)

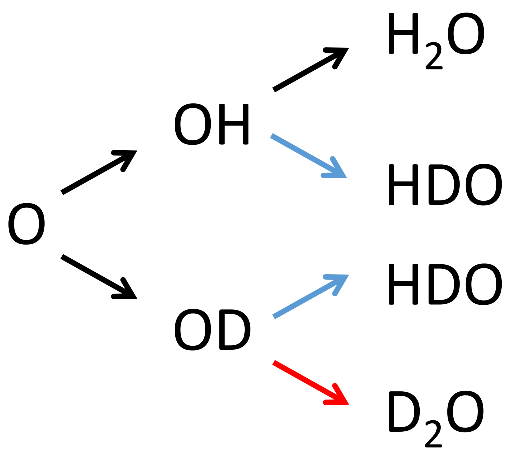
- The ratio is a better probe to distinguish between the two cases (inheritance vs. in-situ formation in disks)

  → D_2O observations toward comets are crucial

  (Furuya+ in prep.)

Constant atomic D/H case

i.e., assumes quasi-steady state



O

OH

OD

H_2O

HDO

HDO

D_2O

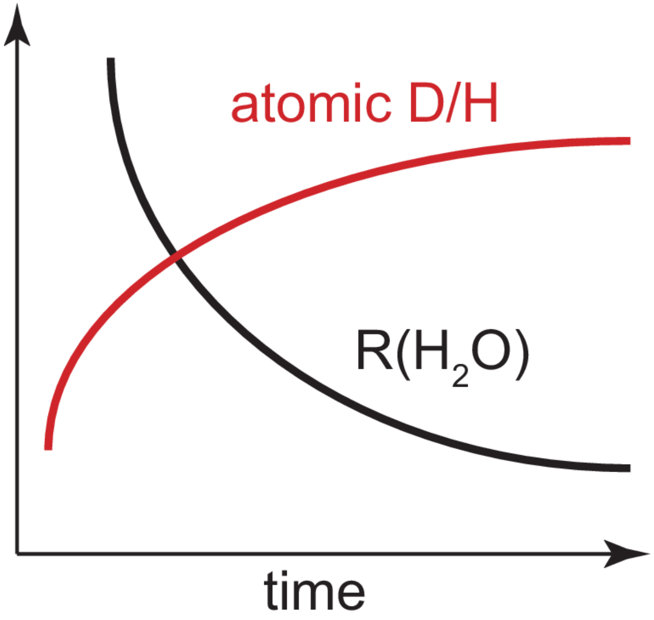
$$\frac{D_2O}{HDO} \leqq \frac{1}{4}\frac{HDO}{H_2O}$$

(e.g., Roberts&Charnley 2002; Oba+2012,2014)

contradicts with the observational relation $\frac{D_2O}{HDO} \sim 7\frac{HDO}{H_2O}$

→ time-dependency of the atomic D/H

Consider chemical evolution



$R(HDO) \propto R(H_2O)*(\text{atomic D/H})$
$R(D_2O) \propto R(H_2O)*(\text{atomic D/H})^2$

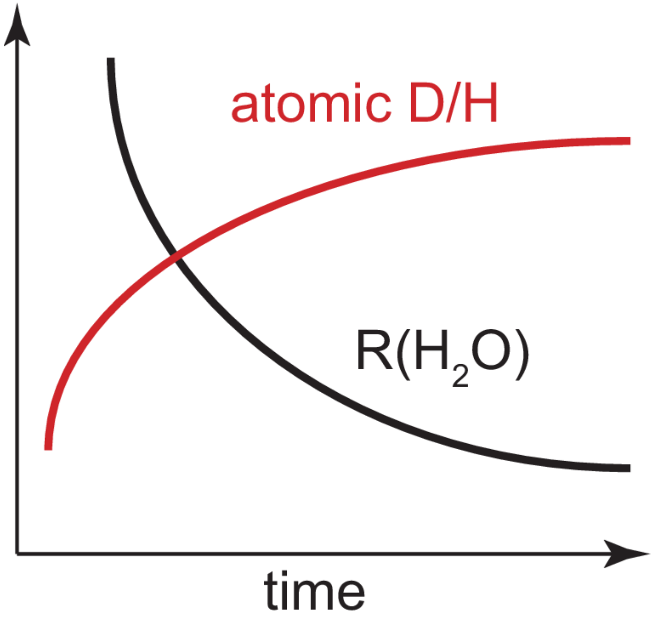
→Production rates of HDO and D_2O do not necessarily follow that of H_2O

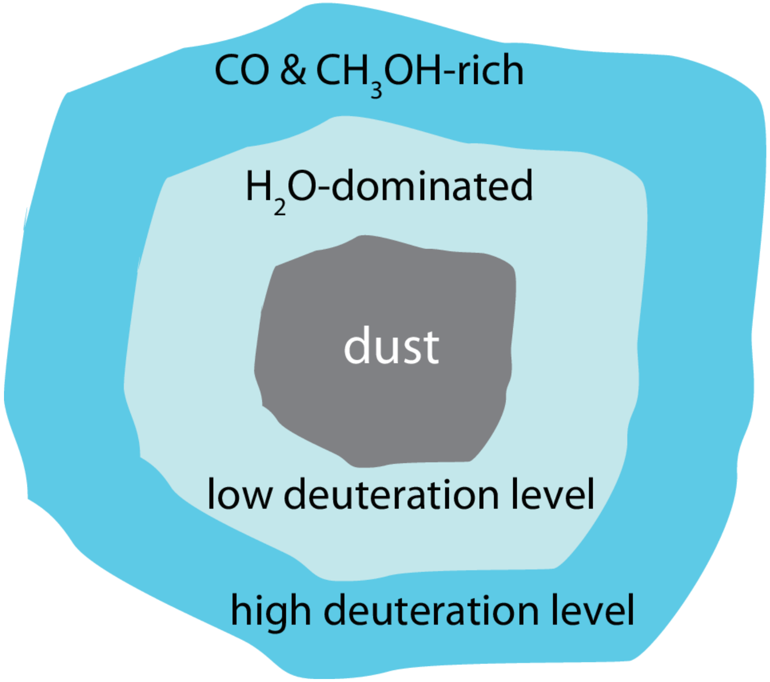
If the production of HDO and D_2O are dominated in late times

D_2O/HDO in the whole ice ~ atomic D/H in late times
HDO/H_2O in the whole ice << atomic D/H in late times

$$\Rightarrow \frac{D_2O}{HDO} \gg \frac{HDO}{H_2O}$$

Consider chemical evolution



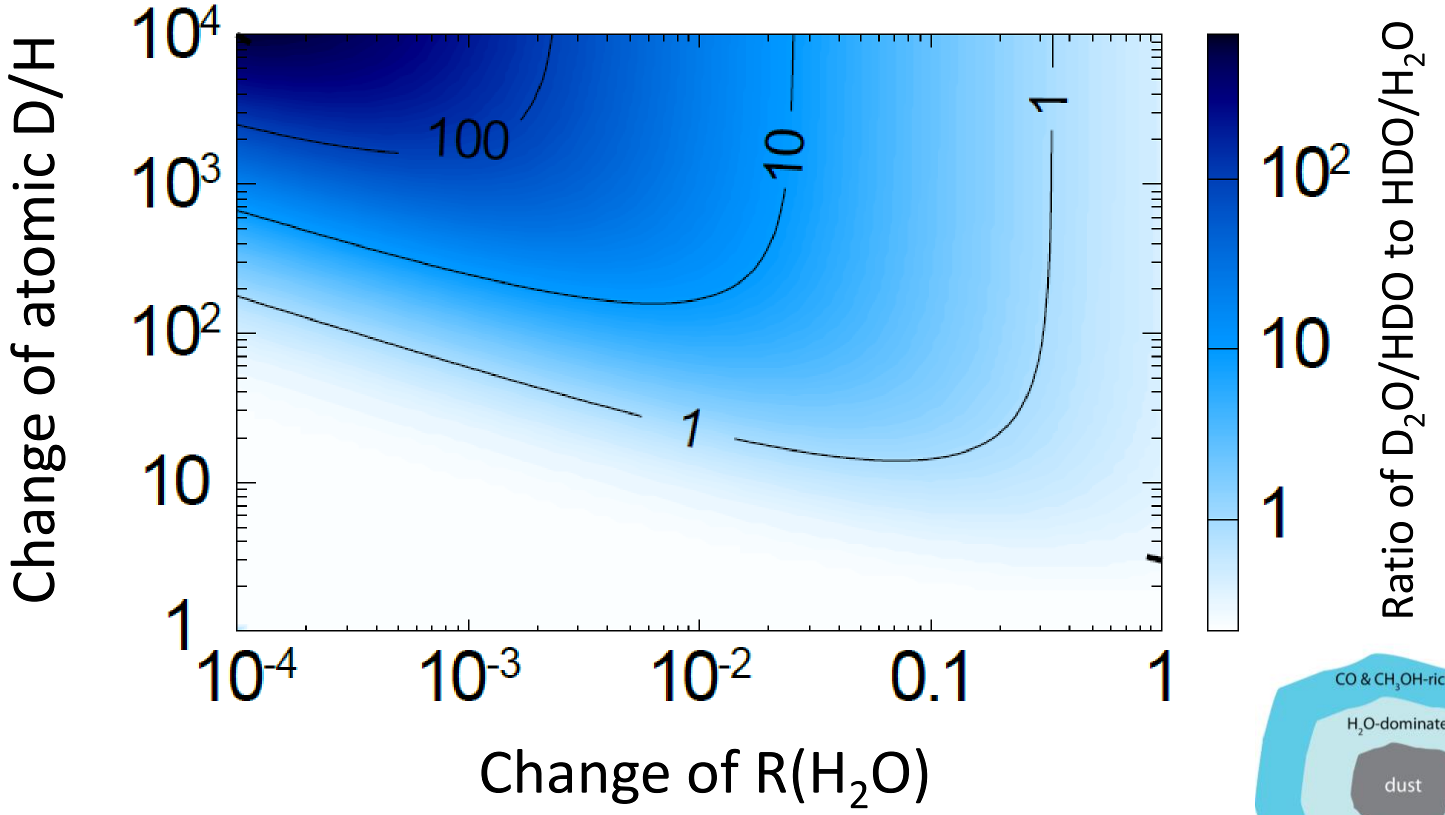


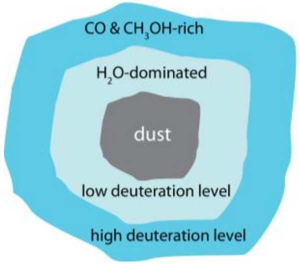
If the production of HDO and D_2O are dominated in late times

D_2O/HDO in the whole ice ~ atomic D/H in late times
HDO/H_2O in the whole ice << atomic D/H in late times

$$\frac{D_2O}{HDO} \gg \frac{HDO}{H_2O}$$

Required conditions for reproducing the observations





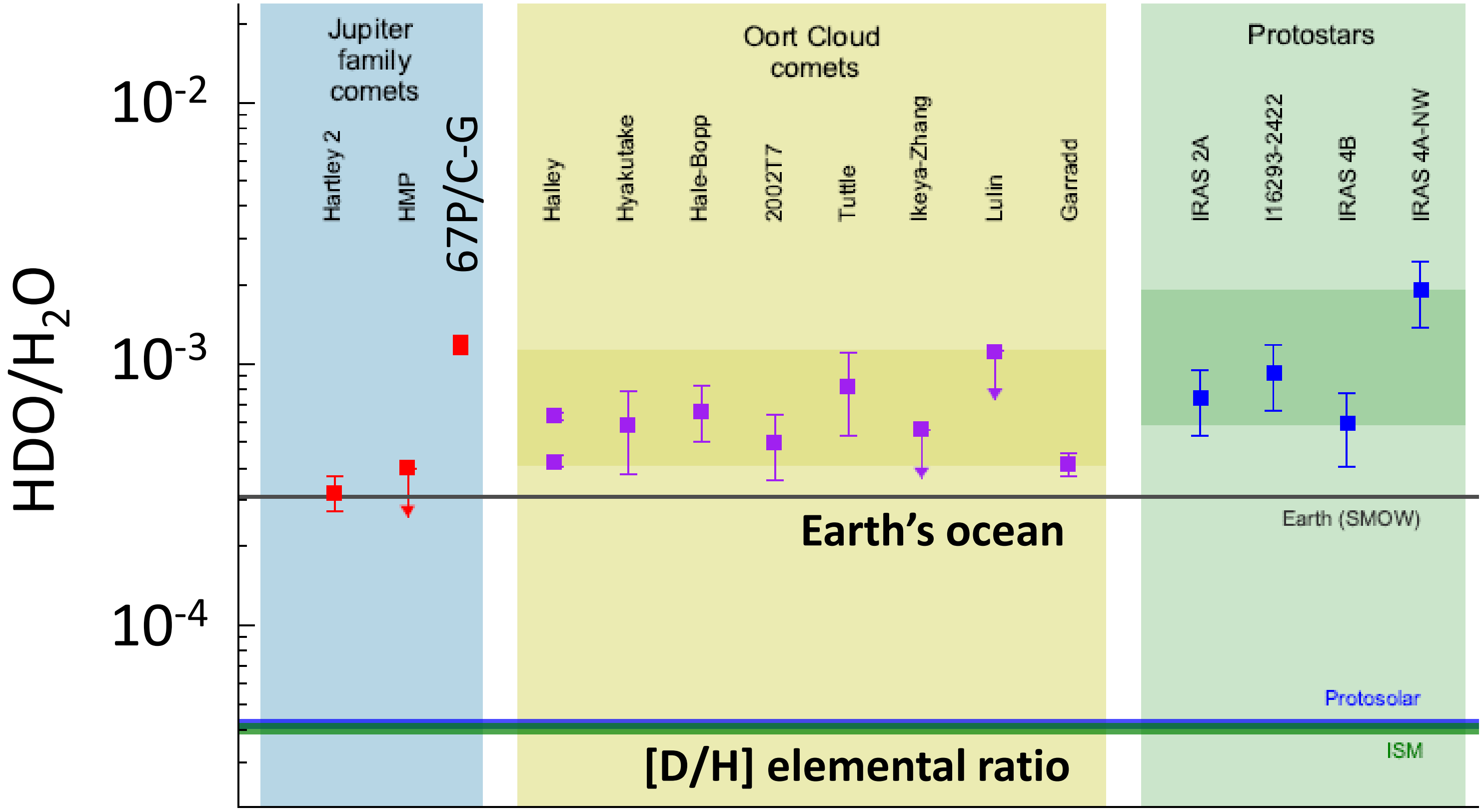
(i) drop of R(H_2O) by a factor of >10

(ii) enhancement of the atomic D/H by a factor of >100

→ very inhomogeneous

Ratio of D_2O/HDO to HDO/H_2O

- The high ratio likely characterizes the ISM ice
  → D_2O observations toward comets are crucial
  for studying the origin of cometary water



(Mumma & Charnley 2011; Altwegg+2015; Persson+ 2014)

Summary

- Water is formed before the stellar birth
- Our model suggests that forming disks contain lots of interstellar H_2O ice
  → favorable for the formation of icy planetesimals (and planets)
- D_2O observations toward comets are crucial for testing the model prediction