Ice deuteration: Models and observations to interpret the protostar history

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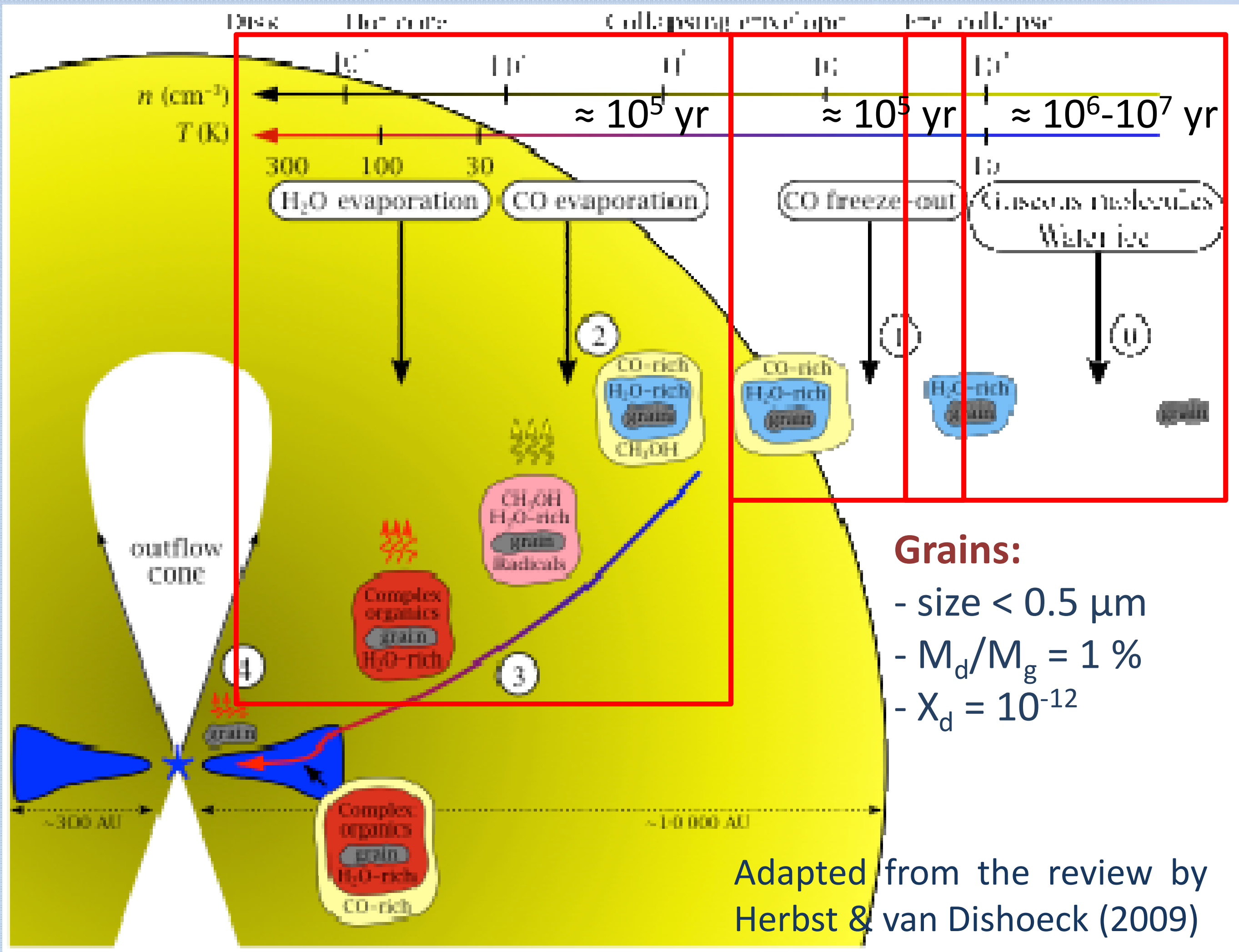
PCMI 2012 Conference

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

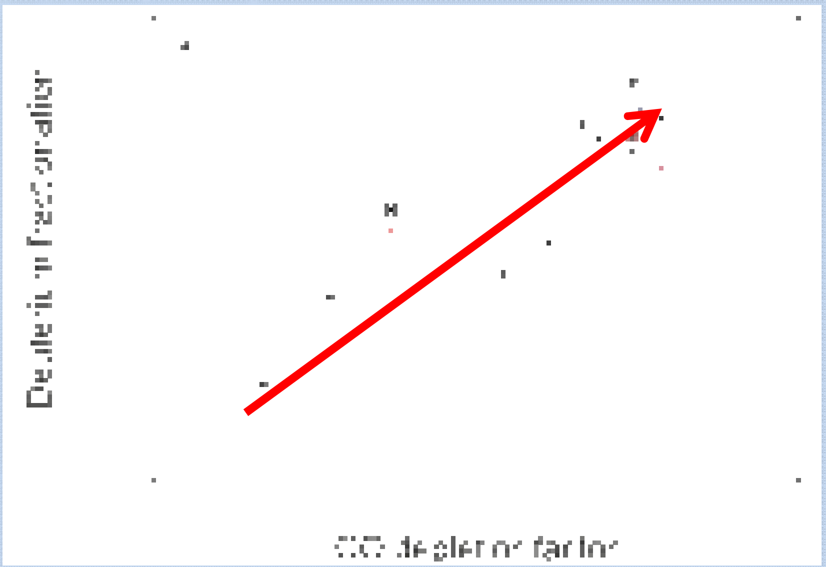
High deuteration is observed for **various species** in **prestellar cores:**

Molecular clouds

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

(Linsky 2003)

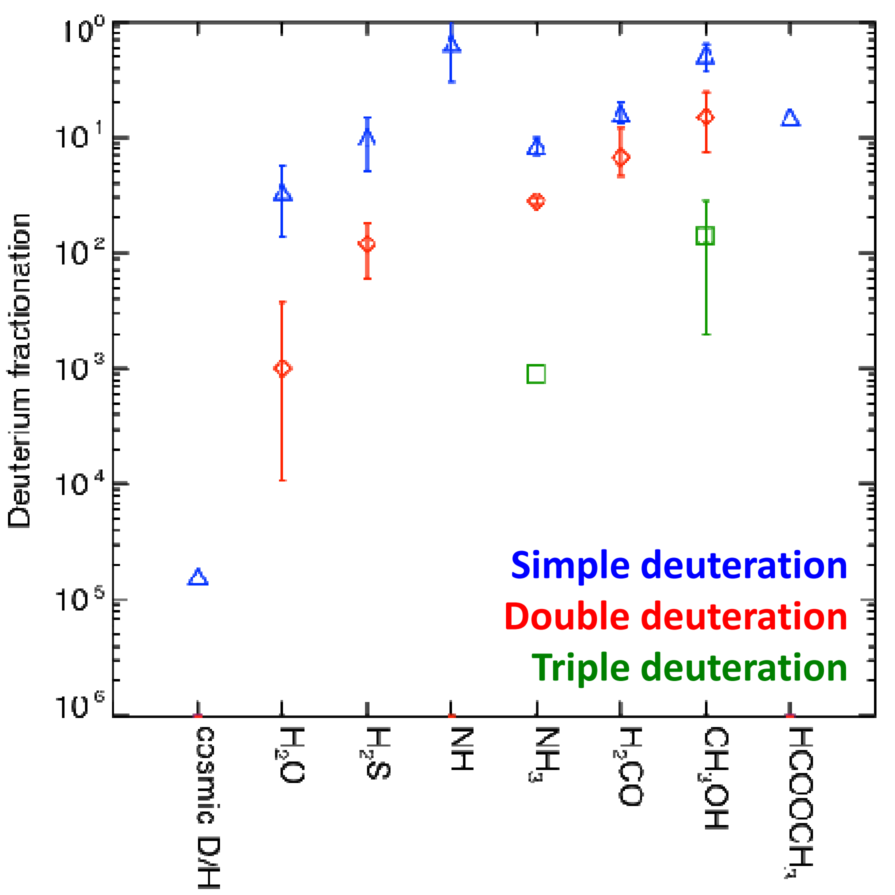
Prestellar cores



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

Deuteration in Class 0 protostars

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



➔ 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**

From Taquet et al. (2012, in press) **see A. Coutens's poster for water deuteration**

The GRAINOBLE model

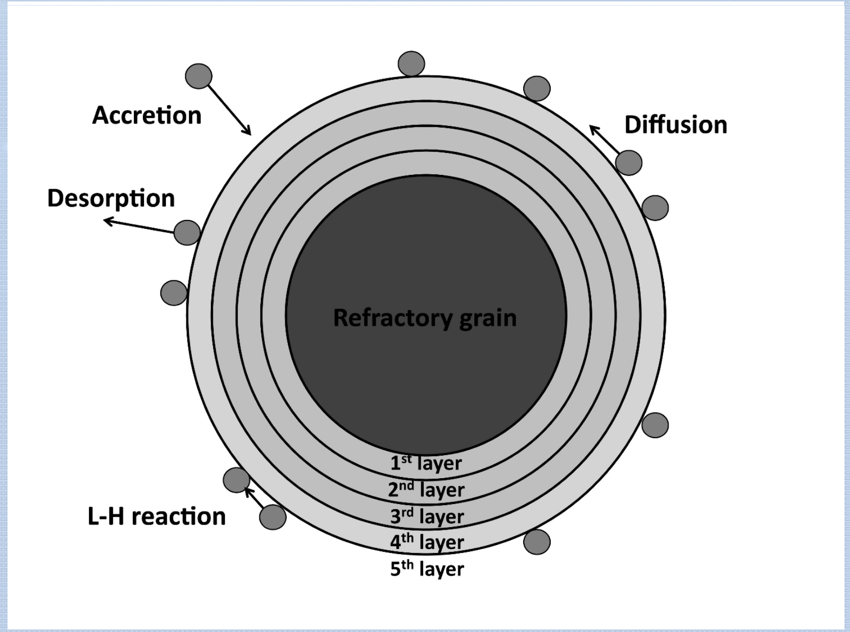
Time-dependent gas-grain astrochemical model based on the **rate equations** (Hasegawa et al. 1992)

- 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

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) (**see A. Faure and L. Gavilan's posters on H_2 o/p**)

Surface chemical network based on recent experimental works:

- **deuterated water** network from i) O (Dulieu+ 2010, Oba+ 2012), ii) O_2 (Miyauchi+ 2008, **see H. Chaabouni's poster**), iii) O_3 (Mokrane+ 2009)
- **deuterated formaldehyde and methanol** network (Watanabe+ 2002, Nagaoka+ 2005, Hidaka+ 2009, Fuchs+ 2009, **see A. Pernet's poster**)
- **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)

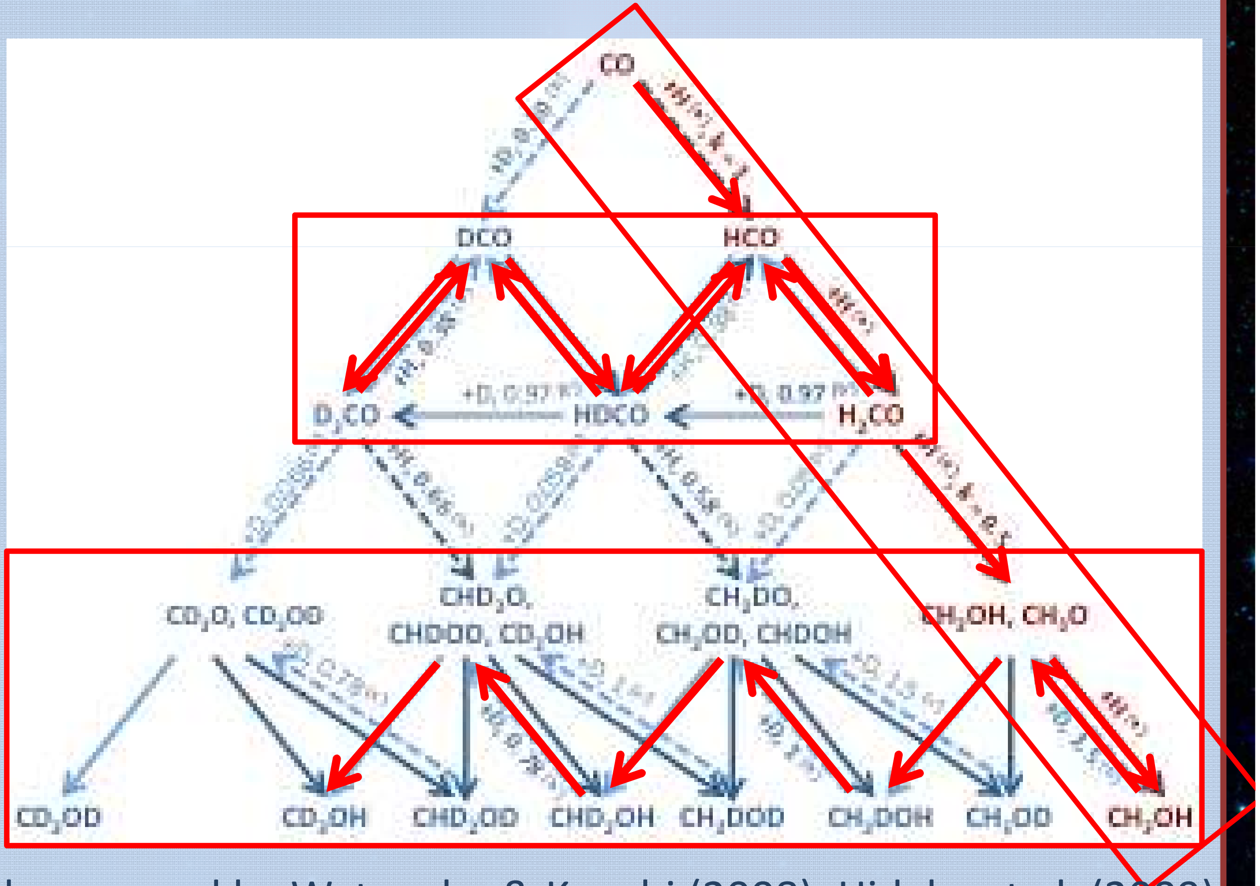
An example:
the methanol network

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)

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

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

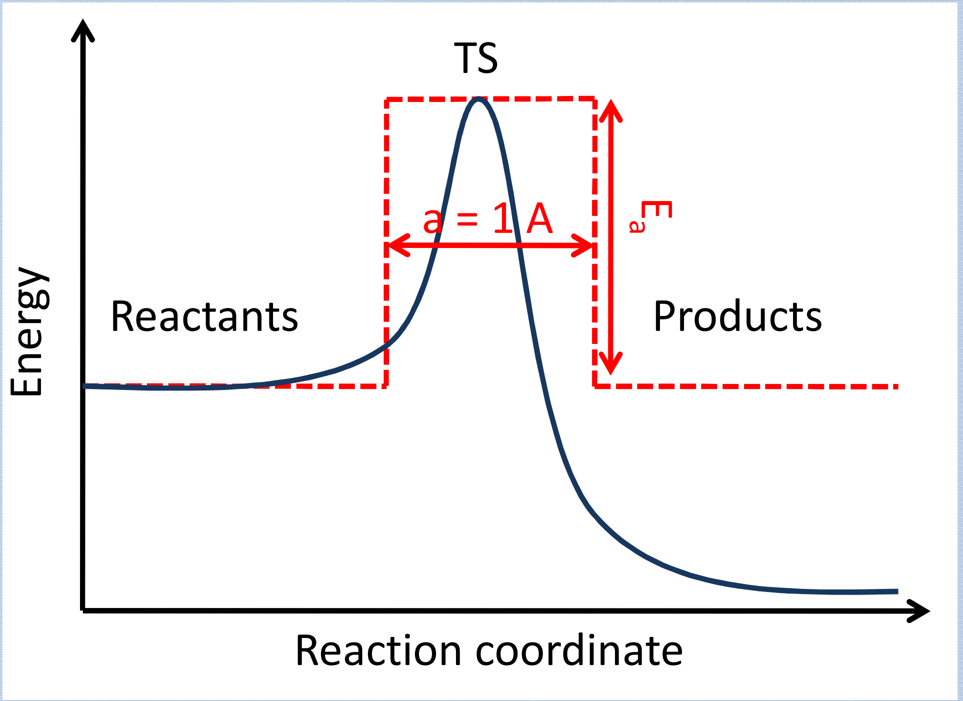
- The **Eckart model** is introduced for all the reactions, from quantum gas phase calculations

➔ 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.

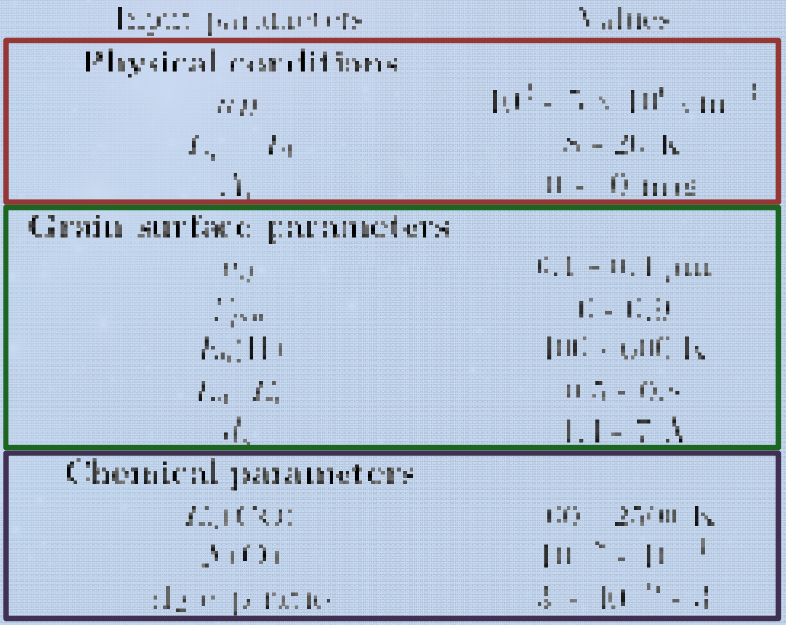
Multiparameter approach

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**

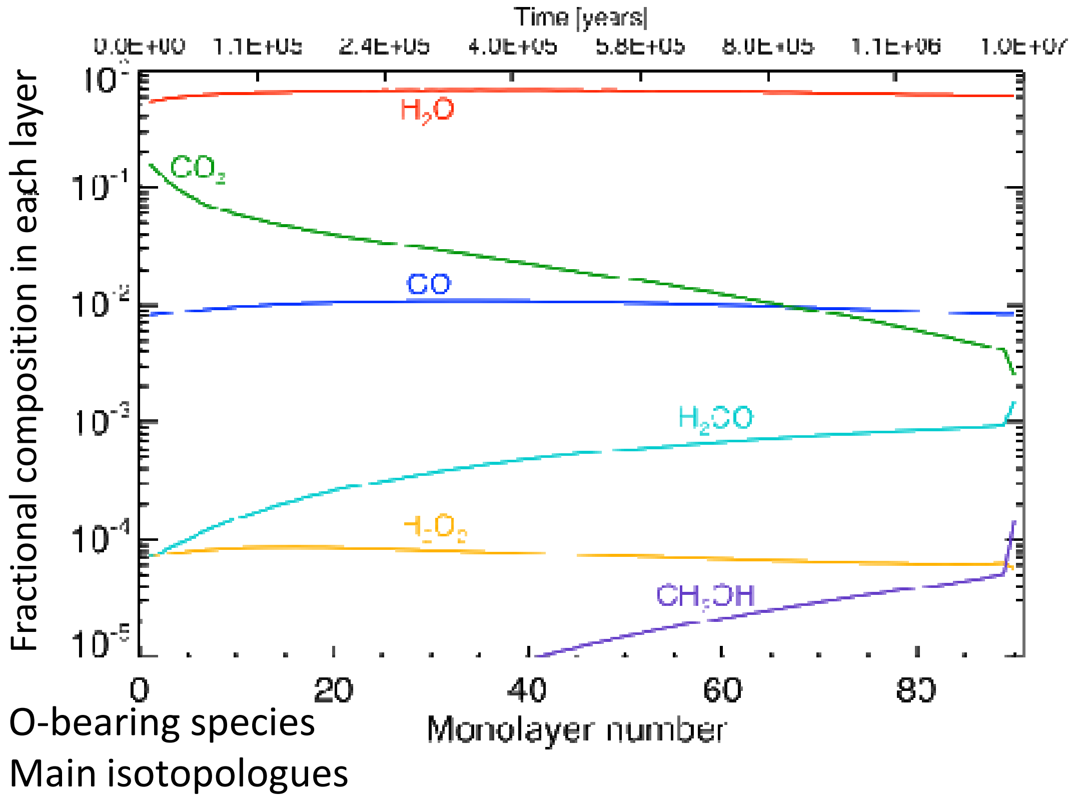


Input parameters	Values
Physical conditions	
[illegible]	[illegible]
[illegible]	[illegible] K
[illegible]	[illegible] mag
Grain surface parameters	
[illegible]	[illegible] μm
[illegible]	[illegible]
[illegible]	100 - 600 K
[illegible]	[illegible]
[illegible]	[illegible] Å
Chemical parameters	
[illegible]	[illegible] K
[illegible]	[illegible]
[illegible]	[illegible]

➔ **Model grid** by varying the input parameter values:
study the **influence of each parameter** on the ice chemistry
(**see also H. Mokrane's poster**)

Chemical differentiation within ices

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



O-bearing species
Main isotopologues

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. 2012c, A&A, accepted

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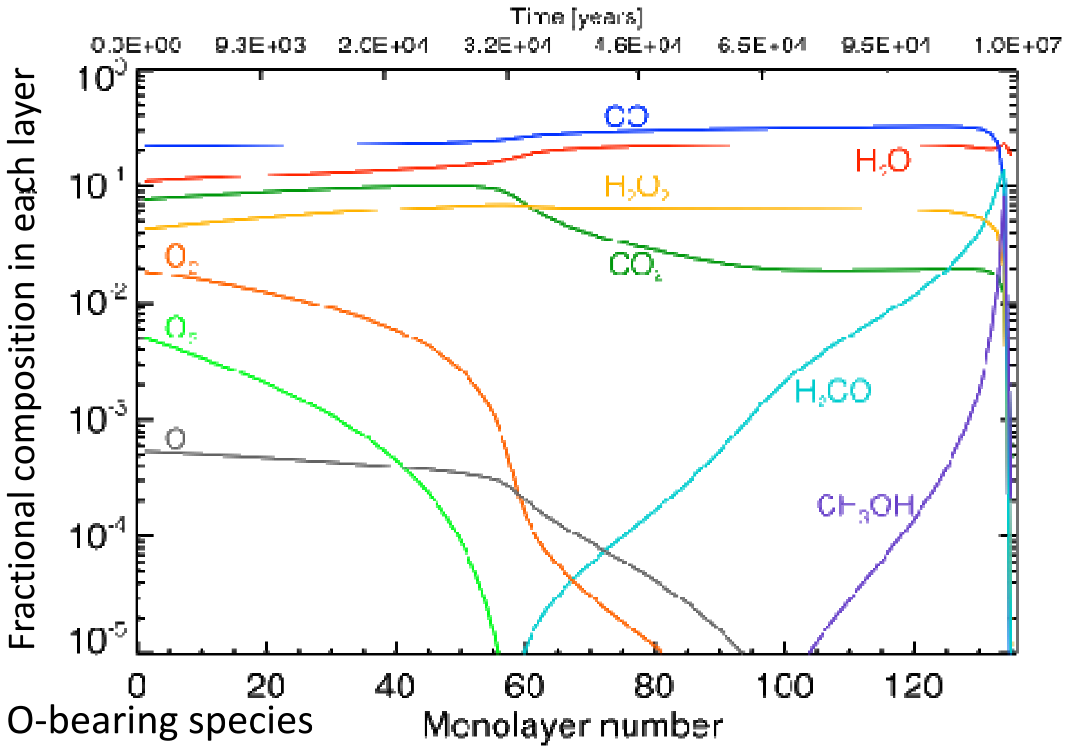


O-bearing species
Main isotopologues

Dense core region

$n_H = 10^5$ cm^{-3}
$T = 10$ K
$A_v = 10$ mag ($A_{v,obs} = 20$ mag)

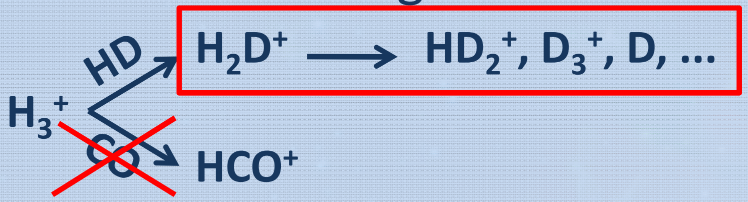
CO-rich ice

(+ 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. 2012c, A&A, accepted

CO depletion and ice deuteration

Deuteration reactions in competition with reactions involving CO



$H_3^+ \xrightarrow{HD} \boxed{H_2D^+ \longrightarrow HD_2^+, D_3^+, D, \ldots}$

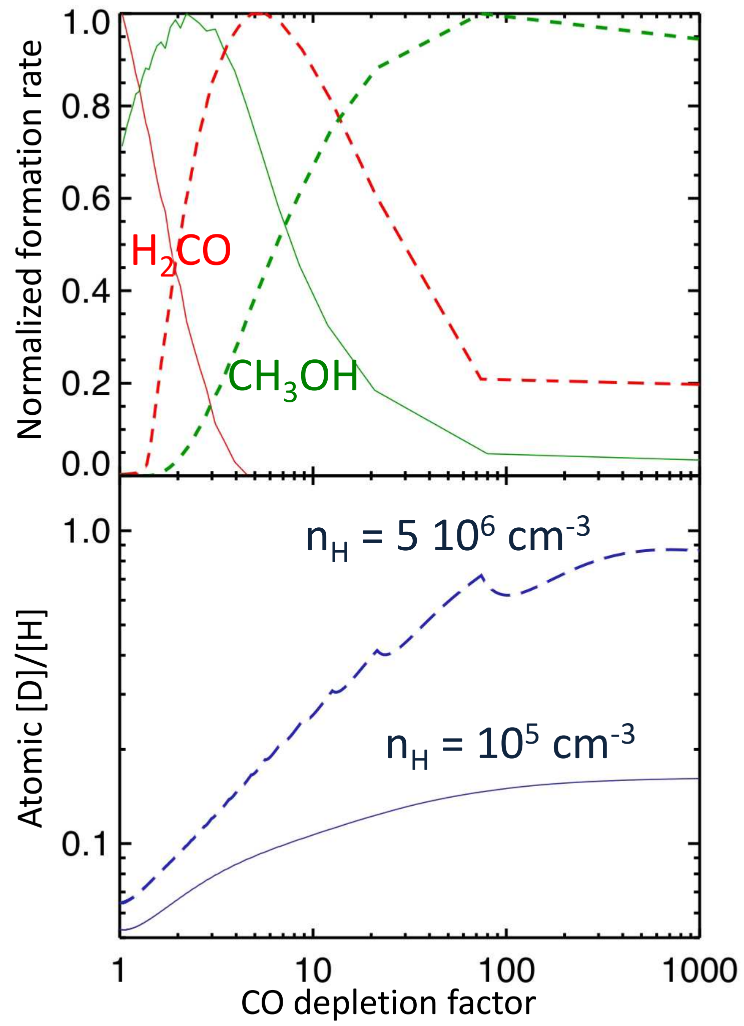
$H_3^+ \xrightarrow{\cancel{CO}} HCO^+$

➔ **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**

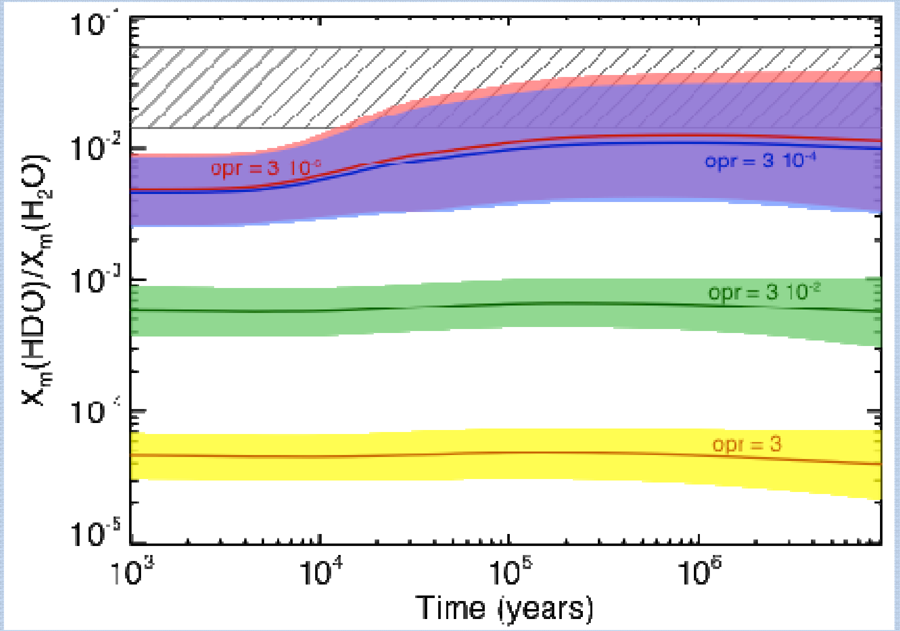


Taquet, Ceccarelli, Kahane 2012b, ApJL, 748, L3

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

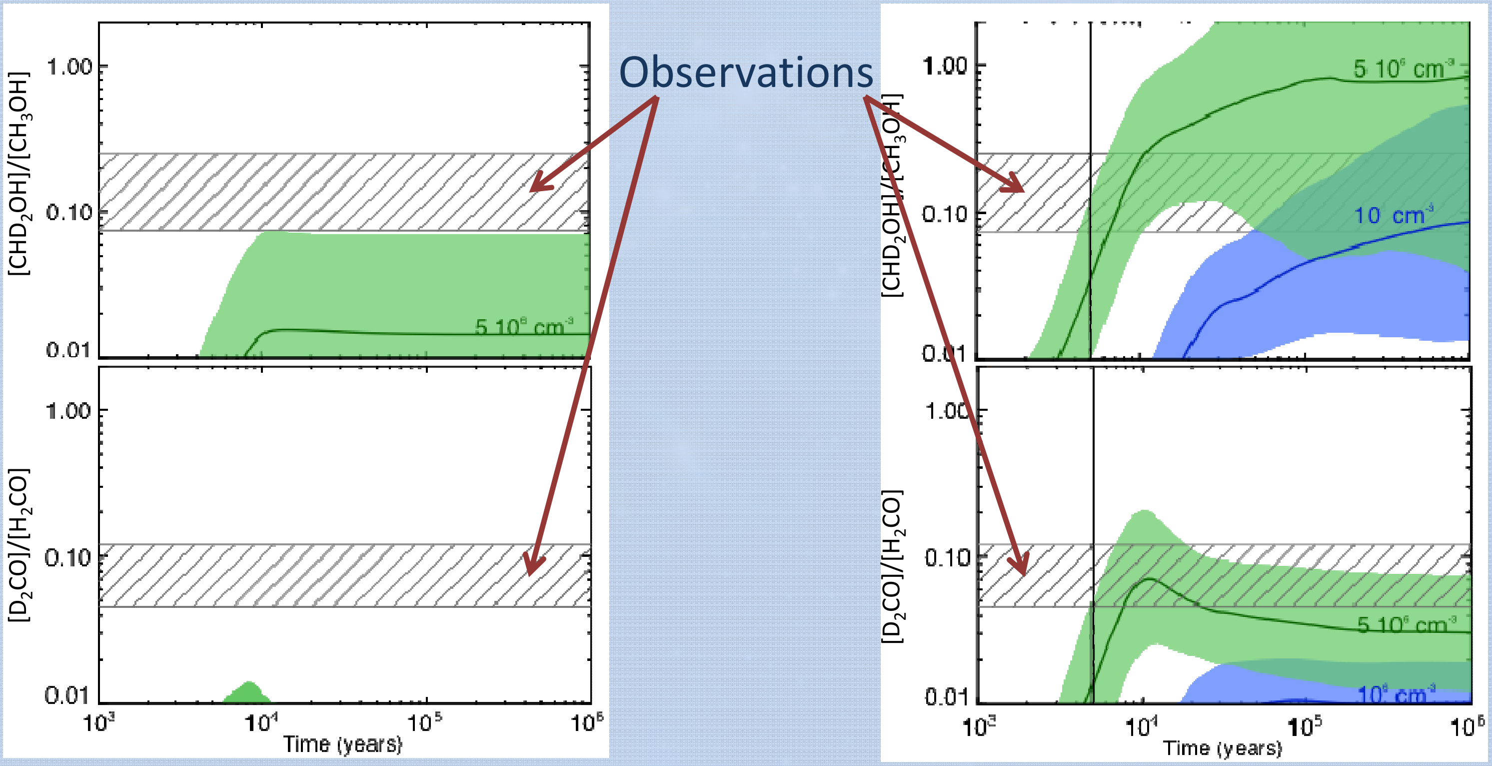
Taquet, Peters, Kahane, Ceccarelli et al. 2012c, A&A, in press.

Abstraction reactions and formaldehyde/methanol deuterations

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

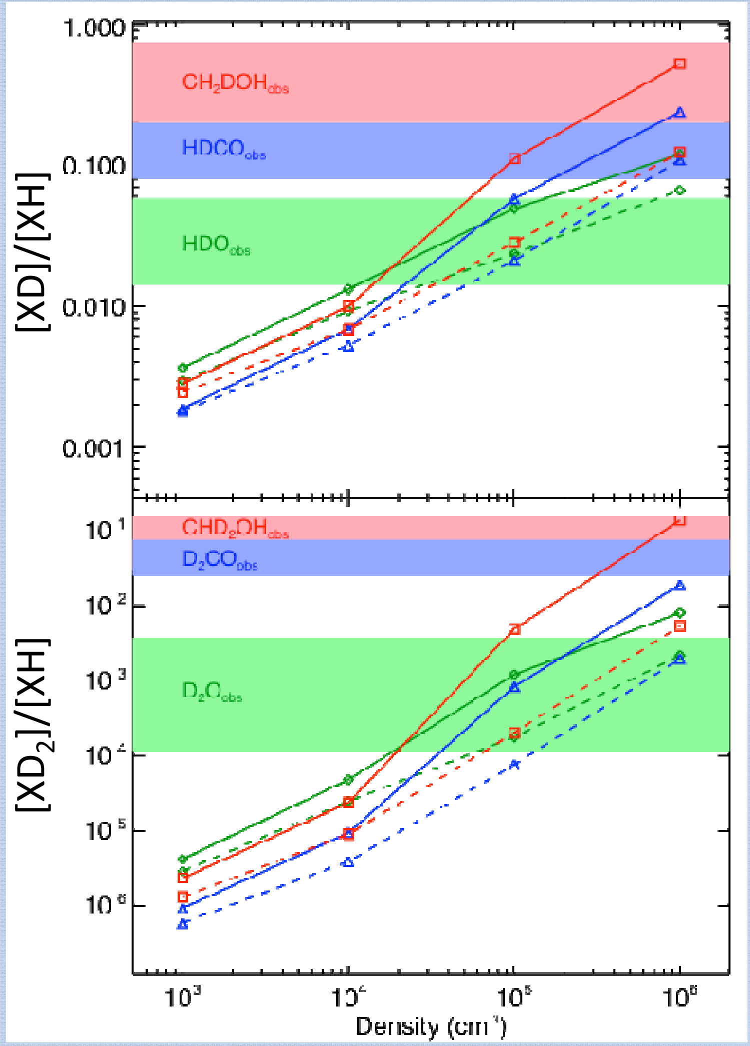
Addition reactions only

Addition + abstraction reactions



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

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. 2012c, A&A, in press.

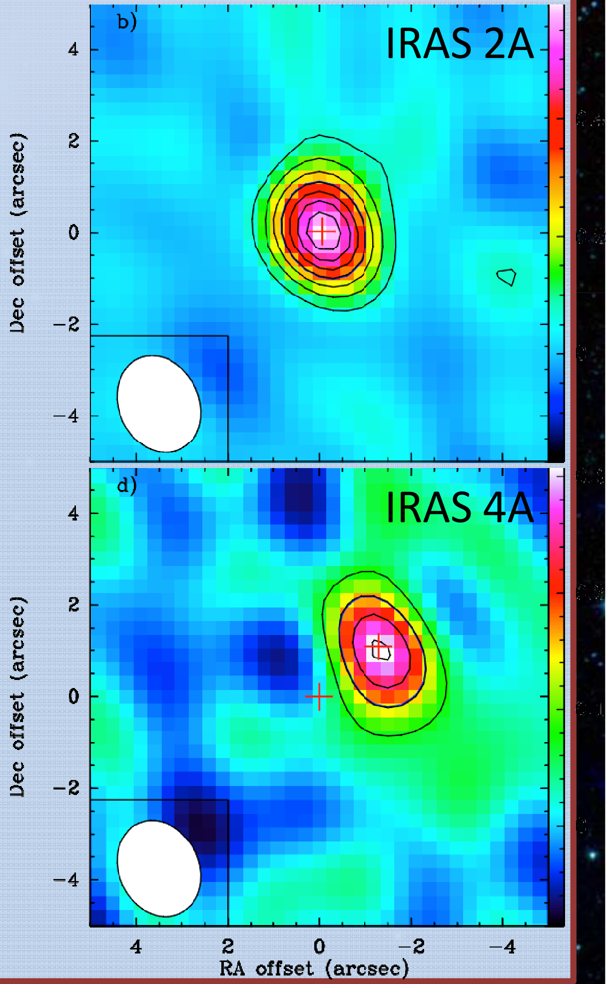
Water deuteration in low-mass protostars

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 **IRAS 16293**

➔ **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**: estimation of the emission coming from the **warm quiescent envelope**



Taquet, López-Sepulcre, Ceccarelli et al. 2012d, ApJL, in prep.

Water deuteration in low-mass protostars

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

→ Although the $H_2{}^{18}O$ emission has also an outflow component, most of the **HDO** and **$H_2{}^{18}O$** emissions originate from the **same quiescent envelope**

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

- **HDO/H_2O = 0.2-0.5 % in IRAS2A**
- **HDO/H_2O = 0.5-1 % in IRAS4A**

Taquet, López-Sepulcre, Ceccarelli et al. 2012d, ApJL, in prep.

Conclusions & Perspectives

✓ The **multilayer approach** shows that **ices** are **heterogeneous**

➔ in good agreement with A_V-dependent **ice observations**

✓ The **high deuteration** is **explained** by recent chemical networks

➔ ex: abstraction reactions are needed to reproduce the observed H_2CO and CH_3OH deuterations

✓ 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**