Ice deuteration: Models and observations to interpret the protostar history

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HDO 2013 workshop

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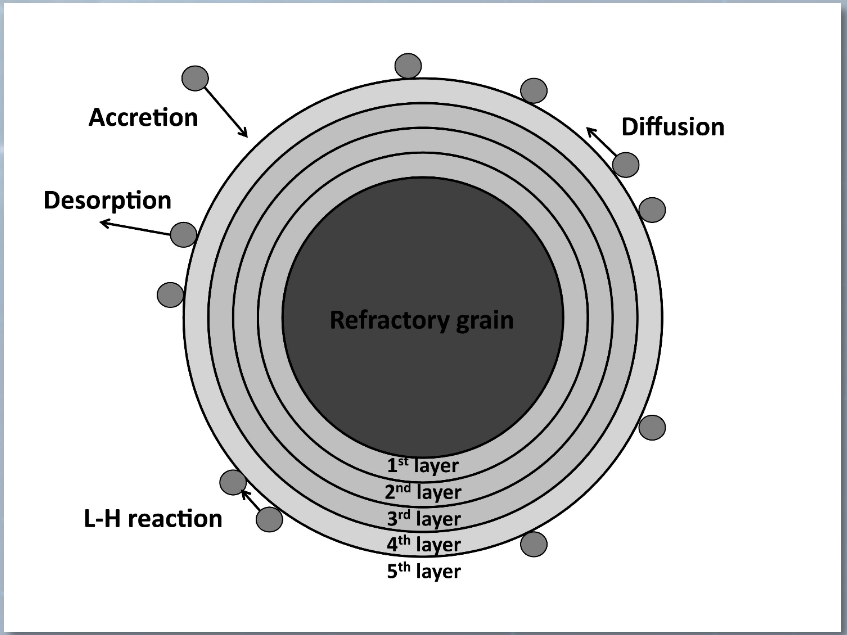
The GRAINOBLE model

Time-dependent gas-grain astrochemical model based on the **rate equations** (Hasegawa et al. 1992)
- gas phase processes
- gas-grain processes ➔ accretion and (thermal+non-thermal) desorption
- bimolecular and exothermic surface reactions

➔ Following surface experiments which show that cold ices are mostly inert (see Watanabe et al. 2003, 2004),
Multilayer approach that:
- distinguishes the processes between surface/ bulk
- traps particles in the bulk
- saves the composition of each layer

➔ accurate for ice photolysis



Taquet, Ceccarelli, Kahane 2012a, A&A, 538, A42

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The chemical network

Gas phase chemical network:

- complex network coming from the **KIDA database** for 7 elements
- **deuterium chemistry** (following Roberts et al. 2000, 2003, 2004)
- **ortho** and **para** spin states of H_2 and key ions (following Hugo et al. 2009)

Surface chemical network based on recent experimental works:

- **deuterated water** network from i) O (Dulieu+ 2010, Oba+ 2012), ii) O_2 (Miyauchi+ 2008, Ioppolo+ 2010), iii) O_3 (Mokrane+ 2009)
- **deuterated formaldehyde and methanol** network (Watanabe+ 2002, Nagaoka+ 2005, Hidaka+ 2009, Fuchs+ 2009)
- **carbon dioxide network** (Oba+ 2010, Ioppolo+ 2011, Raut+ 2011)
- **wavelength-dependent UV photolysis** on ices based on experimental works (Fayolle+ 2011) or MD simulations (Andersson+ 2008)

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Multiparameter approach

Several **input parameters** show a **large range of values**:

- **Physical conditions** vary with time/ object

- **Grain surface parameters** follow distributions depending on grain/ice

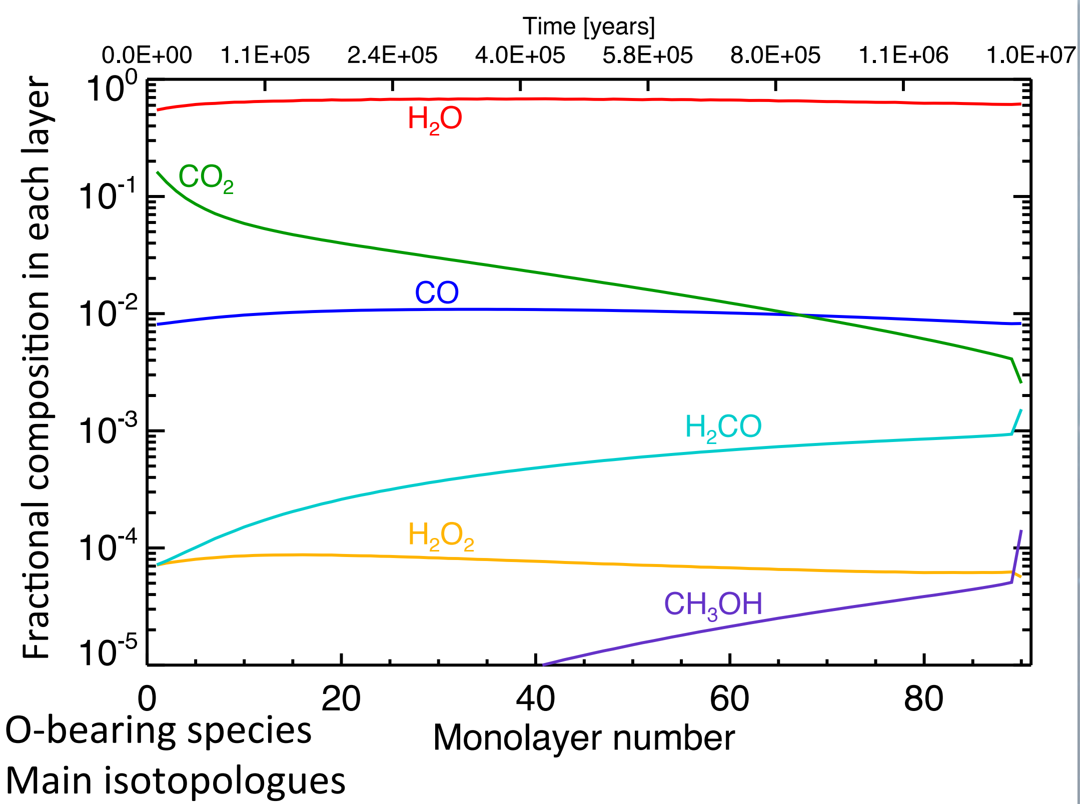
- Uncertain key **chemical parameters**

Input parameters	Values
Physical conditions	
n_H	10^3 - 5×10^6 cm^{-3}
$T_g = T_d$	8 - 20 K
A_v	0 - 10 mag
Grain surface parameters	
a_d	0.1 - 0.4 μm
F_{por}	0 - 0.9
E_b(H)	400 - 600 K
E_d/E_b	0.5 - 0.8
d_s	1.4 - 7 Å
Chemical parameters	
E_a(CO)	400 - 2500 K
X(O)	10^{-8} - 10^{-4}
H_2 o/p ratio	3×10^{-6} - 3

➔ **Model grid** by varying the input parameter values:
study the **influence of each parameter** on the ice chemistry

Chemical differentiation within ices

Ices are very heterogeneous and their **chemical composition depends on the physical conditions**



Translucent cloud region

$n_H = 10^4$ cm^{-3}

T = 15 K

A_v = 2 mag (➔ $A_{v,obs}$ = 4 mag)

Water-rich ice (+ CO_2)

➔ consistent with Av-dependent ice observations (see Whittet et al. 2001, 2007)

Taquet, Peters, Kahane, Ceccarelli et al. 2013, A&A, in press

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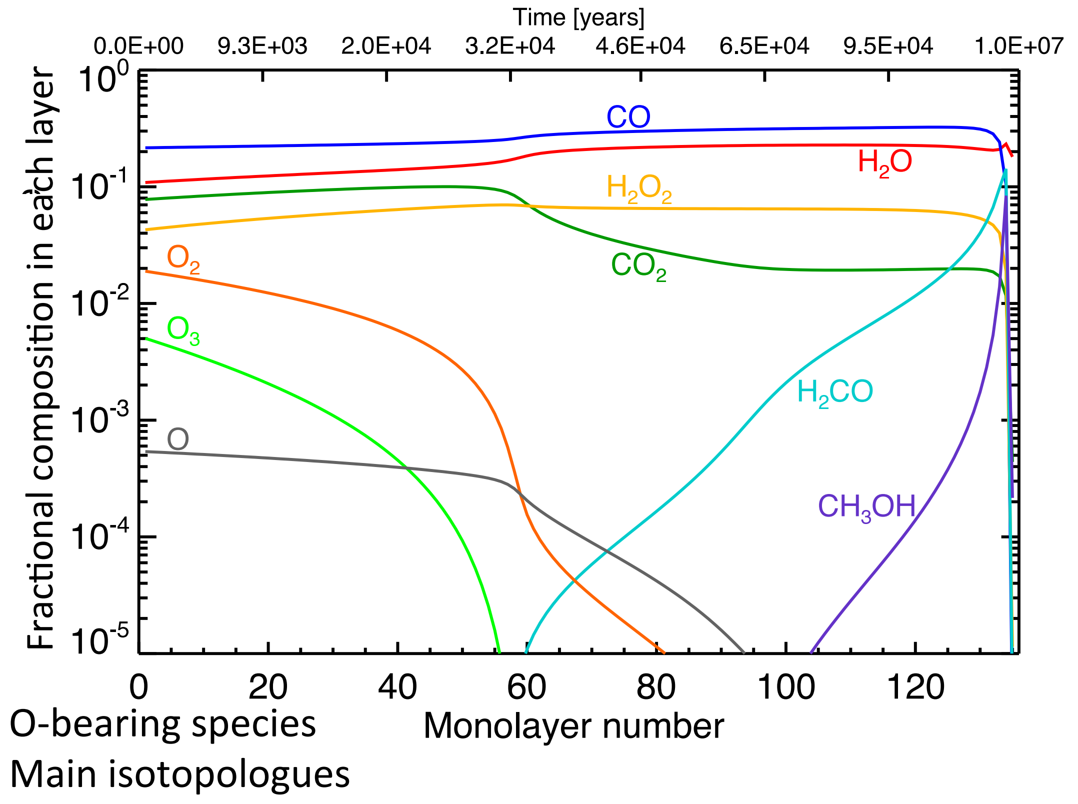


Dense core region

$n_H = 10^5\ cm^{-3}$

$T = 10\ K$

$A_v = 10\ mag\ (A_{v,obs} = 20\ mag)$

CO-rich ice

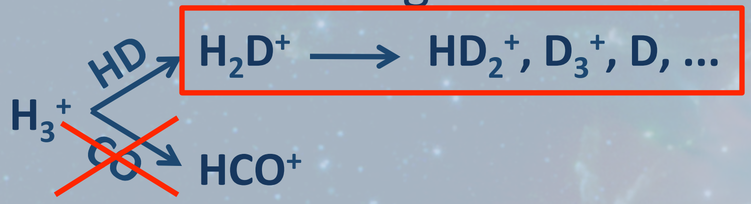
(+ H_2O_2, H_2CO, CH_3OH)

➔ consistent with Av-dependent ice observations (see Whittet et al. 2007, 2011; Boogert et al. 2011)

Taquet, Peters, Kahane, Ceccarelli et al. 2013, A&A, in press

CO depletion and ice deuteration

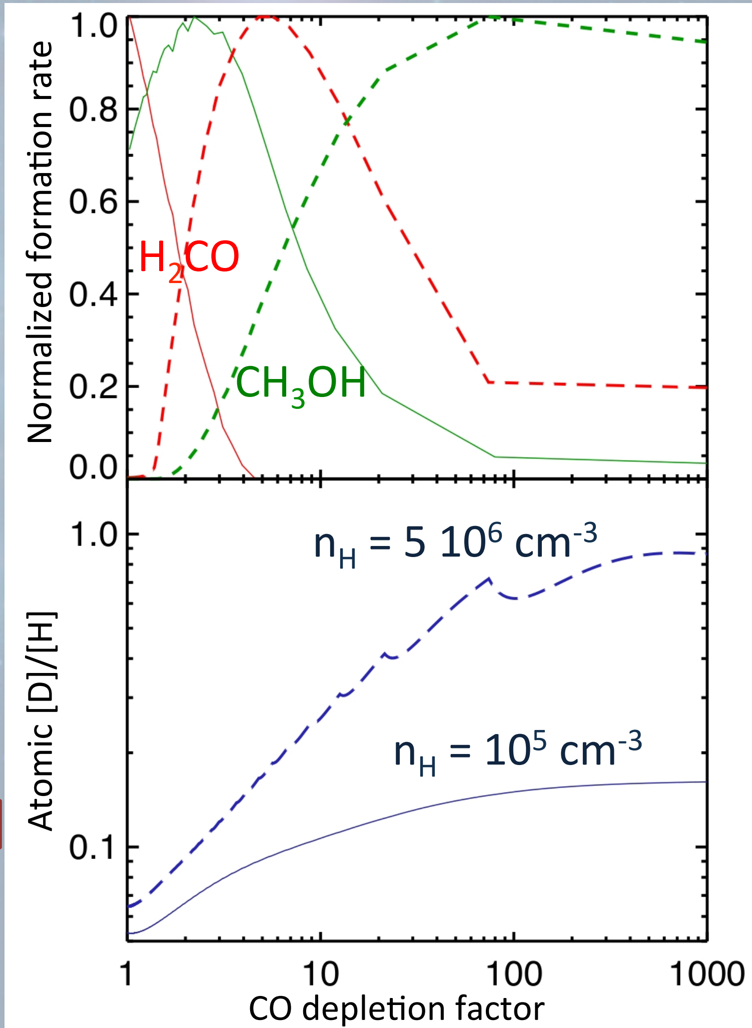
Deuteration reactions in competition with reactions involving CO



➔ **CO depletion increases the deuteration** (see Roberts et al. 2003)

Icy molecules (H_2O, H_2CO, CH_3OH) form via addition **reactions with H, D atoms**

➔ Their **deuteration depend on**:
- the **increase** of the gaseous atomic **[D]/[H]**
- **when they are formed**

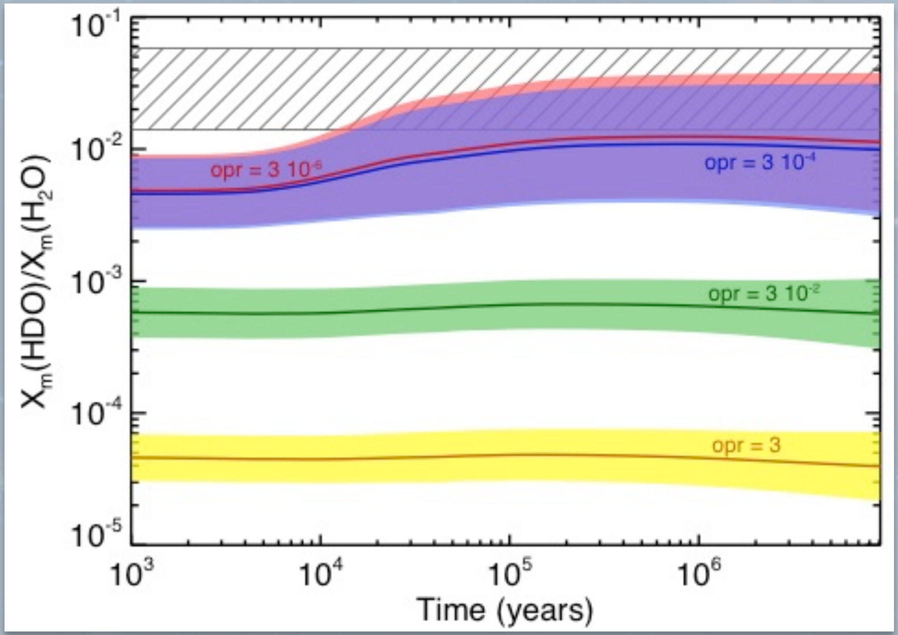


Taquet, Ceccarelli, Kahane 2012b, ApJL, 748, L3

H_2 ortho/para ratio and ice deuteration

Ortho spin state of H_2 has a higher internal energy, allowing **endothermic reactions** to occur at low temperatures

➔ **deuteration** in the gas phase **decreases with the opr(H_2)**



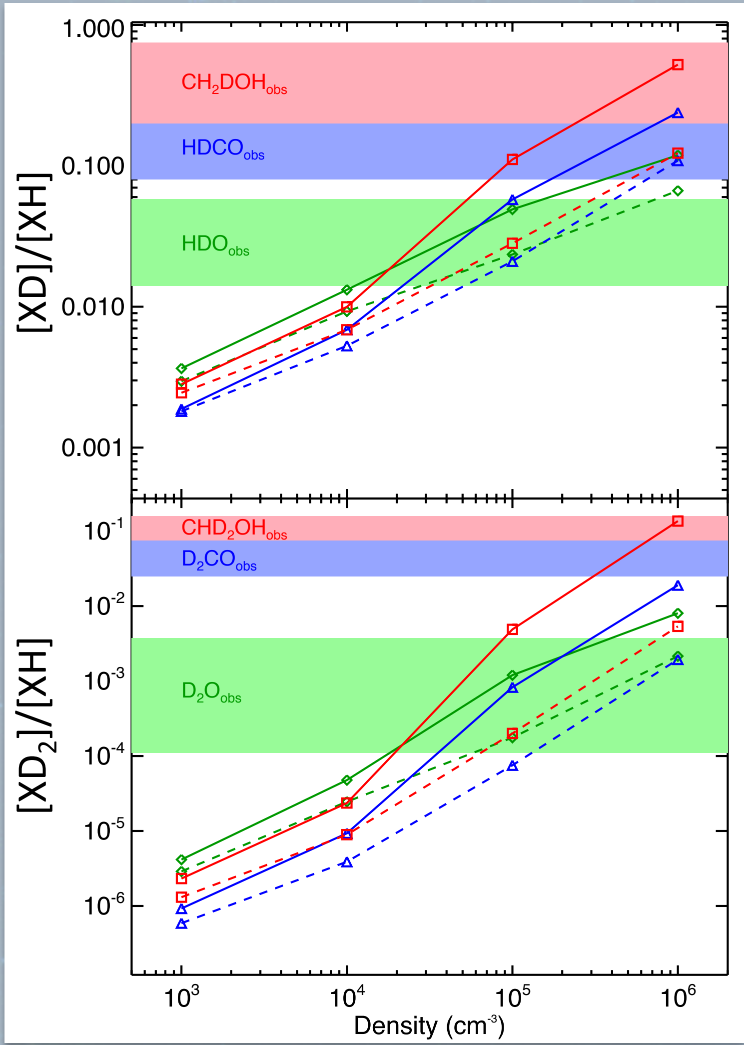
Water deuteration for 4 opr(H_2) values and varying 6 other parameters

The opr(H_2) decreases the water deuteration by several orders of magnitude

➔ stronger decrease than the standard deviations induced by all other parameters

Taquet, Peters, Kahane, Ceccarelli et al. 2013, A&A, in press.

Ice formation in IRAS 16293



Water deuteration is reproduced for:
- a **low H_2 o/p** ($< 3\ 10^{-4}$)
- a **large range of n_H** ($8\ 10^3 < n_H < 3\ 10^5\ cm^{-3}$)
- temperatures between **10 and 20 K**

Formaldehyde and methanol deuteration are reproduced for:
- **higher densities** ($> 5\ 10^5\ cm^{-3}$)
- **lower temperatures** (≈ 10 K)

➔ water forms first in low-density regions while formaldehyde and methanol are mainly formed in cold dark cores

solid: 10 K, dashed: 20 K

Taquet, Peters, Kahane, Ceccarelli et al. 2013, A&A, in press.

Water deuteration in low-mass protostars

Gas phase processes are **not efficient** enough to alter the deuteration after the ice evaporation seen in Class 0 protostars (Charnley+ 1997, André+ 2000, Osamura+ 2004)

➔ The deuteration observed in Class 0 protostars **reflects** the formation in **ices**

HDO/H_2O abundance ratio in Class 0 protostars:
tracer of the water formation in the precursor cold phase

However, **HDO/H_2O** constrained only in a few low-mass protostars
➔ Only **IRAS 16293** shows a value of the ratio; for other protostars lower/upper limits

Taquet, López-Sepulcre, Ceccarelli et al. 2013, ApJL, submitted

HDO in NGC 1333 IRAS 2A and 4A

➔ **PdBI observations** of the **HDO $4_{2,2}$-$4_{2,3}$ transition (at 143 GHz)** toward 2 low-mass protostars: **NGC1333-IRAS2A** and **-IRAS4A**

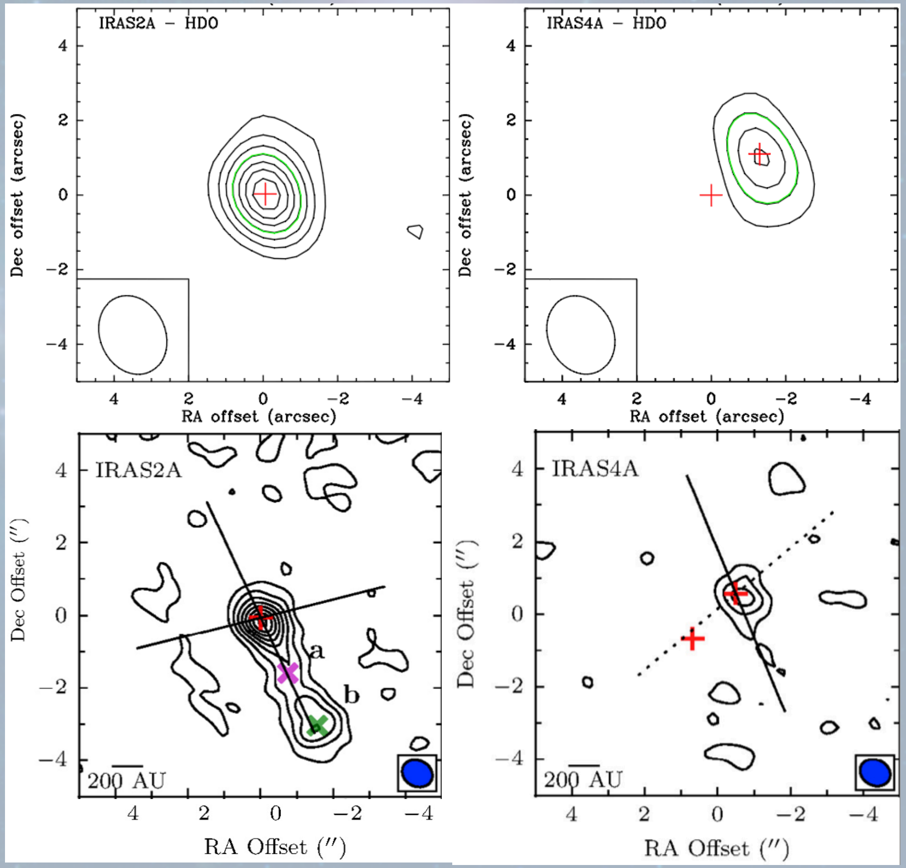
➔ **High angular resolution (2'')**: estimation of the emission coming from the **warm quiescent envelope**

Taquet, López-Sepulcre, Ceccarelli et al. 2013, ApJL, submitted

HDO in NGC 1333 IRAS 2A and 4A

Comparison of our observations with PdBI **$H_2{}^{18}O$ observations** by Persson et al. (2012):

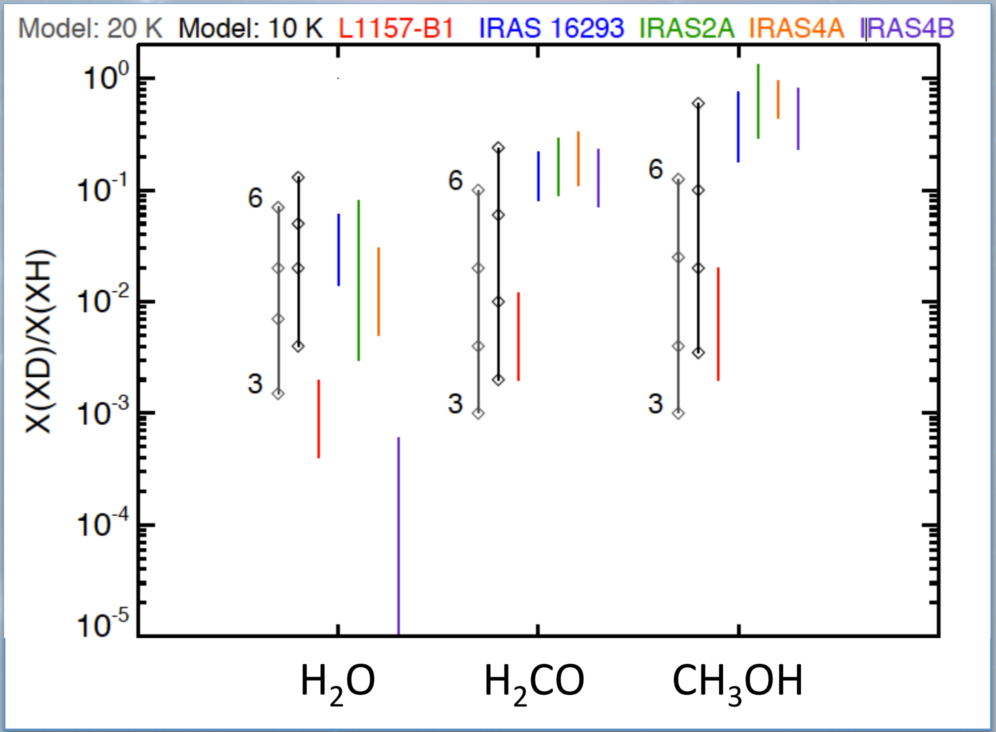
➔ Most of the **HDO** and **$H_2{}^{18}O$** emissions originate from the **same quiescent envelope**



Taquet, López-Sepulcre, Ceccarelli et al. 2013, ApJL, submitted

HDO in NGC 1333 IRAS 2A and 4A

LVG analysis of these emissions combined with single-dish observations of IRAS2A (Liu et al. 2011):



$6 \times 10^5 < n_H < 10^8$ cm^{-3}

T_{kin} = 75-80 K

θ = 0.4 "

➔ $5 \times 10^{17} < N(HDO) < 10^{19}$ cm^{-2}

Depending on the physical case,

- **HDO/H_2O = 0.3 – 8 % in IRAS2A**
- **HDO/H_2O = 0.5 – 3 % in IRAS4A**

Taquet, López-Sepulcre, Ceccarelli et al. 2013, ApJL, submitted

Conclusions & Perspectives

✓ The **multilayer approach** shows that **ices** are **heterogeneous**
➔ in good agreement with A_v-dependent **ice observations**

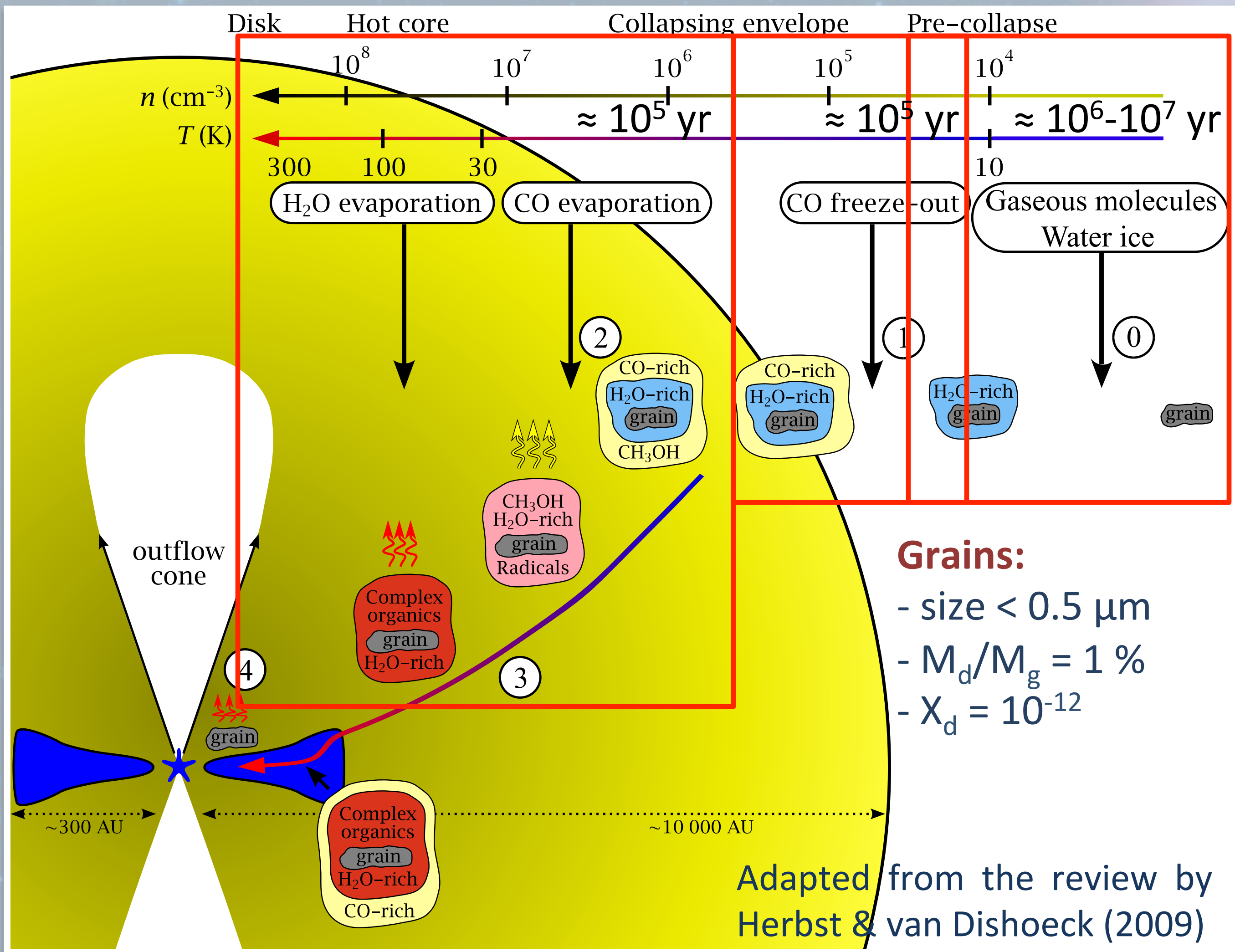
✓ The **deuteration of water** is **explained** by recent chemical networks

✓ The **deuteration** is **very sensitive** to the **physical conditions**
➔ **trace** the physical and chemical **history** of observed **protostars**

- Study of the multilayer formation and deuteration of ices with **evolving physical conditions**
- Use the deuteration to probe **the formation pathways of Complex Organic Molecules**

Spitzer image of the
NGC1333 star-forming region

Interstellar grains and chemical complexity



Grains:
- size < 0.5 µm
- M_d/M_g = 1 %
- $X_d = 10^{-12}$

Adapted from the review by Herbst & van Dishoeck (2009)

Molecular clouds:
- simple molecules
- first ices (H_2O, CO_2)

Prestellar cores:
- CO freeze-out
- other organic ices

Protostellar envelopes:
- COMs formation
- ice sublimation

Deuteration in prestellar cores

Deuterium fractionation: **Abundance ratio** between an **hydrogenated species** and its **deuterated isotopologue** including D atom(s)

Ex: water ➔ HDO/H_2O or D_2O/H_2O

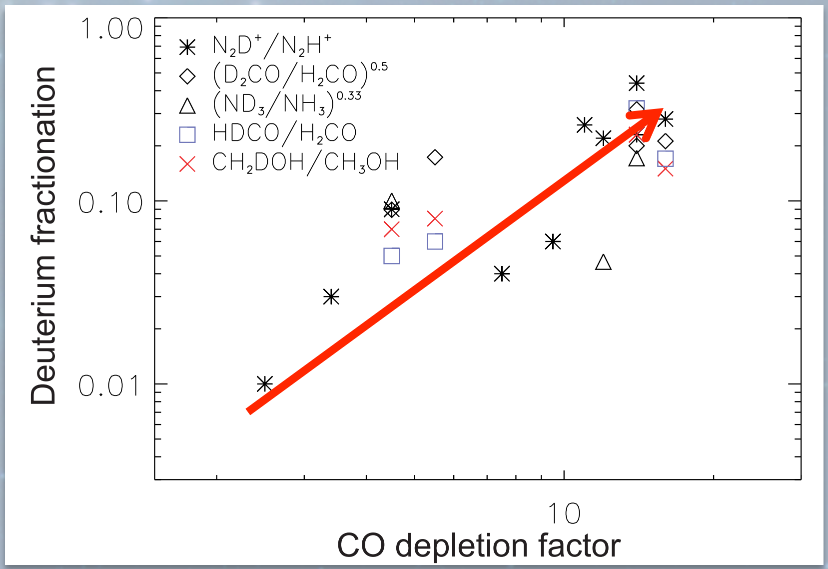
High deuteration is observed for **various species** in **prestellar cores:**

Molecular clouds

Cosmic D/H reservoir: 10^{-5}

(Linsky 2003)

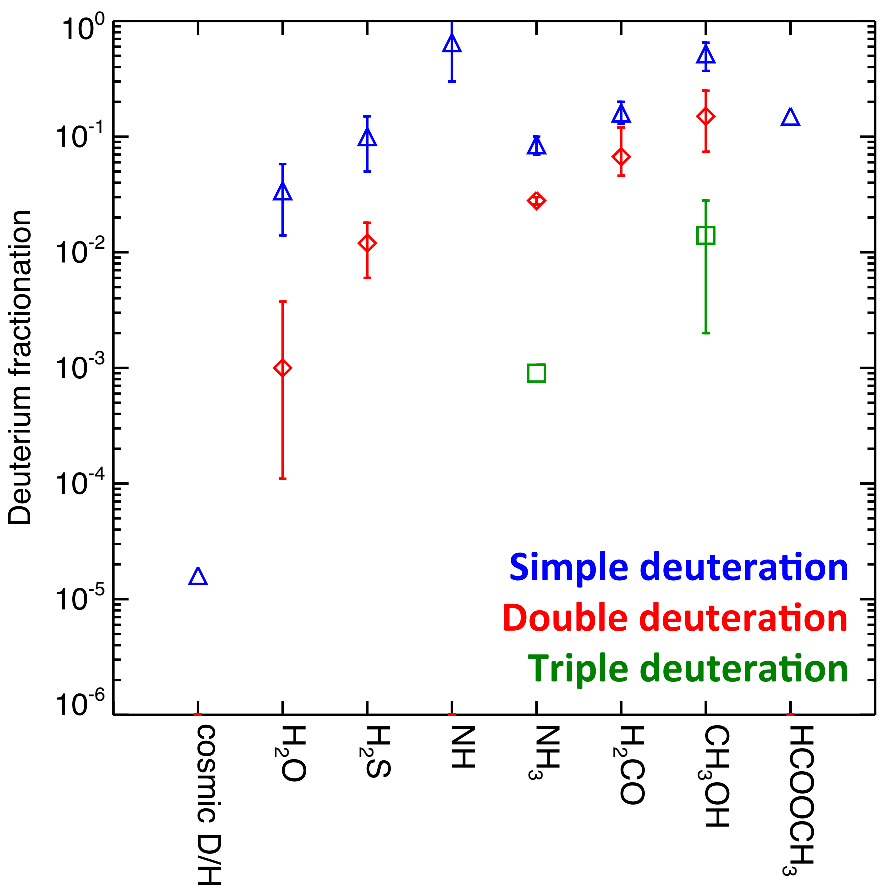
Prestellar cores



see Ceccarelli et al. (2007); Bacmann et al. (2007)

Deuteration in Class 0 protostars

Very high molecular deuteration is observed **in Class 0 protostars**:



From Taquet et al. (2012, in press)

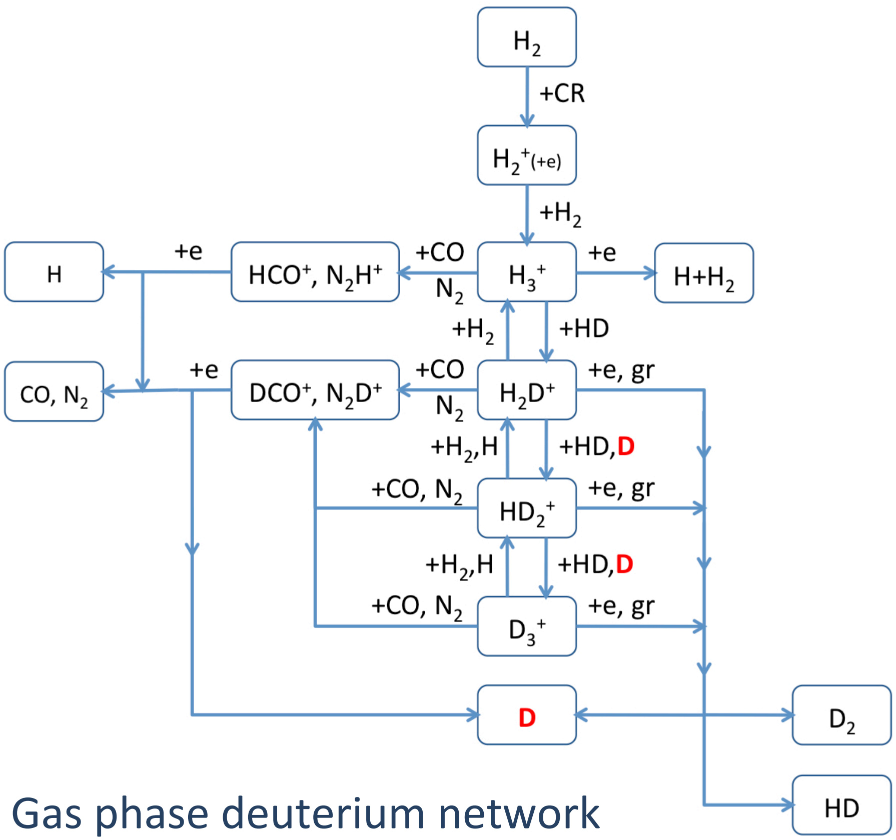
➔ Why do the **grain surface molecules** show **different fractionations** ?

Gas phase processes are **not efficient** enough to alter the deuteration after the ice evaporation seen in Class 0 protostars
(Charnley+ 1997, André+ 2000, Osamura+ 2004)

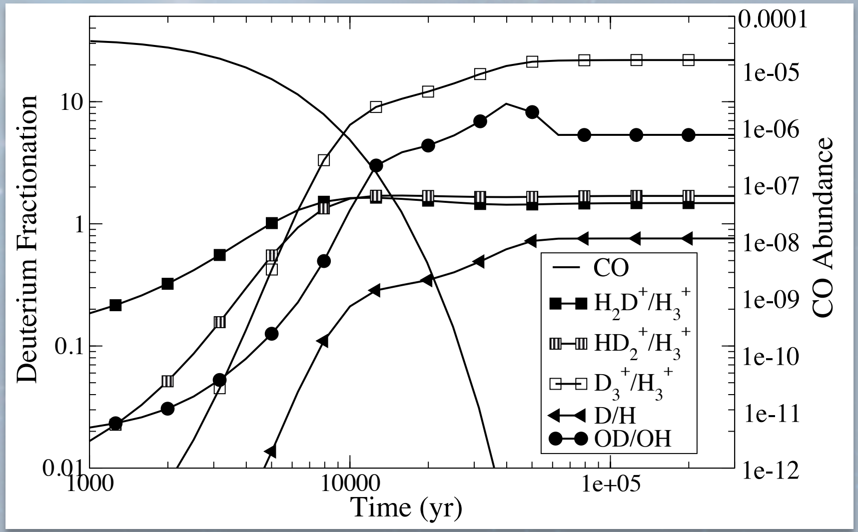
➔ The deuteration observed in Class 0 protostars **reflects** the formation in **ices**

Deuterium chemistry

The deuteration reactions are in competition with reactions involving CO ➔ its depletion increases their reactivity



Gas phase deuterium network



Model predictions computed by Roberts et al. (2004) with a gas phase model for $n_H = 2\ 10^6\ cm^{-3}$, T = 10 K

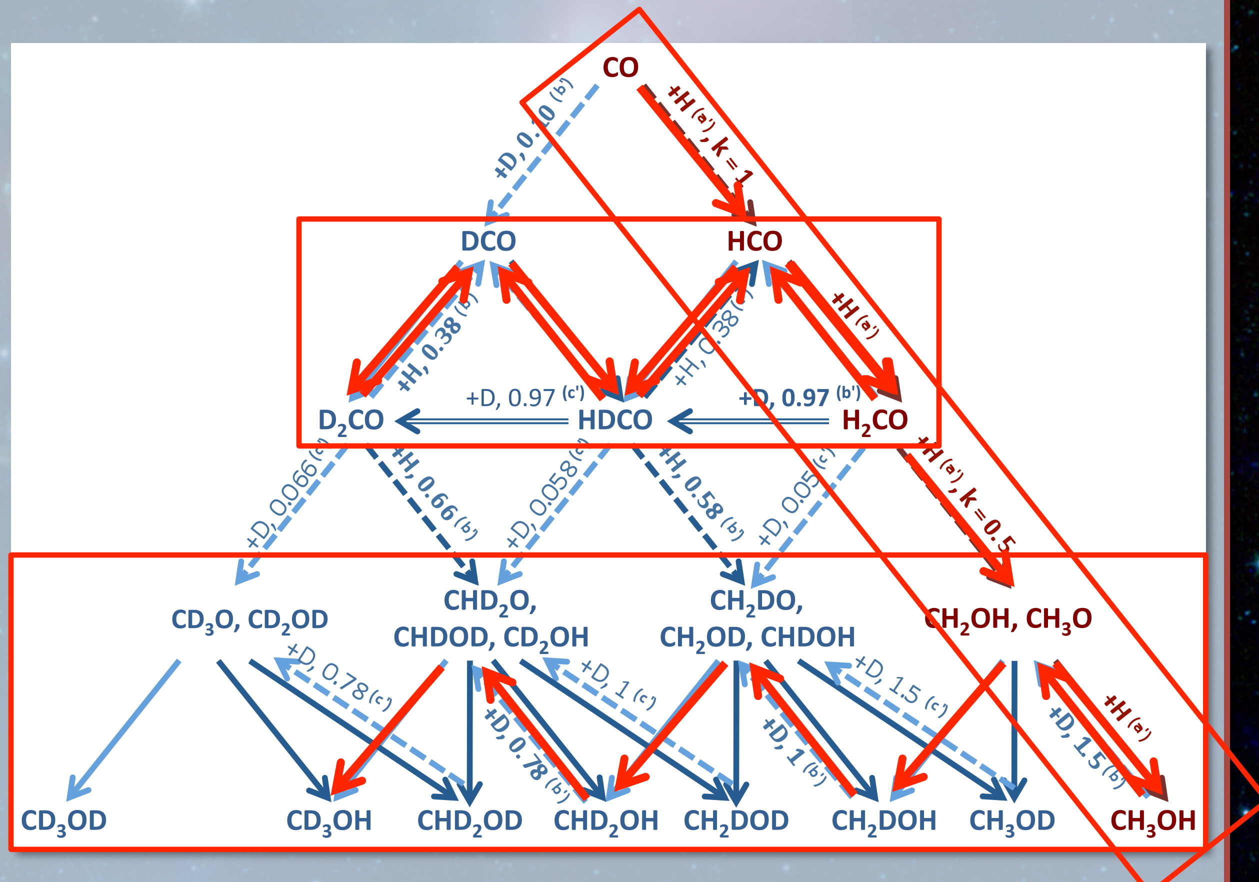
An example: the methanol network

Chemical network based on **recent experimental studies**:

- Hydrogenation of CO
(Watanabe+ 2002, 2004, 2006, Fuchs+ 2009)

- H_2CO deuteration via addition/abstraction reactions
(Hidaka+ 2009)

- CH_3OH deuteration via addition/abstraction reactions
(Nagaoka+ 2005, 2007)



Chemical network proposed by Watanabe & Kouchi (2008), Hidaka et al. (2009)

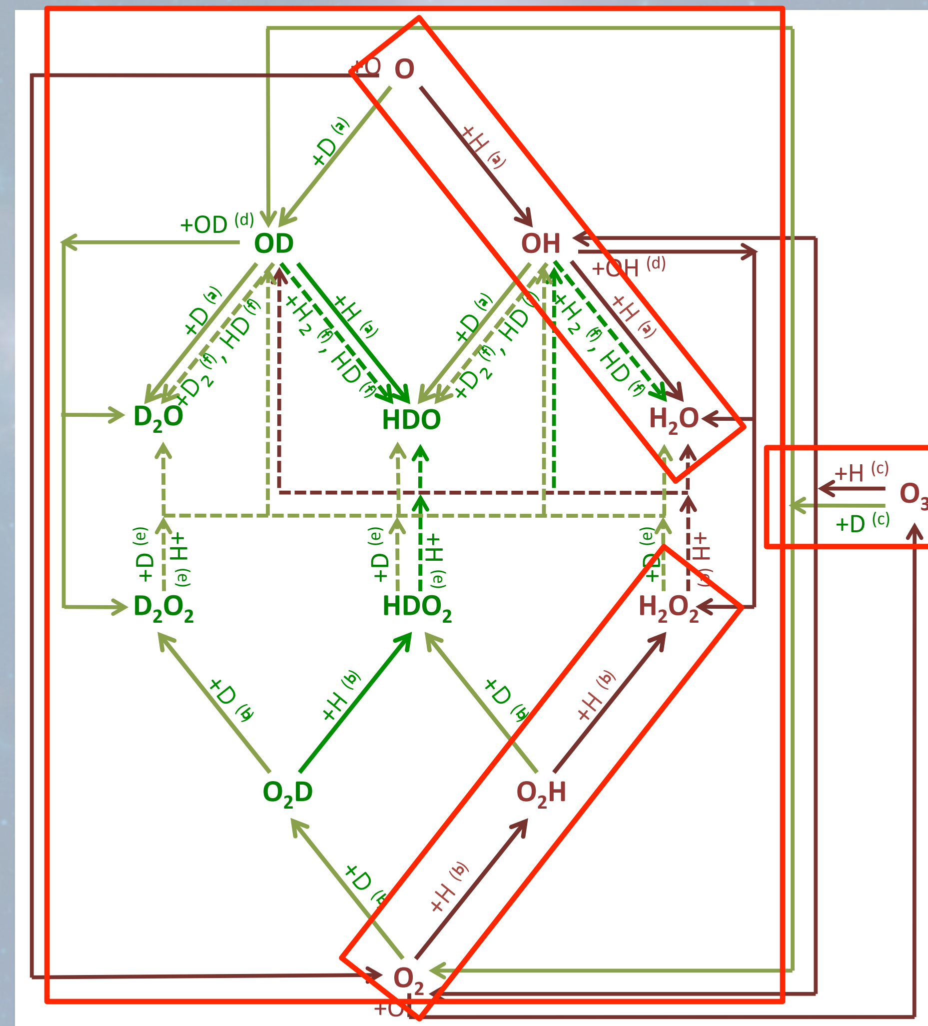
Formation and deuteration of water ice

Chemical network based on recent experimental works:

- Hydrogenation of atomic O
(Dulieu+ 2010, Jing+ 2011, Oba+ 2012)

- Hydrogenation of O_2, O_3
(Miyauchi+ 2008, Ioppolo+ 2008, Mokrane+ 2009, Cuppen+ 2010, Romanzin+ 2011)

- Deuteration of O, O_2
(Miyauchi+ 2008, Matar+ 2008, Oba+ 2012)



Reaction probabilities

Some key reactions show activation energy barriers

- In **previous models**, reaction probability computed assuming a **rectangular energy barrier** with a **width arbitrary fixed** to 1 A

➔ $P_r = \exp\left(-\frac{2a}{\hbar}\sqrt{2\mu E_a}\right)$

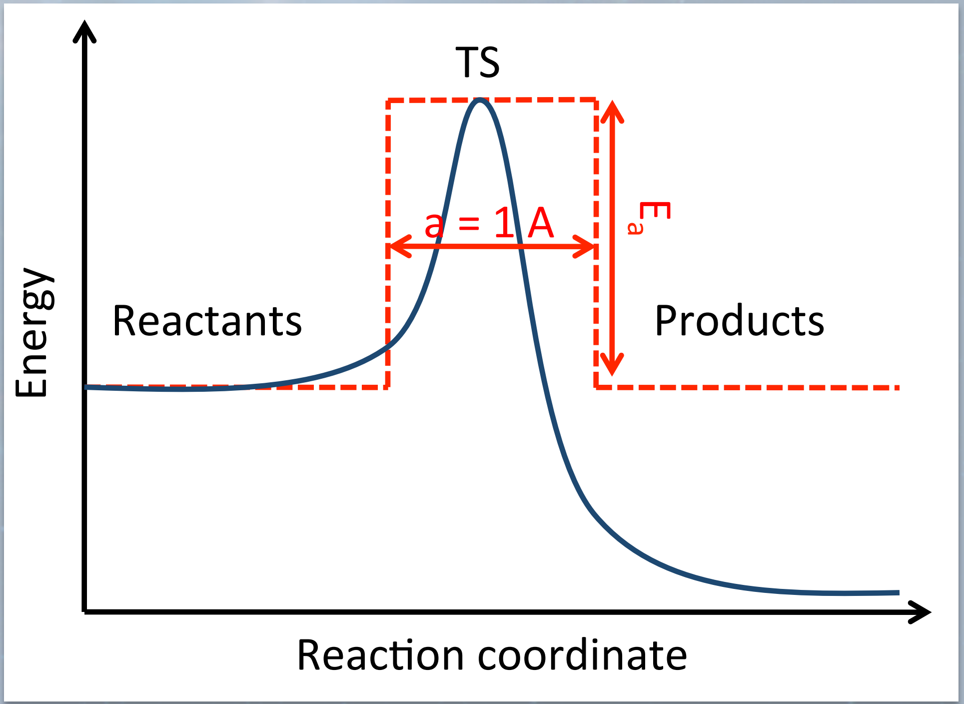
- The **Eckart model** is introduced for all the reactions, from quantum gas phase calculations

➔ fit an approximate PES

➔ compute an accurate reaction probability

ex: $H_2O_2 + H \rightarrow H_2O + OH$

$P_{r,square} = 1.2\ 10^{-8}$; $P_{r,Eckart} = 1.4\ 10^{-7}$

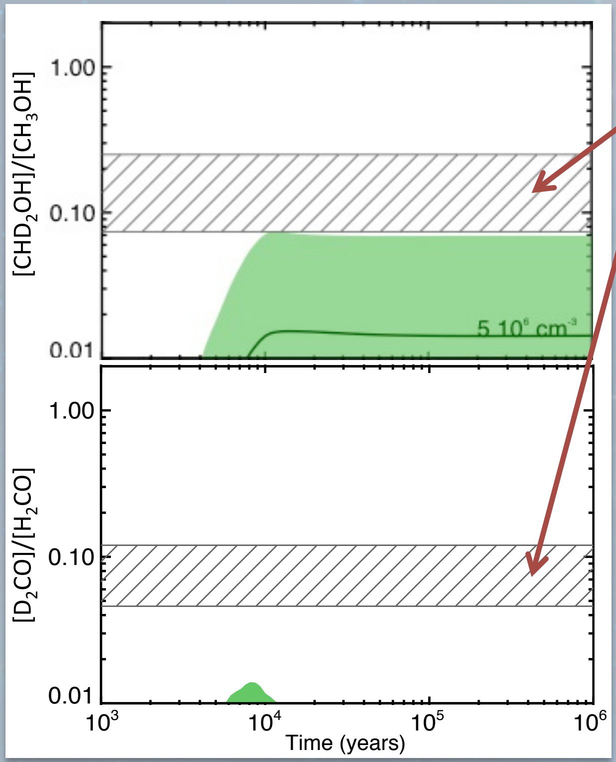


Taquet, Peters, Kahane, Ceccarelli et al. 2012c, A&A, in press.

Abstraction reactions and formaldehyde/methanol deuterations

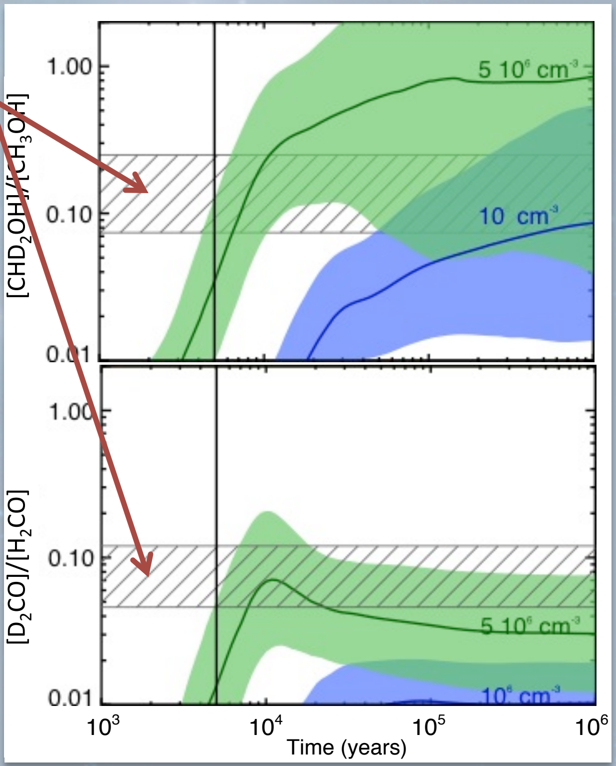
Abstraction reactions ➔ needed to reproduce the **high observed H_2CO and CH_3OH deuterations**

Addition reactions only



Observations

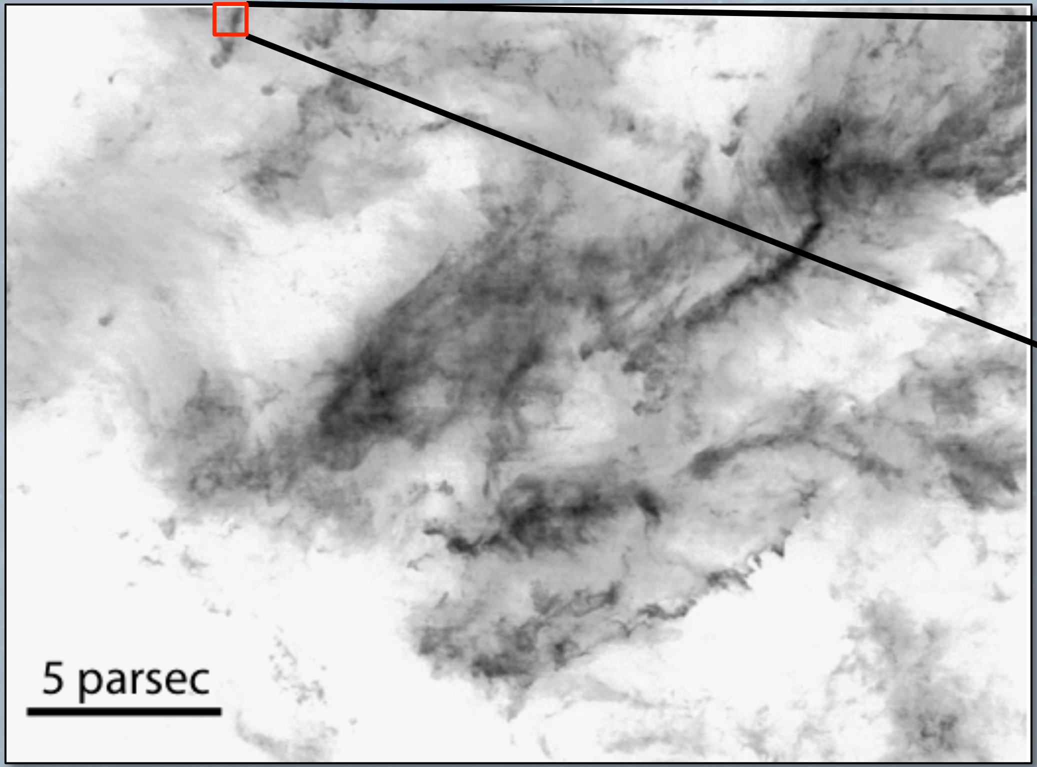
Addition + abstraction reactions



Taquet, Ceccarelli, Kahane 2012b, ApJL, 748, L3

The formation of Sun-like stars

Low-mass protostars usually form in cold dark clouds, also called molecular clouds



Densities n_H: $10^3 – 10^4$ cm^{-3}
Temperature T: 10 – 30 K

Taurus Molecular Cloud seen in ^{13}CO J=1-0 emission (Goldsmith et al. 2008)

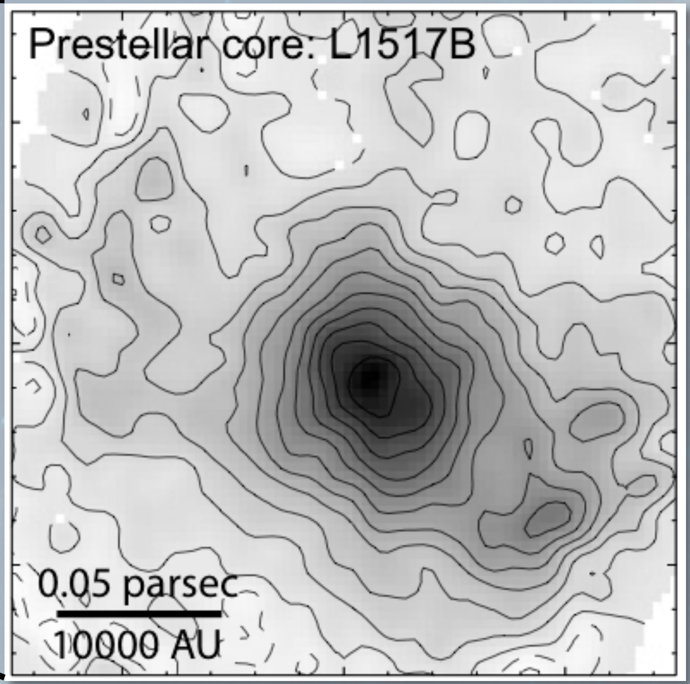
Interstellar grains and chemical complexity

Infrared, sub-millimetric, and millimetric observations have revealed a **chemical evolution with the evolutionary stage of stars**

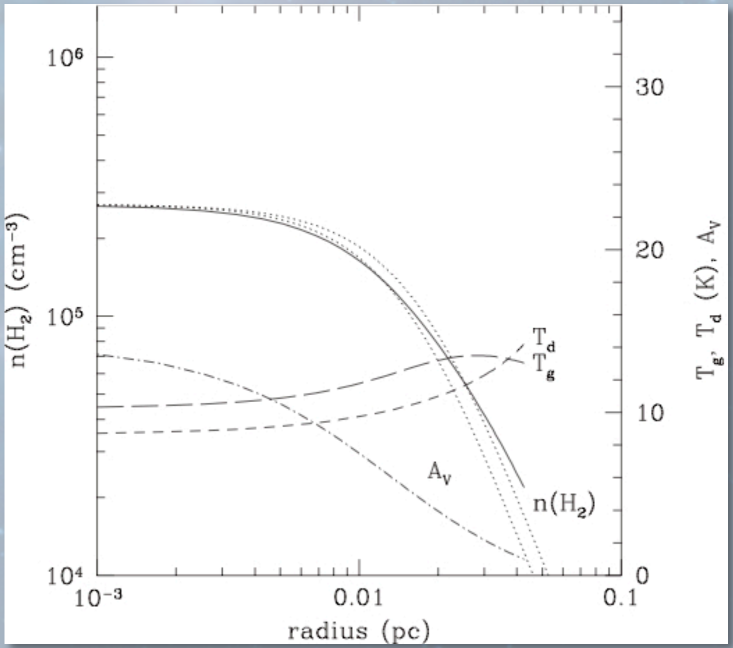
➔ In spite of their tiny sizes (< 0.5 µm), and their low abundances (1% in mass, < 10^{-12} in abundances), **interstellar grains play a crucial role in this chemical evolution**

The formation of Sun-like stars

Cold dark cores form via the progressive accumulation of matter:



1.2 mm continuum map of L1517B (Tafalla et al. 2004)



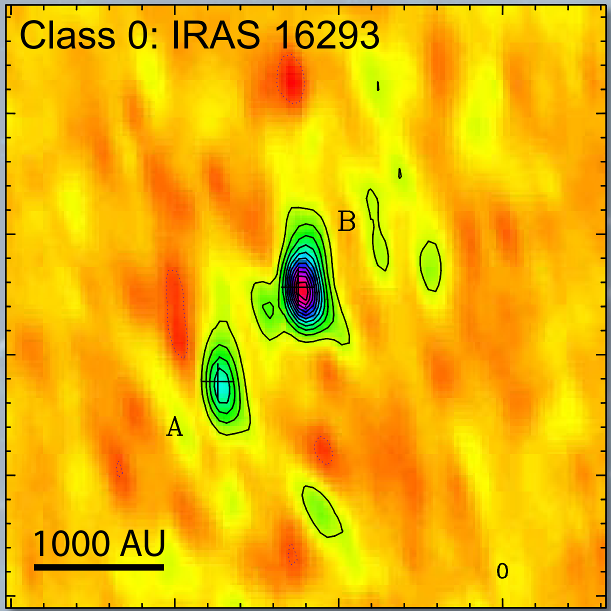
Density, temperature and A_V structure computed by Galli et al. (2002)

The formation of Sun-like stars

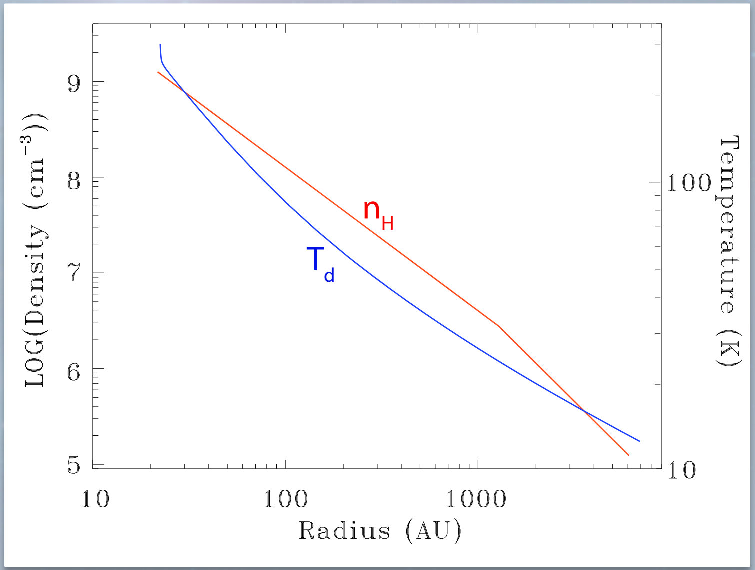
A protostar borns at the center and starts to warm-up its envelope

Gravitational collapse

and protostar birth



1.3 mm continuum map of IRAS 16293 (Bottinelli et al. 2004)

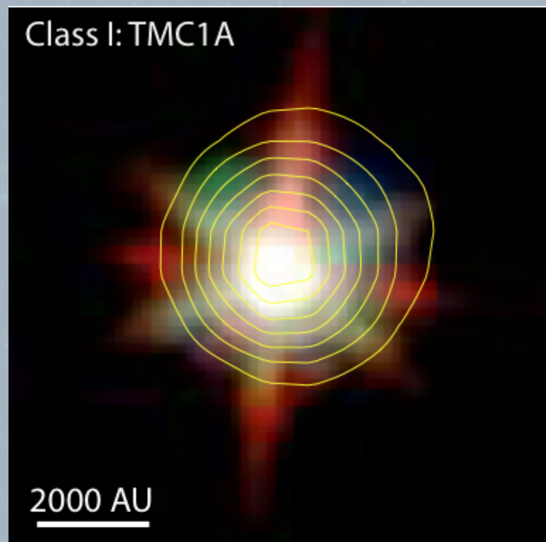


Density and temperature structures derived by Crimier et al. (2010)

The formation of Sun-like stars

Envelope progressively accreted by the protostar

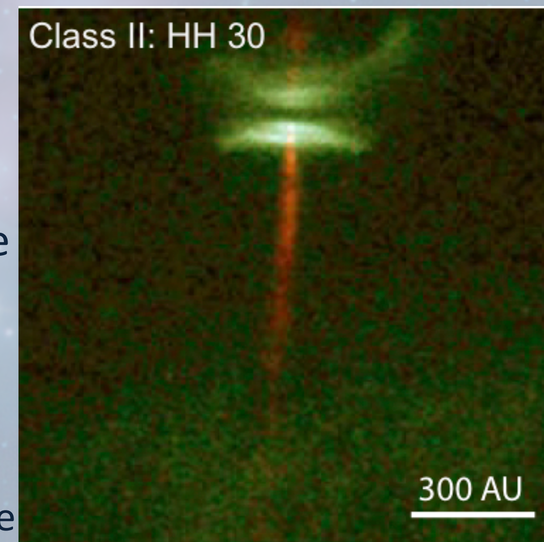
Disk formation
Bipolar outflows



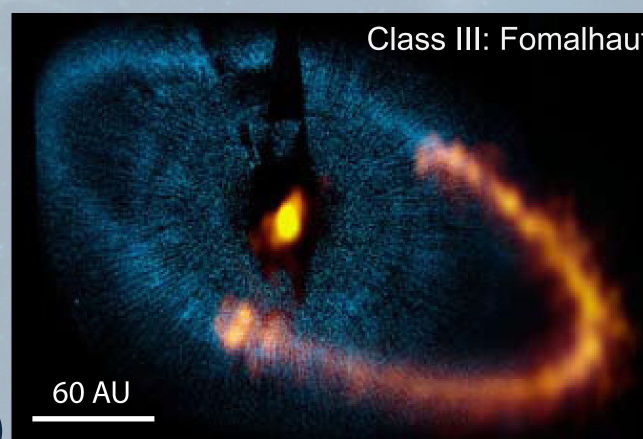
di Francesco et al. (2008)

Almost of spherical envelope

Evolved disk



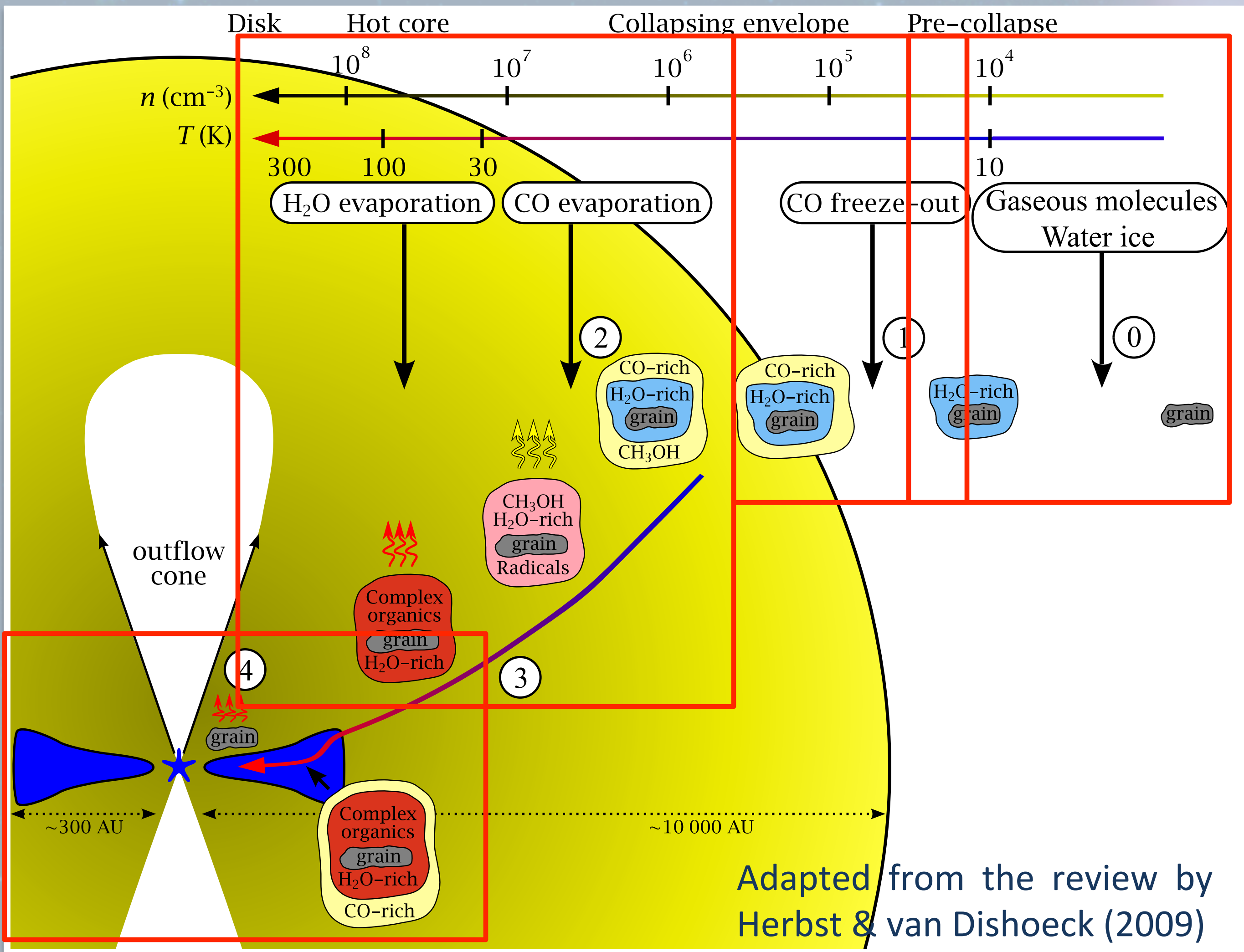
Hubble website



Boley et al. (2012)

Formation of planetesimals, debris disks, and then planetary sytems

Deuteration: why bothering ?



Adapted from the review by Herbst & van Dishoeck (2009)

Molecular clouds:
- cosmic D/H ≈ 10^{-5}

Prestellar cores:
- deuteration increase

Protostellar envelopes:
- superdeuteration

Solar System:
- deuteration probes its molecular origin
- deuteration probes Earth's water origin

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Deuteration: why bothering ?

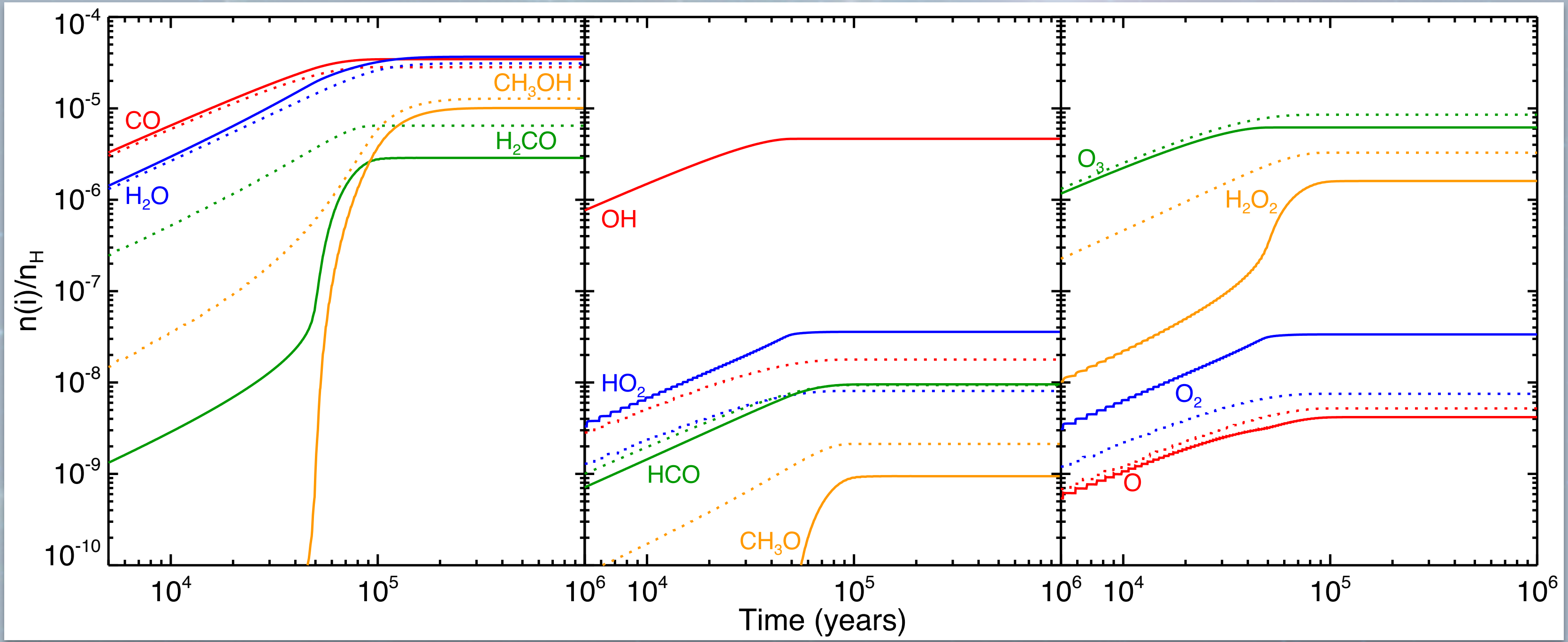
Molecular deuteration refers to the **abundance ratio between a hydrogenated species and its deuterated isotopologue**, including one (or several) deuterium atoms
ex: water ➔ HDO/H_2O

Deuteration can probe the physical conditions at the moment of formation of specific molecules and their eventual reprocessing
➔ Investigate the origin of the molecular content in the Solar System by comparing the deuteration in the ISM and Solar System bodies (comets/meteorites)
➔ Evaluate the contribution of comets for transferring water in Earth's oceans by comparing the water deuteration on the Earth and in comets

Porous versus non-porous grain

Pores trap volatile species (H atoms) increasing their abundances

➔ slightly increase the formation of main hydrogenated species



Absolute abundances for a reference model ($n_H = 10^5$ cm^{-3}, T = 15 K) and a small network.
Solid: smooth grain, dotted: porous grain.

Taquet, Ceccarelli, Kahane 2012 A&A, 538, A42

Abundance distributions

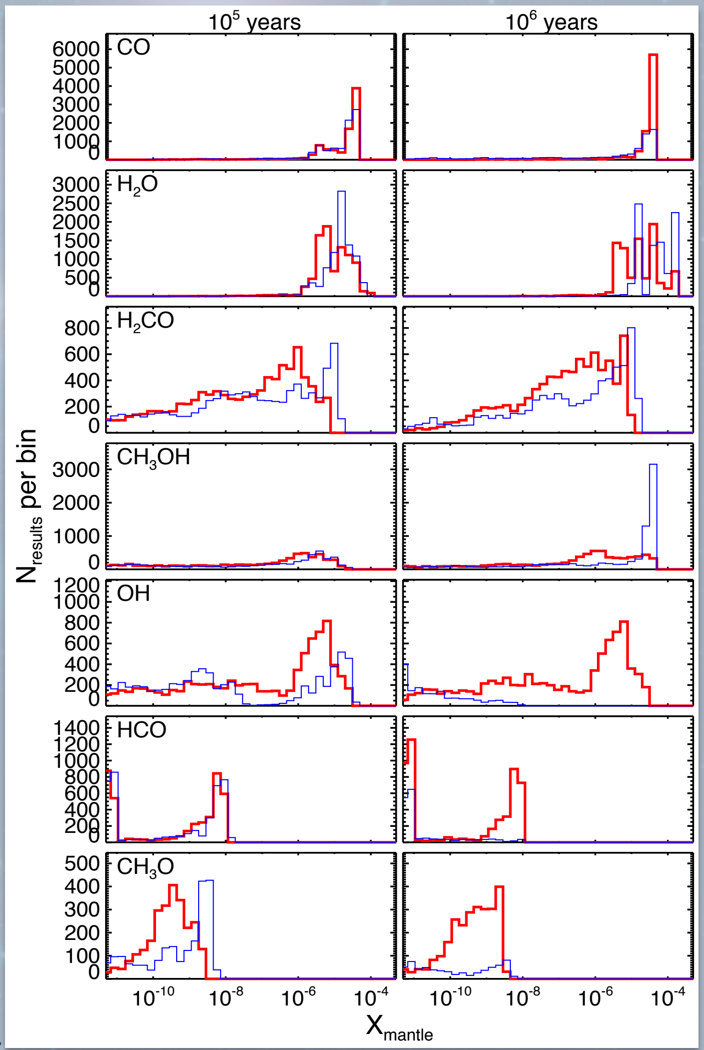
Thanks to the fast computation, large grids of models are run

➔ allow us to study the impact of each parameter on ice chemistry

ex: Abundance distributions for the old "bulk" (blue) and the new "multilayer" (red) approaches

➔ Range of 8 parameters is varied ≈ 18000 runs

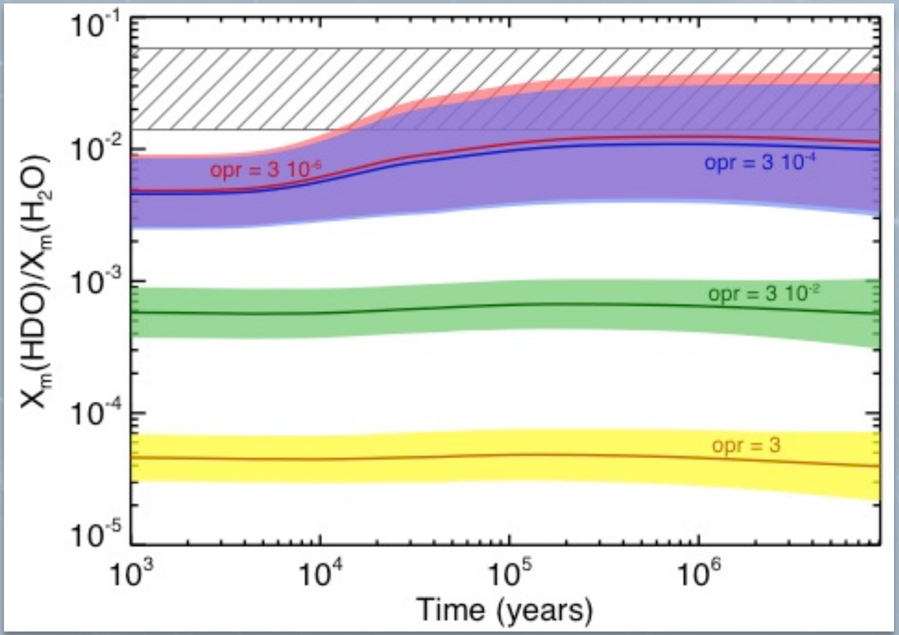
➔ H_2O, H_2CO, CH_3OH abundances are lower with the multilayer approach but radicals can survive



Taquet, Ceccarelli, Kahane 2012 A&A, 538, A42

H_2 ortho/para ratio and ice deuteration

Ortho spin state of H_2 has a higher internal energy, allowing endothermic reactions to occur at low temperatures
➔ deuteration in the gas phase decreases with the opr(H_2)



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➔ stronger impact than the standard deviations induced by all other parameters

Taquet, Peters, Kahane, Ceccarelli et al. A&A, submitted

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- The **Eckart model** is introduced
➔ fit an approximate PES
➔ accurate reaction probability

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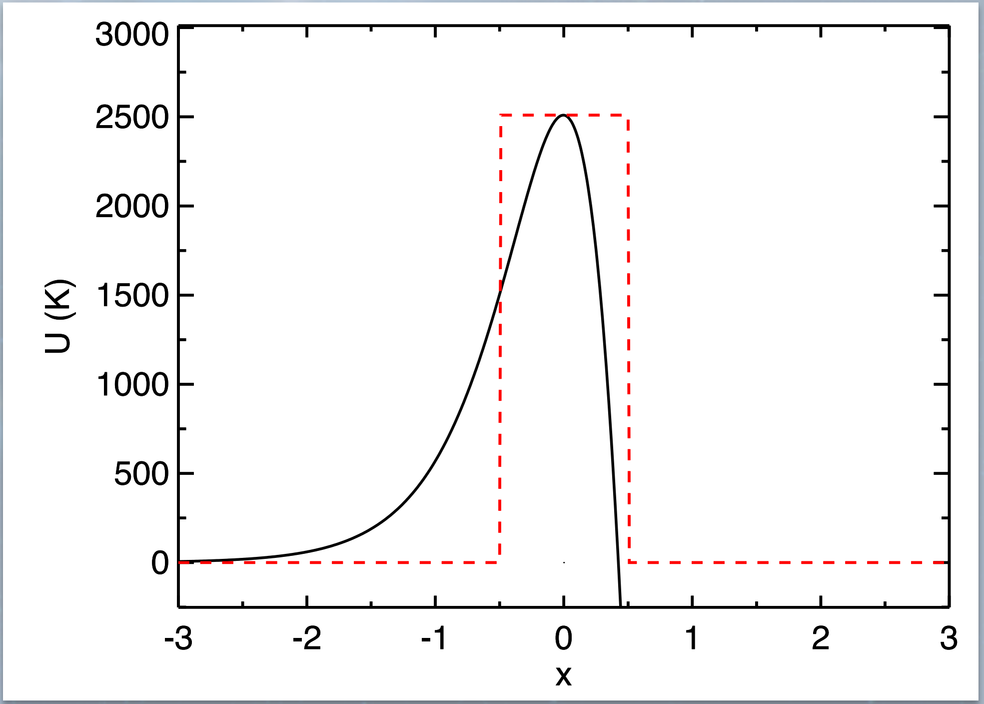

Taquet, Peters, Kahane, Ceccarelli et al. 2012c, A&A, submitted