2. TIME FOR PLANTING: WATER AND ORGANIC MOLECULES IN PRESTELLAR CORES

2. Time for planting

1. What are the Prestellar Cores?
2. Mantle formation
3. The super-deuteration phenomenon
4. Organic molecules

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NOTE: This is NOT a review
=> references illustrative and NOT exhaustive

PREFACE: definition of "Molecular Deuteration"

2. Time for planting

2.0 Preface

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DEFINITION
The molecular deuteration is the ratio of the abundance of the molecule with D-atoms with respect to that with only H-atoms.
Exemple: HDO/H_2O ou D_2O/H_2O

ABUNDANCE RATIO OF DEUTERIUM AND HYDROGEN
Various observations, including those connected to cosmology, indicate that $D/H = 1.5x10^{-5}$.
Exemple: If the atoms of deuterium and hydrogen were statistically distributed one would have:
$HDO/H_2O=3.2x10^{-5}$ et $D_2O/H_2O=2.6x10^{-10}$

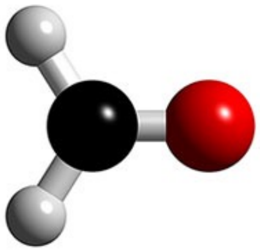
NOTE
In the molecular gas (molecular clouds, regions of star formations…) deuterium is mainly in the HD molecule.

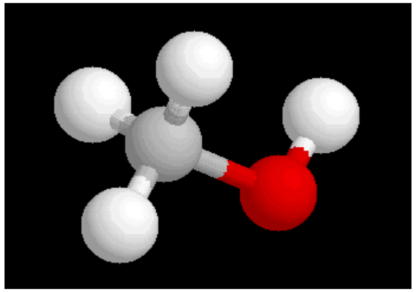
PREFACE: definition of "Complex Organic Molecule" (COM)

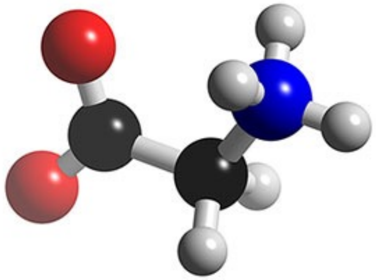
ORGANIC: A molecule containing at least one atom of carbon and connected with life (this definition has some arbitral sides).

COMPLEX: For the astronomers, molecules with more than 5 atoms are considered complex. Of course, a chemist would laugh at us.

EXEMPLES:
Formaldehyde (H_2CO), methanol (CH_3OH), glycine (NH_2CH_2COOH)







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2.0 Preface

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2.1 WHAT ARE THE PRESTELLAR CORES (PSC)?

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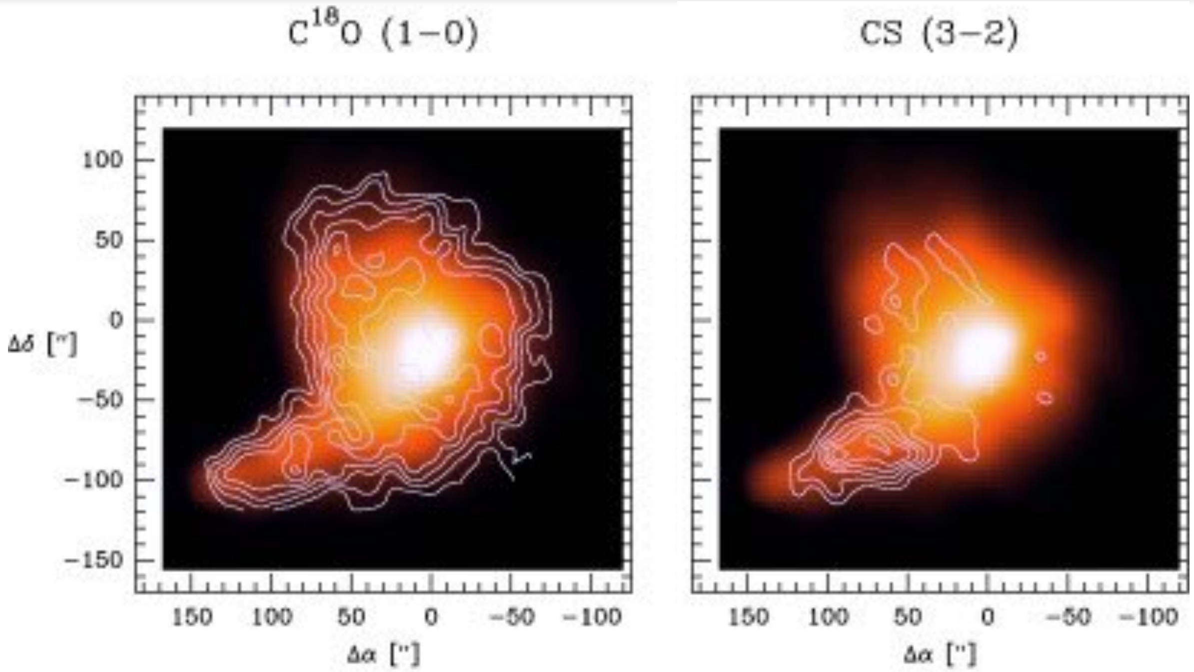
APPEARANCE of PRE-STELLAR CORES

PSC ARE BLACK SPOTS ON OPTICAL PLATES, INDICATING THE PRESENCE OF DENSE PATCHES OF DENSE AND COLD MATERIAL

PSC are the seeds from which stars are born and from which molecular complexity starts

APPEARANCE of PRE-STELLAR CORES

Continuum observations show that the dust and gas density **increases** towards the center (color in the figure).



Bergin et al. 2002
Bergin & Tafalla 2008

Line observations show that the abundance of some molecules **decreases** towards the center (contours in the figure).

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2.1 Prestellar Cores

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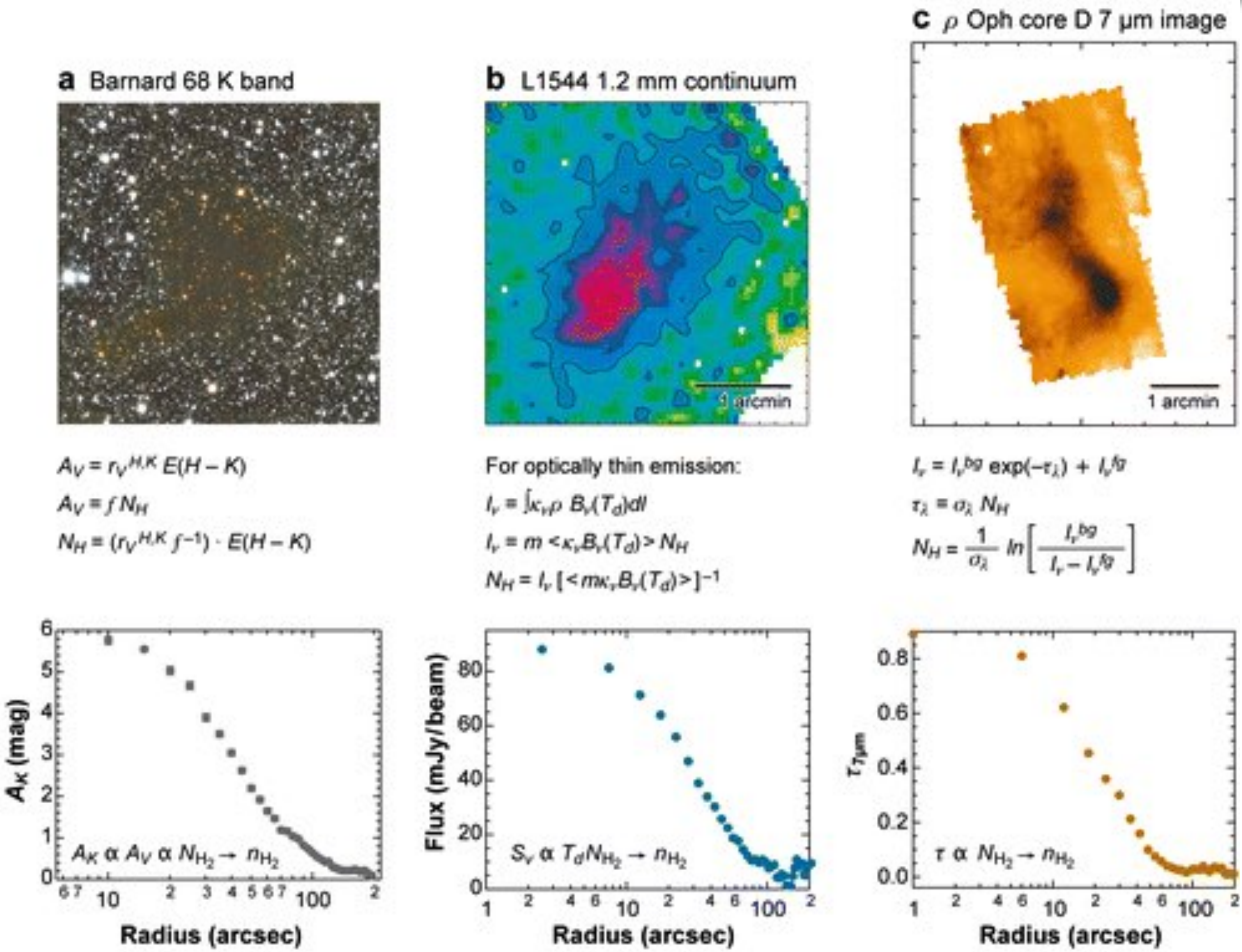
APPEARANCE of PRE-STELLAR CORES



Three methods are used to derive the PSC density profile:

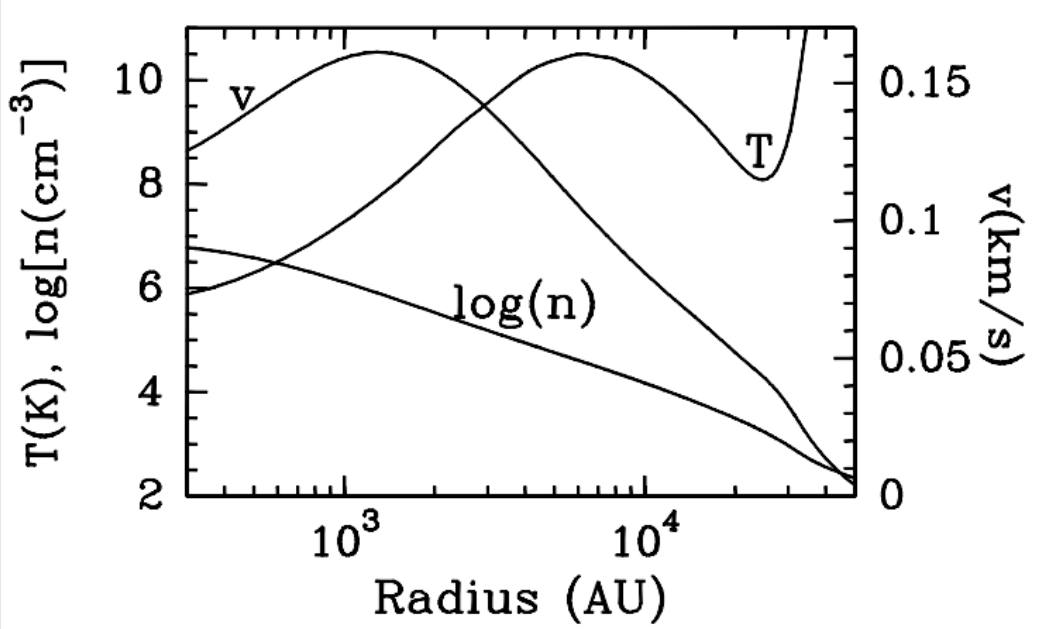
1) Observations in the NIR: measures of the H-K excess of the background stars, to derive the extinction A_V, and, consequently, $N(H+2H_2)$.

2) Observations of continuum at 1.3mm: the intensity gives N(dust) and, assuming a gas-to-dust ratio = 100, $N(H+2H_2)$.

3) Absorption at MIR: measures of the absorption of the MIR radiation, which gives again $N(H+2H_2)$.

THE DENSITY n IS DERIVED, ASSUMING THE SPHERICAL SYMMETRY, FROM THE $N(H+2H_2)$ 1D PROFILE

PHYSICAL STRUCTURE



Caselli et al. 2012

THE DENSITY INCREASES WHILE THE TEMPERATURE DECREASES GOING INWARDS

=> AT THE CENTRE, n_{H2} ~ 10^7 cm^{-3} , T_{gas} ~ 6 K

(evidence of inward matter movements)

MOLECULAR FREEZE-OUT

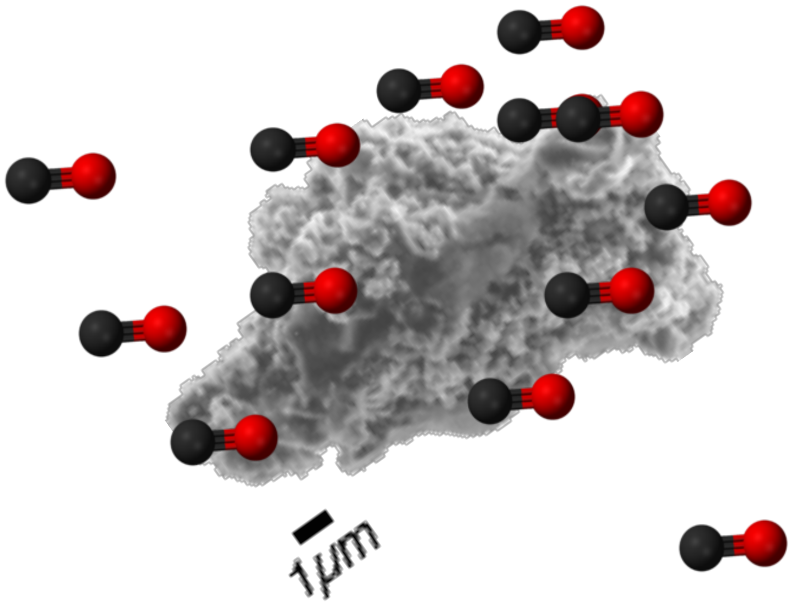
At PSC centre, molecules freeze-out onto the grain surfaces, forming the grain mantles, at a rate:

$$k_{ac} = S\,\pi a^2_{grain}\; n_{grain}\; v_x \quad s^{-1}$$

In absence of a mechanism that desorbs the mantles CO molecules would disappear from the gas phase on a time scale:

$$n_{CO}(t) = 10^{-4}\, n \cdot \exp\left[\frac{-t_{yr}}{4 \cdot 10^9}\, n\right]$$

where n is the gas density and t_{yr} is the time in years.



FOR A GAS DENSITY OF $10^5 cm^{-3}$, CO WOULD DISAPPEAR FROM THE GAS PHASE IN ABOUT FEW 10^4yr, IN ABSENCE OF MECHANISMS THAT REINJECT CO IN THE GAS

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MOLECULAR DESORPTION

Desorption occurs:

1) because of thermal evaporation -which depends on the molecule binding energy to the grain surface:

$$\tau_{ev} = \nu_0^{-1} \exp(E_b / kT_d)$$

2) thanks to the Cosmic Rays that hit the grains:

$$k_{cr} = 9.8 \cdot 10^{-15} \frac{\xi}{3 \cdot 10^{17} s^{-1}}$$

3) because of UV-photo-desorption for water, CO and perhaps other molecules, at the PSC border, where UV photons can penetrate.

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MOLECULAR DEPLETION

THE BALANCE BETWEEN MOLECULAR FREEZE-OUT AND DESORPTION GIVES THE MOLECULAR DEPLETION

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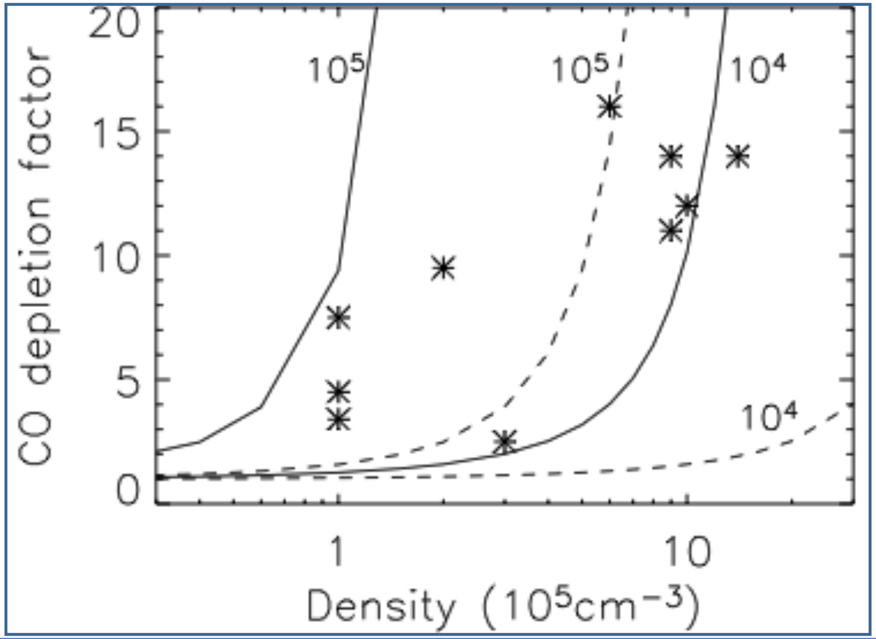

Ceccarelli et al. 2007, PP5

CO depletion factor, defined as the ratio between the non-depleted (A_{CO}) and the actual CO abundance, as function of the density and for different times. The solid lines refer to standard grains, whereas the dashed lines refer to grains 3 times larger in sizes. Stars show measures in a few PSCs.

2.2 MANTLE FORMATION

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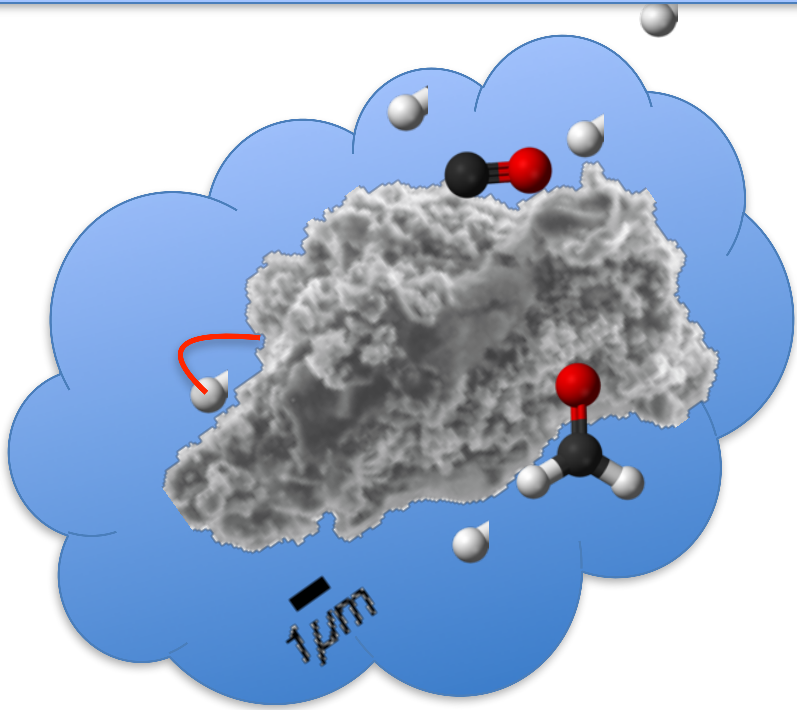
GRAIN MANTLE FORMATION

FROZEN O/CO/N/C ARE HYDROGENATED ON THE GRAIN SURFACES
=> **SIMPLE MOLECULES FORMATION:** WATER (H_2O), FORMALDEHYDE (H_2CO) and METHANOL (CH_3OH), AMMONIA (NH_3), METHANE (CH_4)...



THE ASSUMPTION IS THAT H-ATOMS SCAN THE GRAIN SURFACE AND REACT WITH THE CONDENSED SPECIES

NOTE: HEAVIER ATOMS DO NOT HAVE ENOUGH ENERGY TO MOVE AROUND, AT T_{dust}<40K

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2.2 Mantle formation

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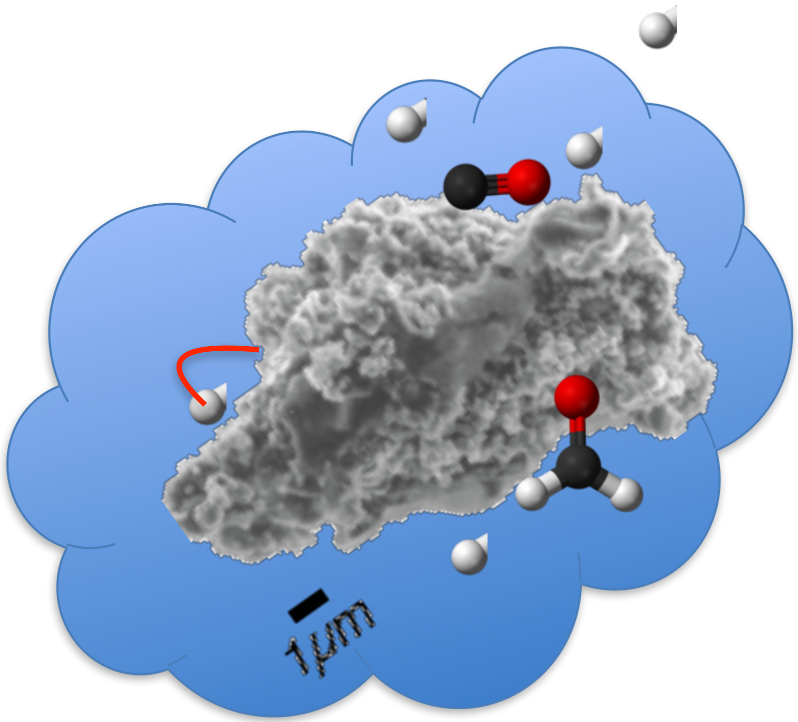
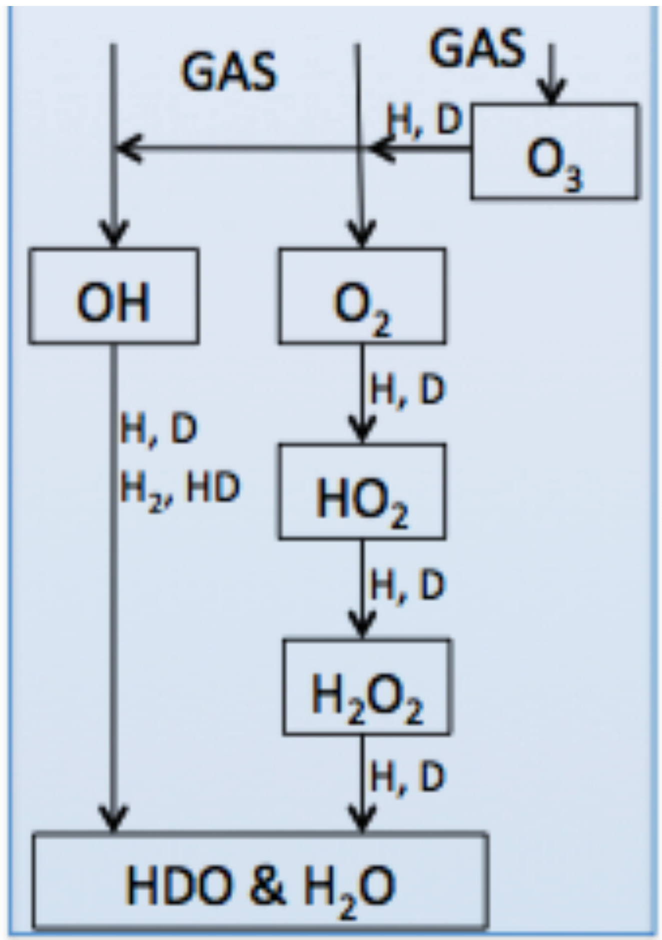
WATER MANTLE FORMATION

WATER (MAINLY) FORMS ON THE GRAIN SURFACES FROM GASEOUS O (and O_2 and O_3) STICKING ON THE GRAINS





Ceccarelli et al. 2014, PP6

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WATER OBSERVATIONS

FIRST (AND ONLY) DETECTION WITH HERSCHEL

Caselli et al. 2012

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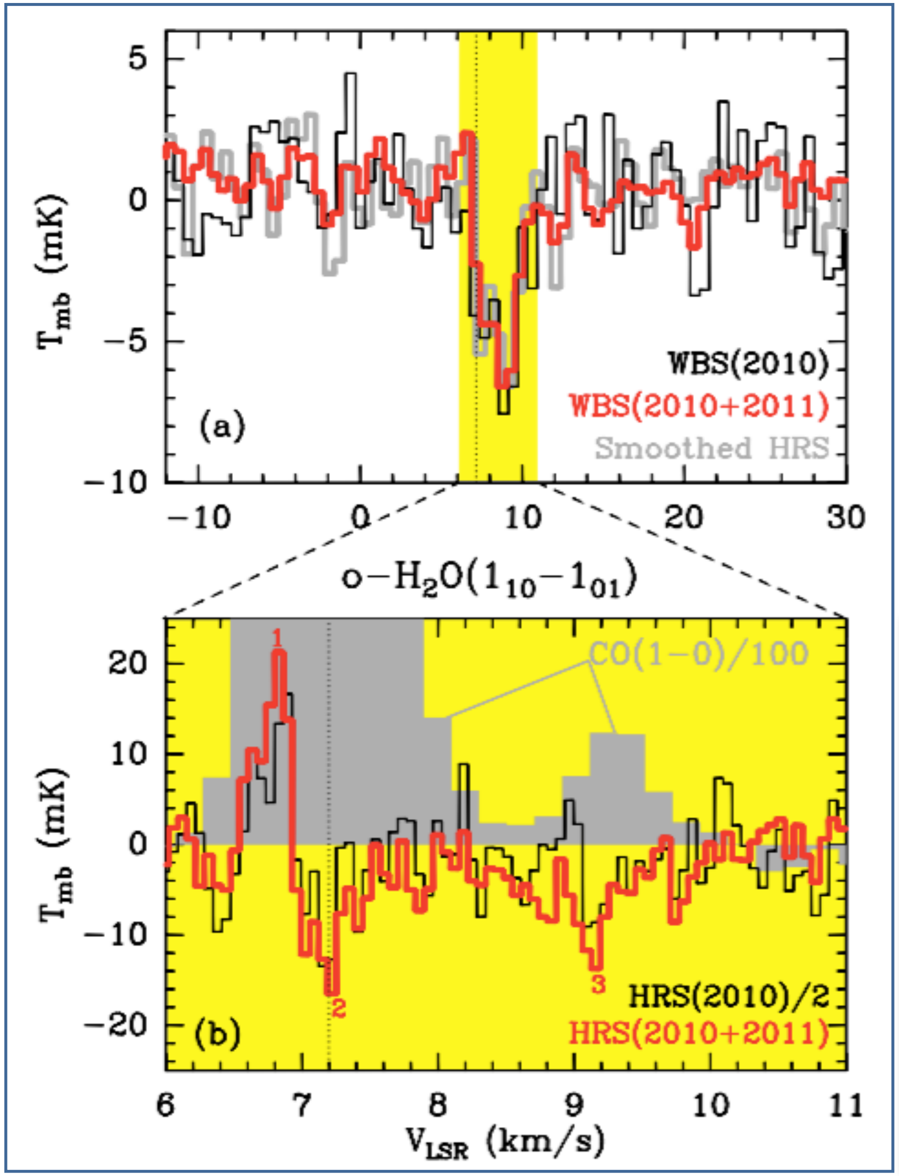
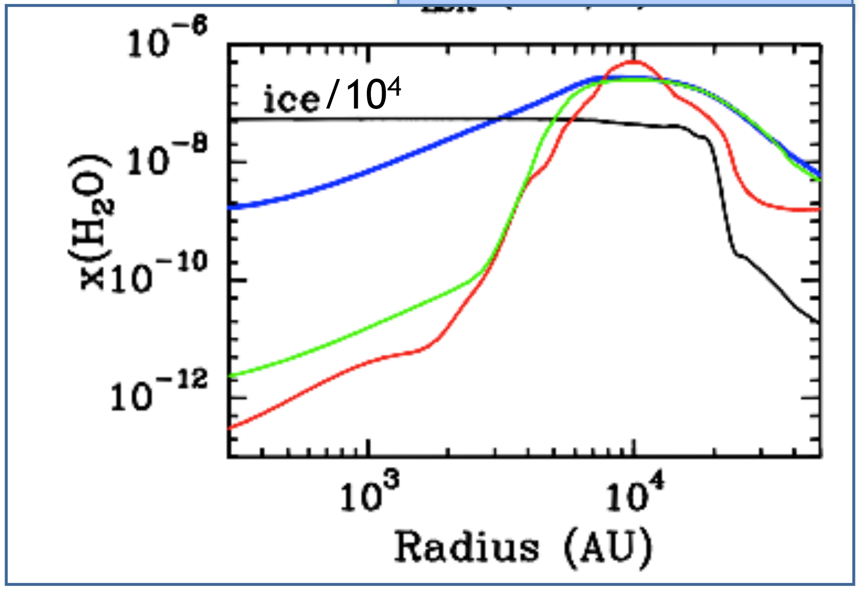
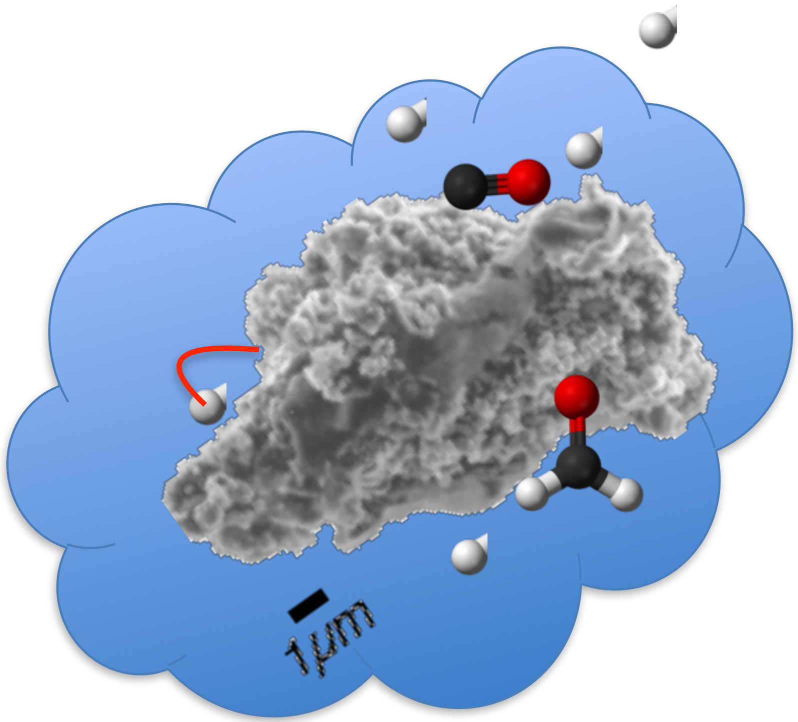




1) THE BULK OF WATER VAPOR IS AT THE BORDER, PHOTO-EVAPORATED BY THE IS UV-PHOTONS
2) THE BULK OF WATER IS FROZEN AROUND GRAINS

METHANOL FORMATION

FROZEN CO IS HYDROGENATED ON THE GRAIN SURFACES, FORMING FORMALDEHYDE AND THEN METHANOL



TIME

$CO + H = HCO$

$HCO + H = H_2CO$

$H_2CO + H = CH_3O$

$CH_3O + H = CH_3OH$

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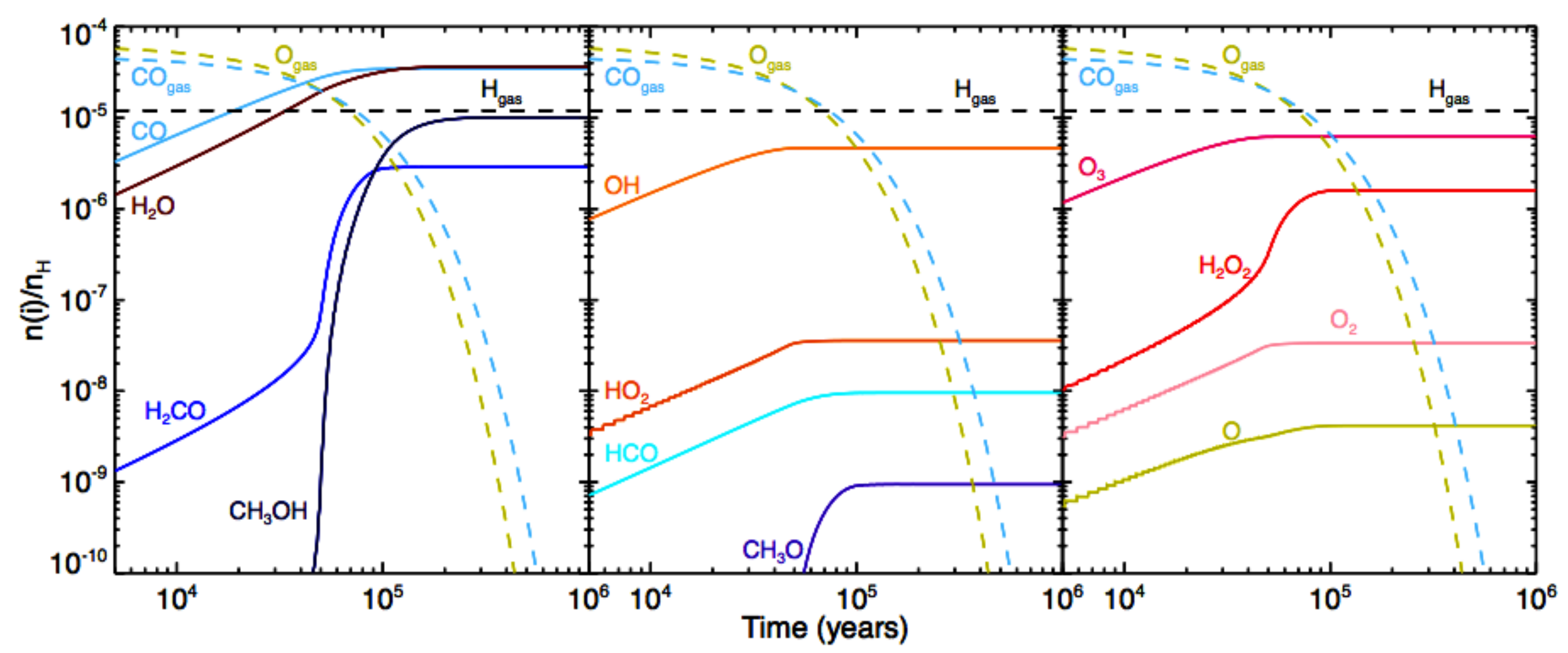
METHANOL FORMATION

FROZEN CO IS HYDROGENATED ON THE GRAIN SURFACES, FORMING FORMALDEHYDE AND THEN METHANOL



Taquet et al. 2012,2013

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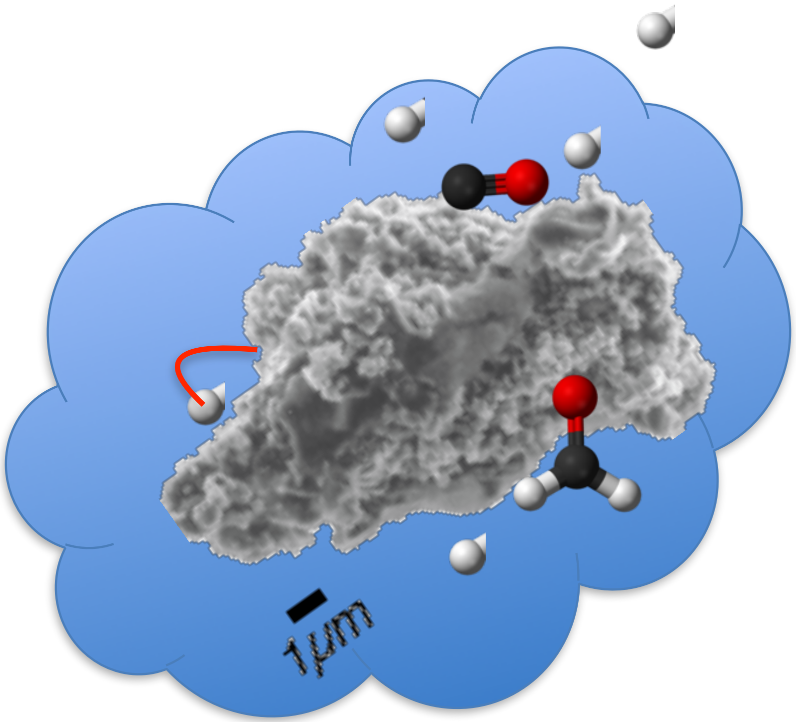
METHANOL FORMATION

LABORATORY EXPERIMENTS + THEORY + MODELING ARE INDISPENSABLE TO UNDERSTAND WHAT HAPPENS



TIME

$CO + H = HCO$

$HCO + H = H_2CO$

$H_2CO + H = CH_3O$

$CH_3O + H = CH_3OH$

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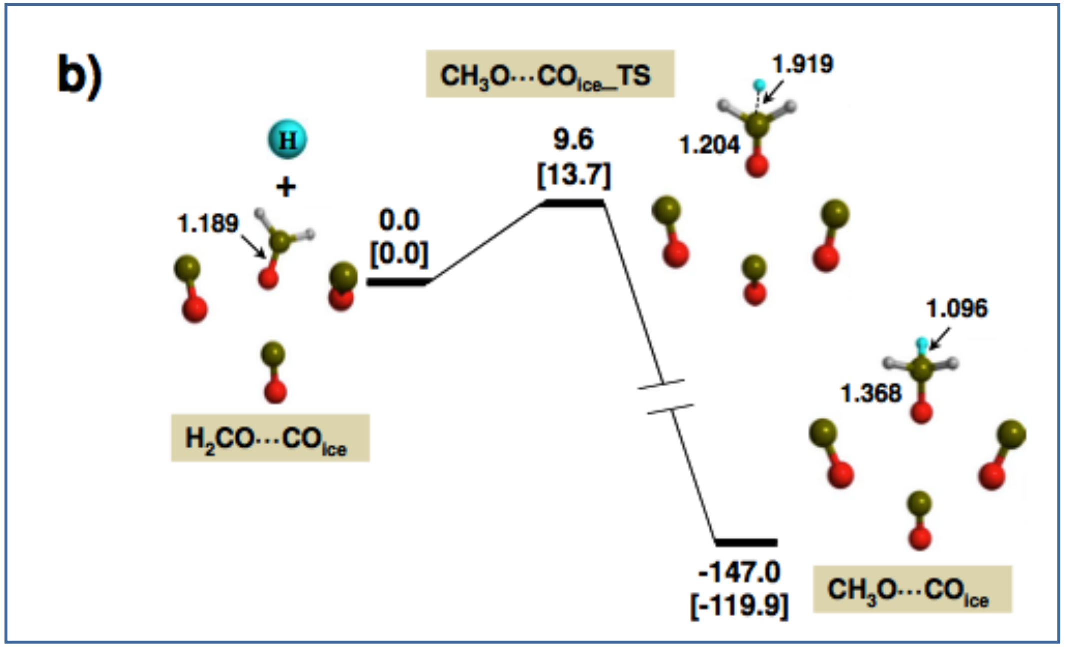
METHANOL FORMATION

LABORATORY EXPERIMENTS + THEORY + MODELING ARE INDISPENSABLE TO UNDERSTAND WHAT HAPPENS



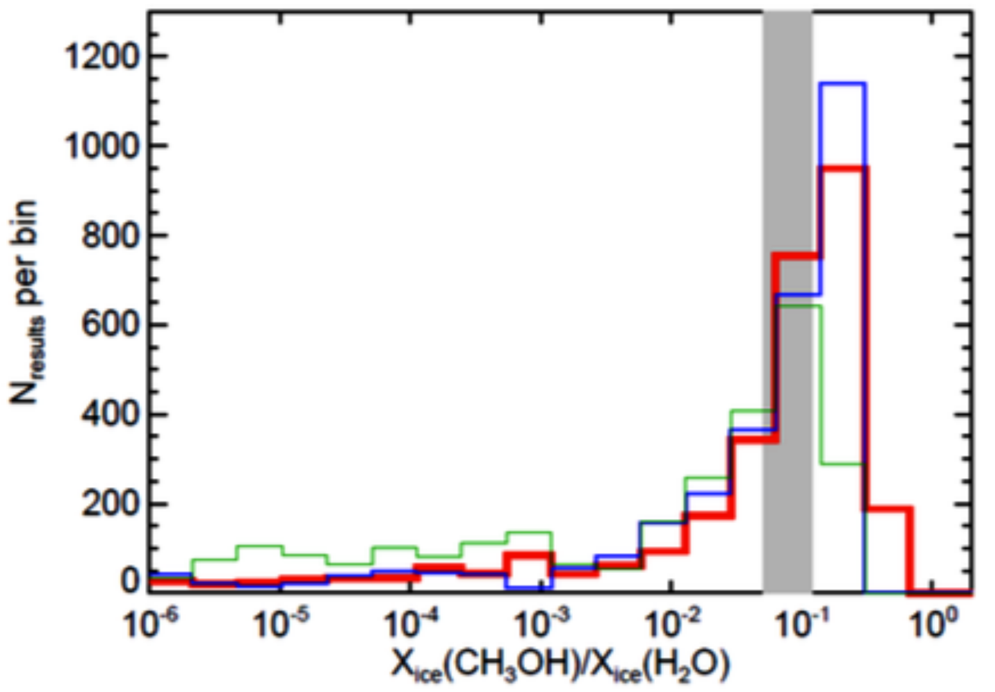
Rimola et al. 2014

H_2CO + H = CH_3O

THE REACTION HAS AN ENERGY BARRIER DIFFICULT TO SURMOUNT AT 10K

METHANOL FORMATION

LABORATORY EXPERIMENTS + THEORY + MODELING ARE INDISPENSABLE TO UNDERSTAND WHAT HAPPENS



Rimola et al. 2014

WHEN CONSIDERING THE (MANY) UNCERTAIN PARAMETERS ENTERING IN THE ASTROCHEMICAL MODELS, STATISTICALLY IT IS POSSIBLE

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2.2 Mantle formation

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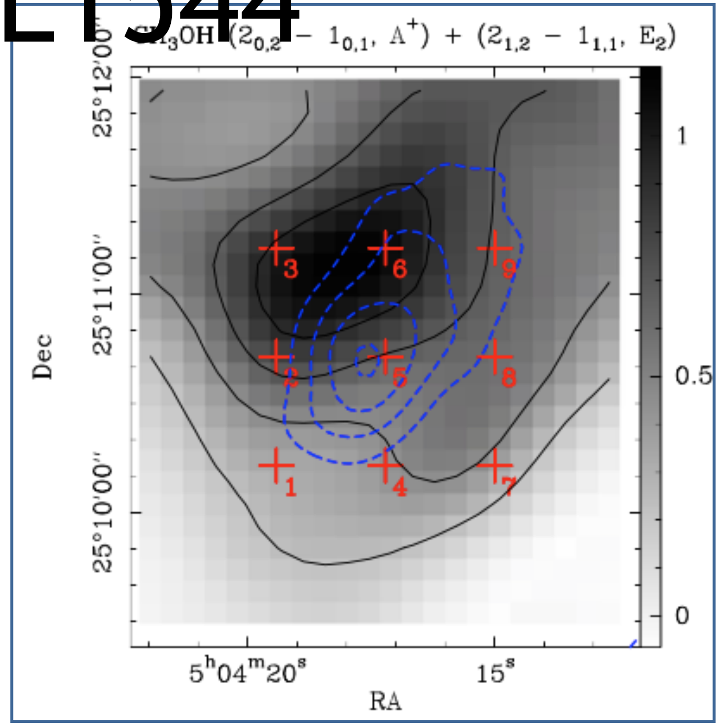
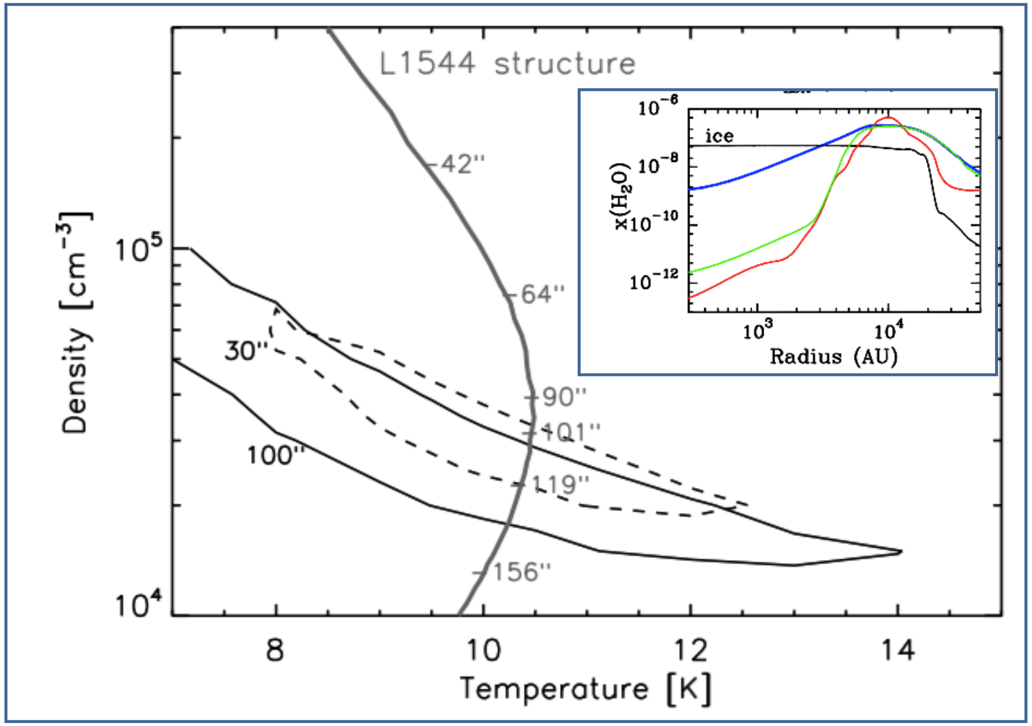
METHANOL OBSERVATIONS

OBSERVED IN SEVERAL PSCs, DETAILED ANALYSIS IN ONE

L1544



Bizzocchi et al. 2014



Vastel et al. 2014

METHANOL EMISSION ORIGINATES AT THE BORDER OF THE CONDENSATION
=> LIKELY PHOTO-DESORBED LIKE THE WATER

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2.3 THE SUPER-DEUTERATION PHENOMENON

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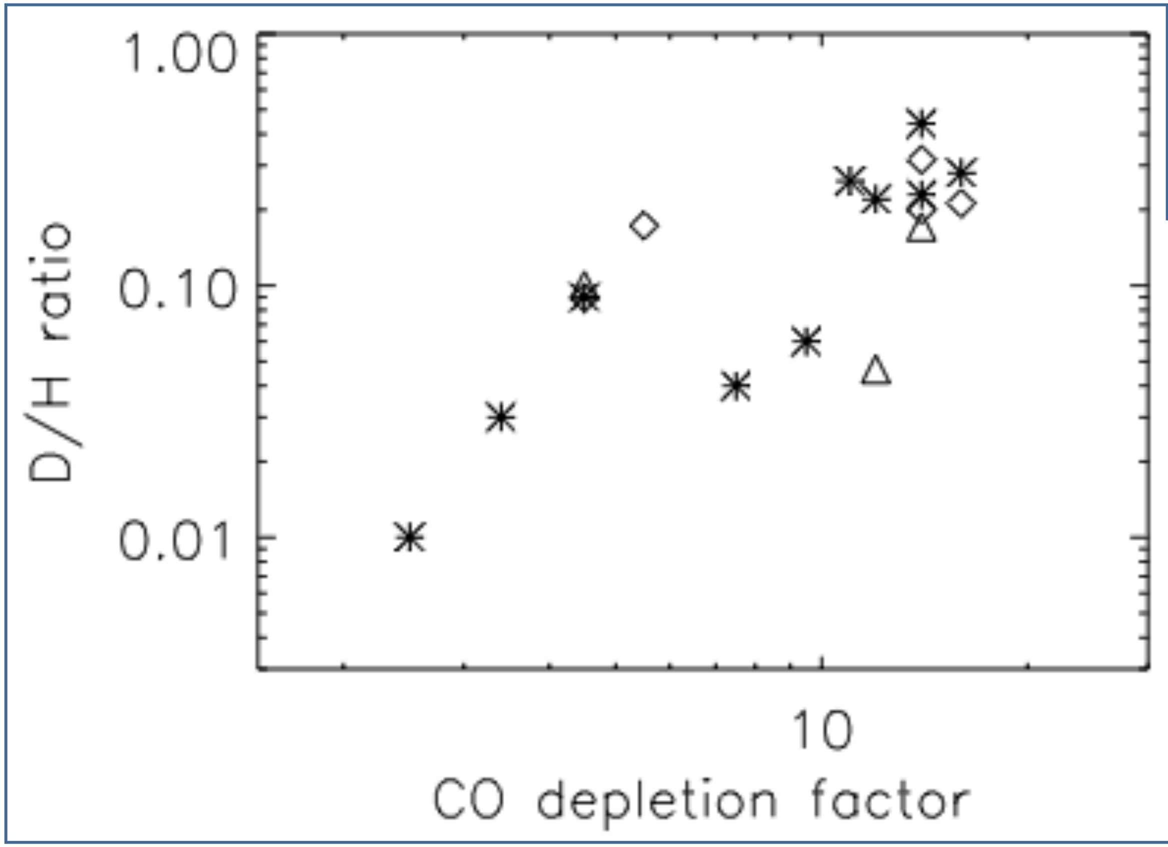
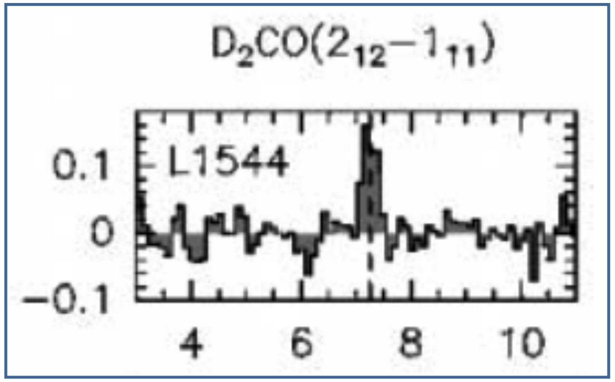
SINGLY & DOUBLY DEUTERATED MOLECULES

SINCE ABOUT 2000, SEVERAL MOLECULES WITH A HIGH MOLECULAR DEUTERATION WERE DETECTED IN PSCs
e.g. D_2CO/H_2CO~0.3 (instead of ~10^{-10} based on D/H)



D_2CO Bacmann et al. 2003
ND_2H Roueff et al. 2005
N_2D^+ Crapsi et al. 2005



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DEUTERATION REACTIONS

2. Time for planting

2.3 Super-deuteration

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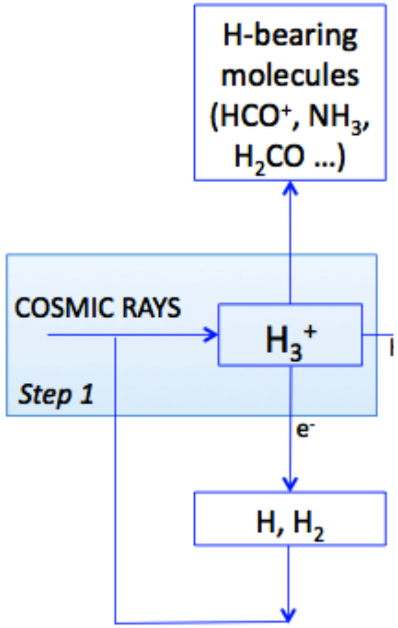
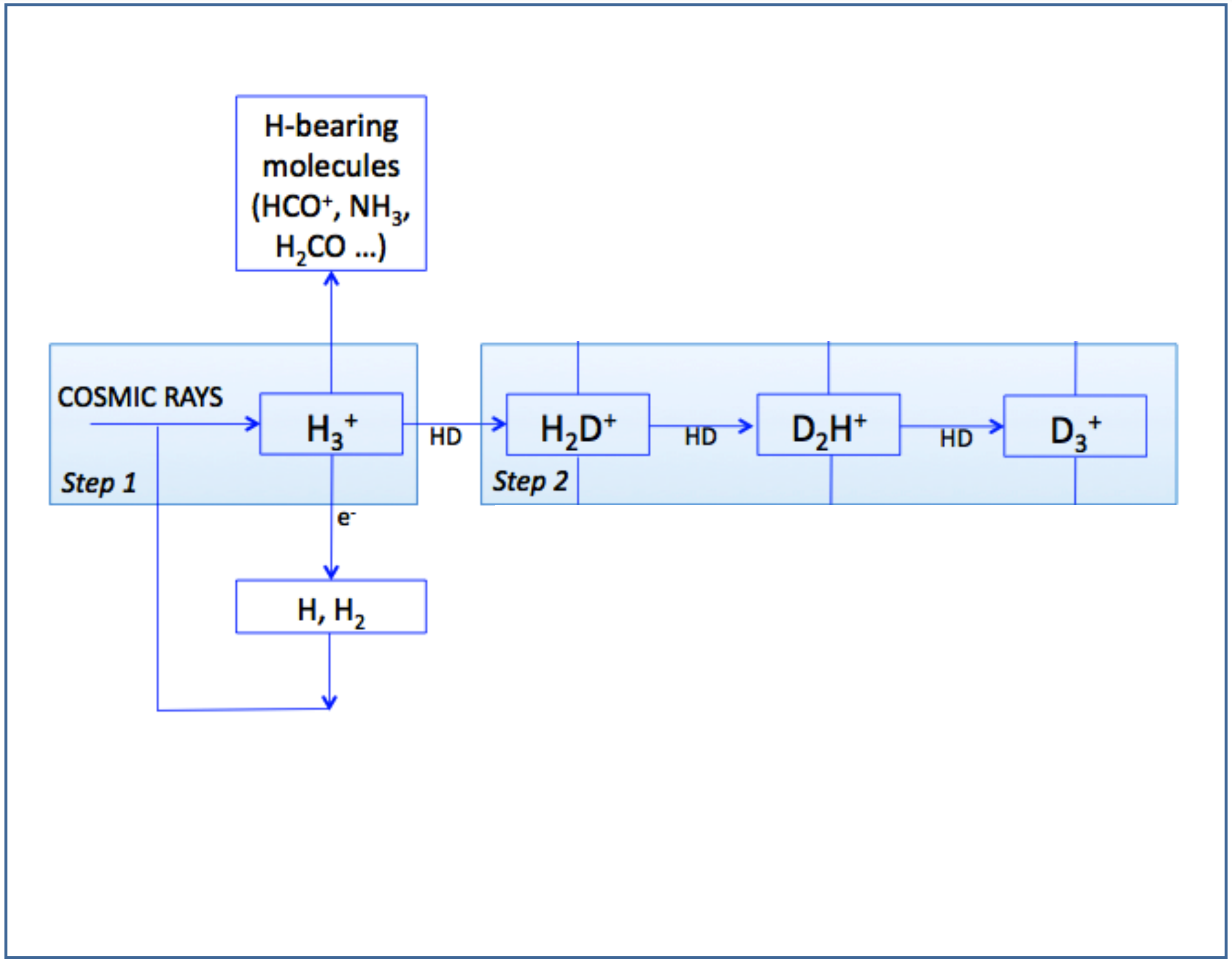


THREE STEPS:

1) Cosmic rays ionisation of H_2 and H

DEUTERATION REACTIONS



THREE STEPS:

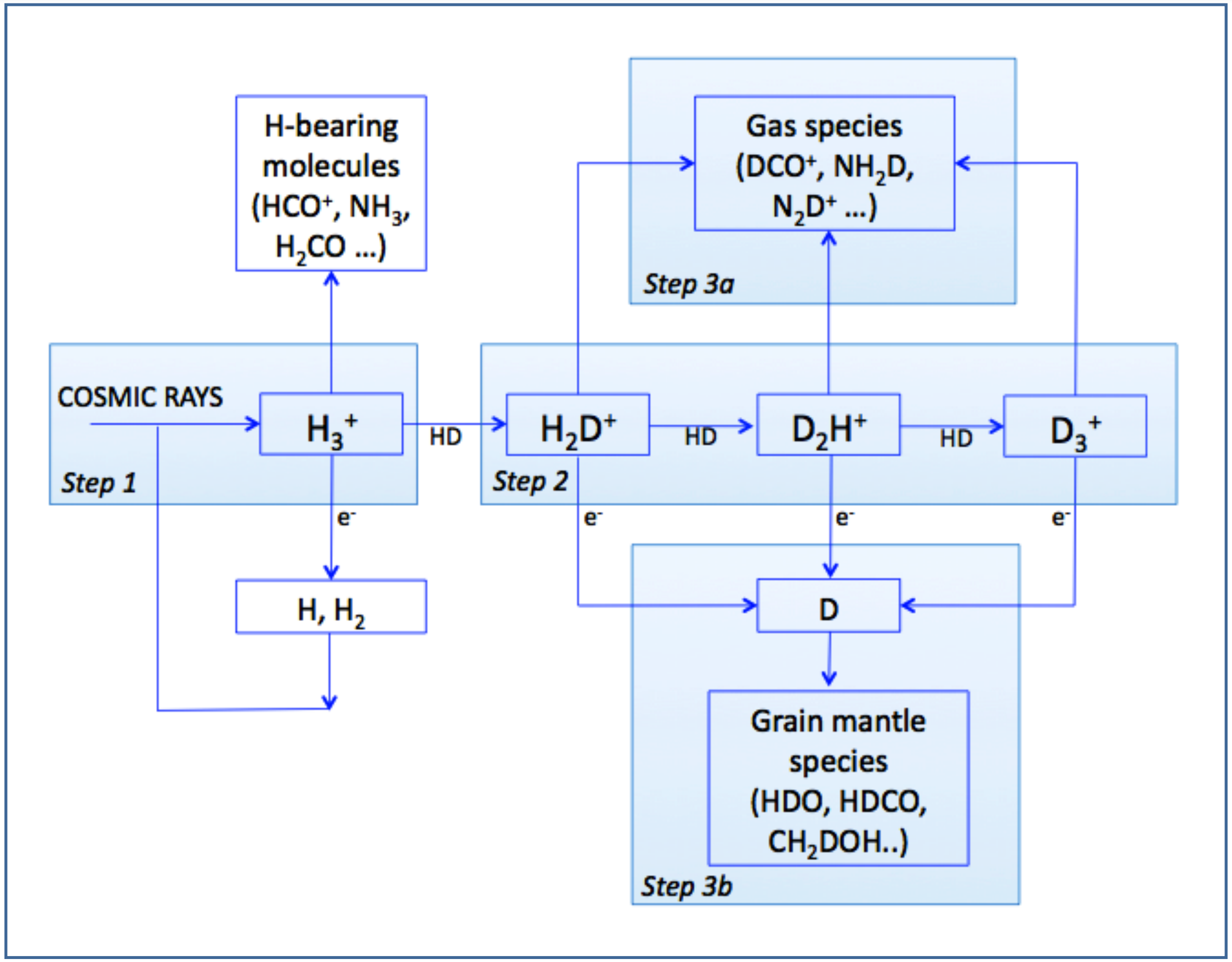
1) Cosmic rays ionisation of H_2 and H

2) Formation of the deuterated forms of H_3^+

DEUTERATION REACTIONS

2. Time for planting

2.3 Super-deuteration



Ceccarelli et al. 2014, PP6

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THREE STEPS:

1) Cosmic rays ionisation of H_2 and H

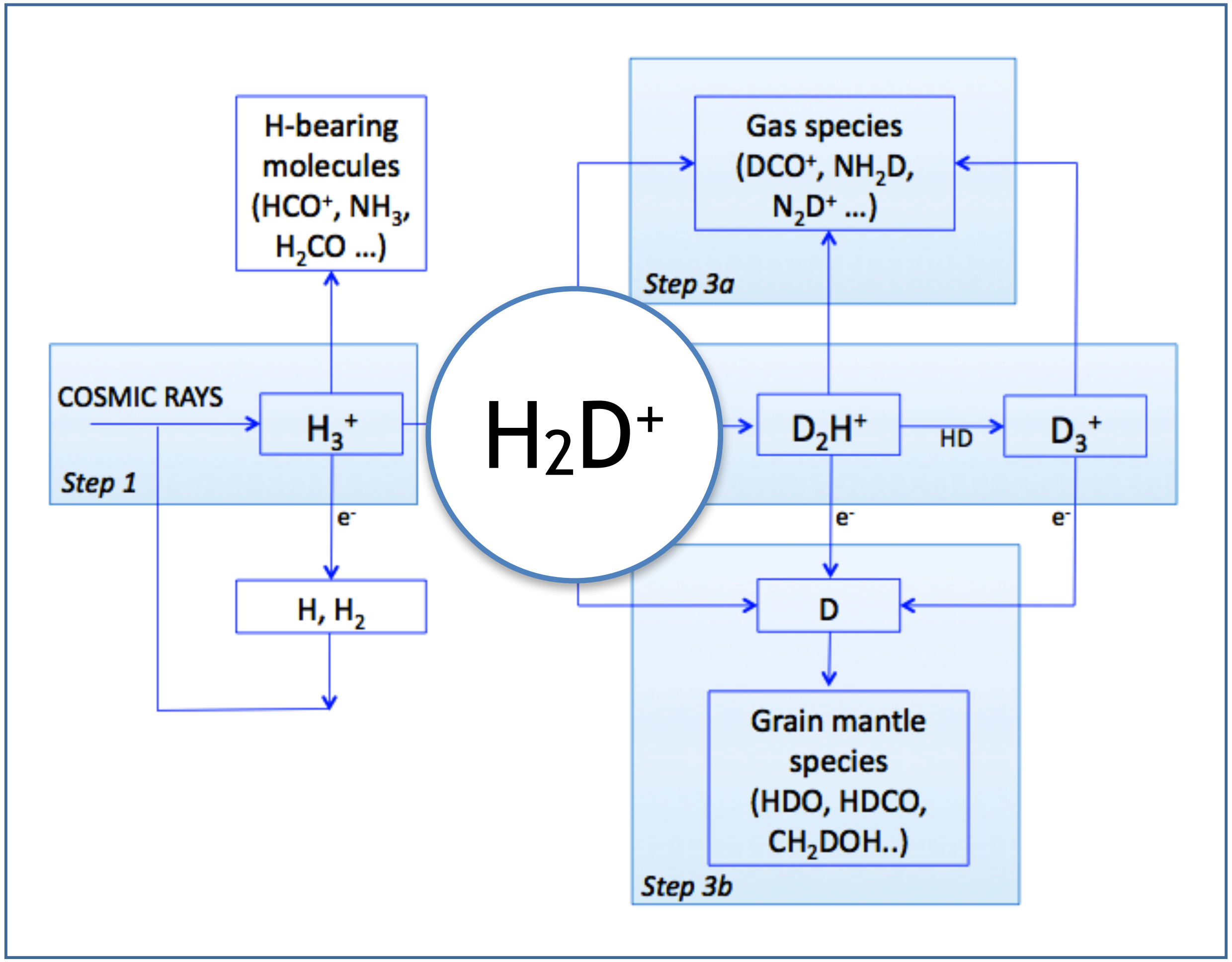
2) Formation of the deuterated forms of H_3^+

3) Transfer of D-atoms from the deuterated H_3^+ to other species

THE KEY MOLECULE: H_2D^+

2. Time for planting

2.3 Super-deuteration



Ceccarelli et al. 2014, PP6

TRACE MOLECULES MOLECULES ARE DEUTERATED BECAUSE OF

$H_2D^+/H_3^+ >> D/H$

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THE (SIMPLE) CHEMISTRY OF H_2D^+

$HD + H_3^+ \longrightarrow H_2D^+ + H_2$

$H_2D^+ + HD \longrightarrow HD_2^+ + H_2$

$H_2D^+ + H_2 \longrightarrow HD + H_3^+$ Energy barrier ~220K

$H_2D^+ + CO \longrightarrow DCO^+ + H_2$

$H_2D^+ + e^+ \longrightarrow H + H + D$

THE (SIMPLE) CHEMISTRY OF H_2D^+

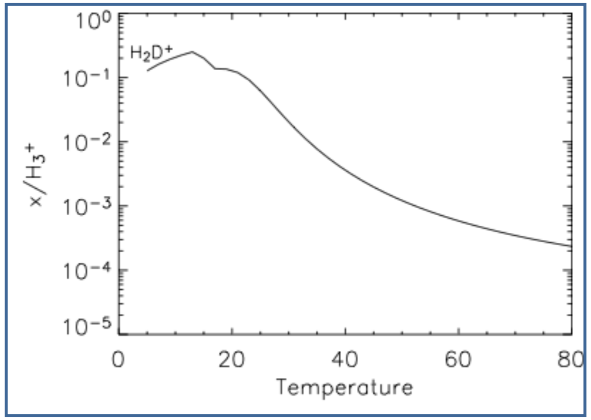
$HD + H_3^+ \longrightarrow H_2D^+ + H_2$

$H_2D^+ + HD \longrightarrow HD_2^+ + H_2$

$H_2D^+ + CO \longrightarrow DCO^+ + H_2$

$H_2D^+ + e^+ \longrightarrow H + H + D$

IN COLD GAS, THE REACTION $H_2D^+ + H_2$ IS INEFFICIENT



2. Time for planting

2.3 Super-deuteration

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THE (SIMPLE) CHEMISTRY OF H_2D^+

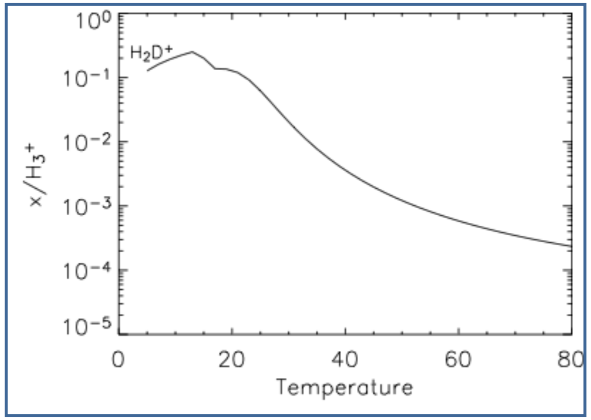
$HD + H_3^+ \longrightarrow H_2D^+ + H_2$

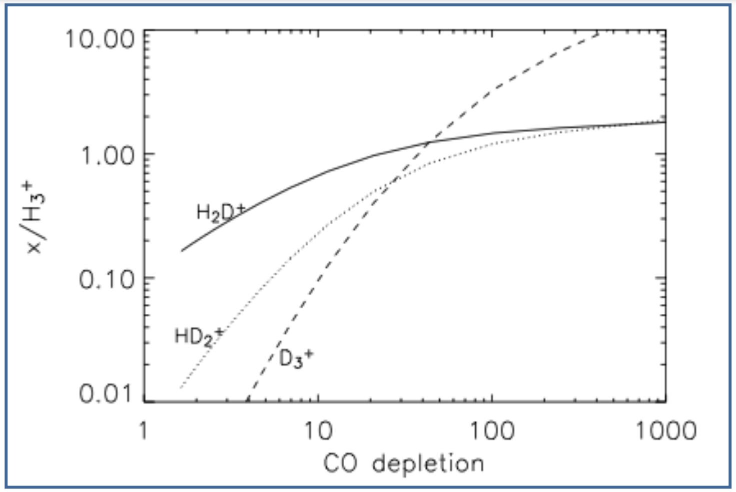
$H_2D^+ + HD \longrightarrow HD_2^+ + H_2$

$H_2D^+ + e^+ \longrightarrow H + H + D$

IN COLD GAS, THE REACTION $H_2D^+ + H_2$ IS INEFFICIENT

IN CO DEPLETED GAS, THE REACTION $H_2D^+ + CO$ IS INEFFICIENT





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2.3 Super-deuteration

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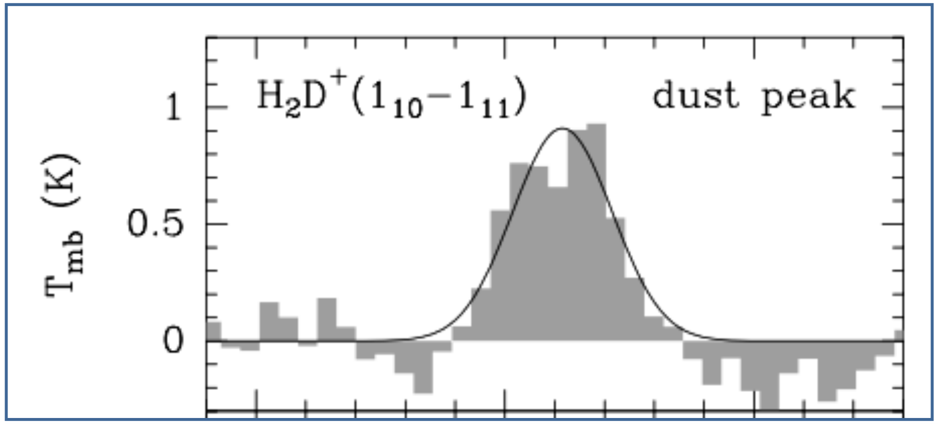
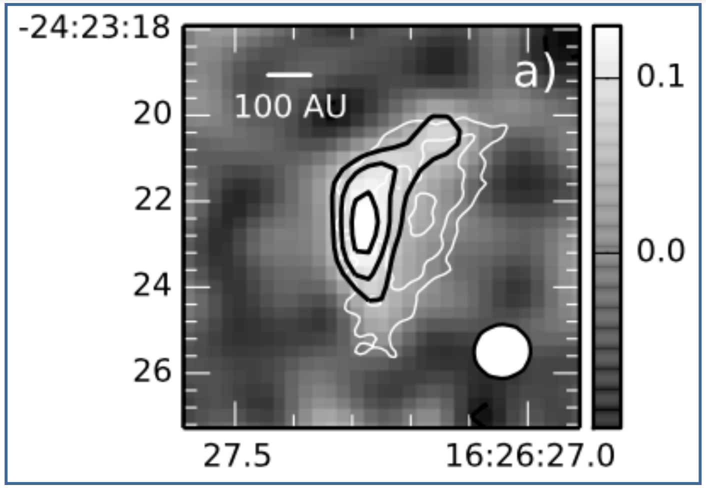
THE KEY MOLECULE: H_2D^+

Caselli et al. 2003





Friesen et al. 2015

OBSERVED H_2D^+/H_3^+ >> D/H IN PSCs
(the line is much brighter than in high mass star forming regions like Orion, SgrB2 etc)

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2.3 Super-deuteration

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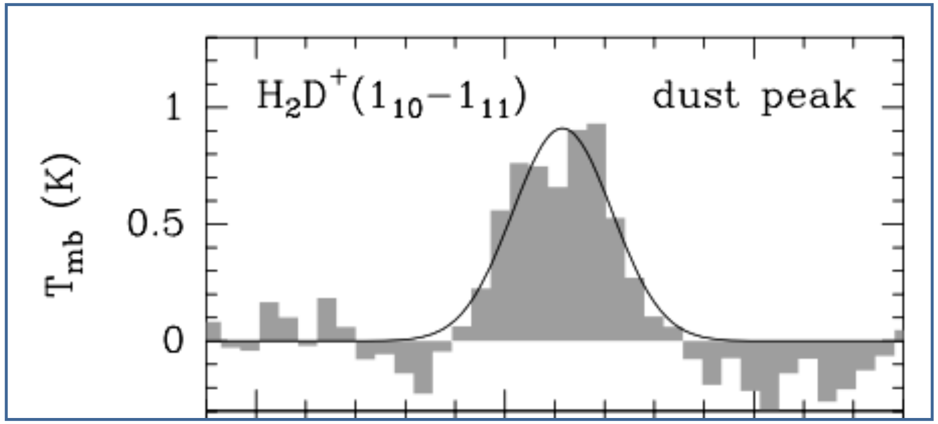
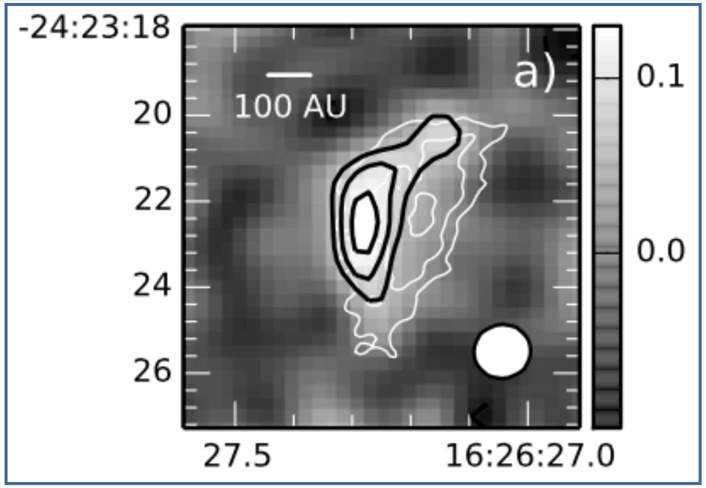
THE KEY MOLECULE: H_2D^+

2. Time for planting

2.3 Super-deuteration

Caselli et al. 2003





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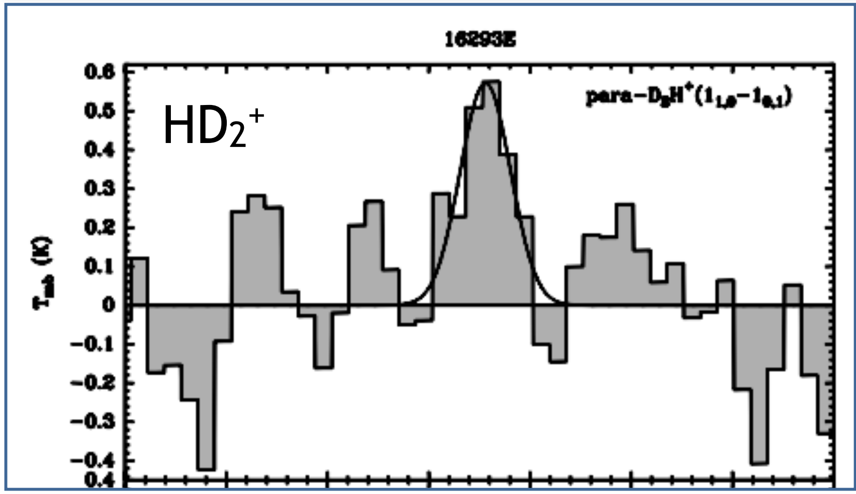

Vastel et al. 2004

DETECTED EVEN HD_2^+

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DEUTERATION ON THE GRAIN SURFACES

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2.3 Super-deuteration

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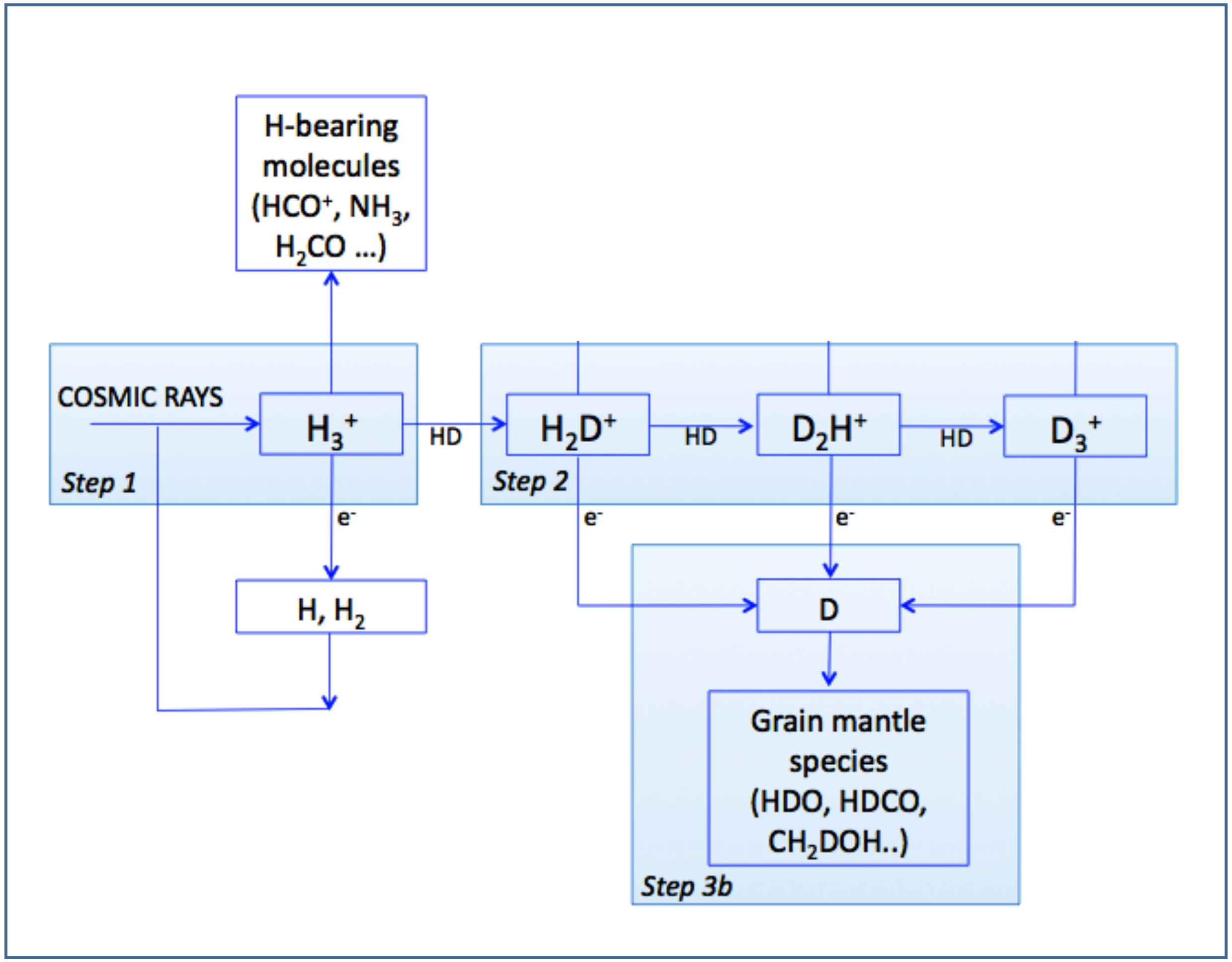

Ceccarelli et al. 2014, PP6

THE DEUTERATION OF THE SPECIES FORMED ON THE GRAIN SURFACES DEPEND IN FIRST INSTANCE ON THE GAS ATOMIC D/H ABUNDANCE RATIO

DEUTERATION OF WATER

Quenard, Taquet, Vastel et al. in prep.

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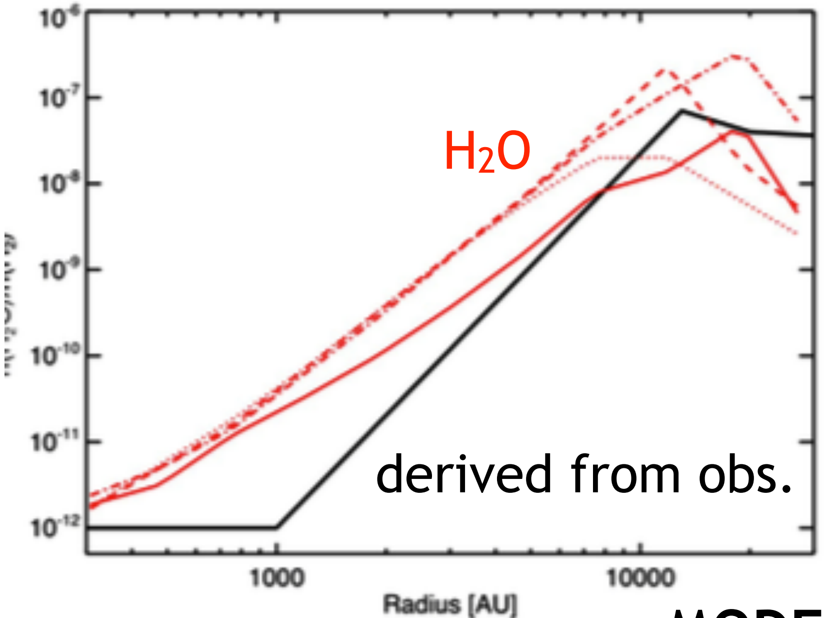
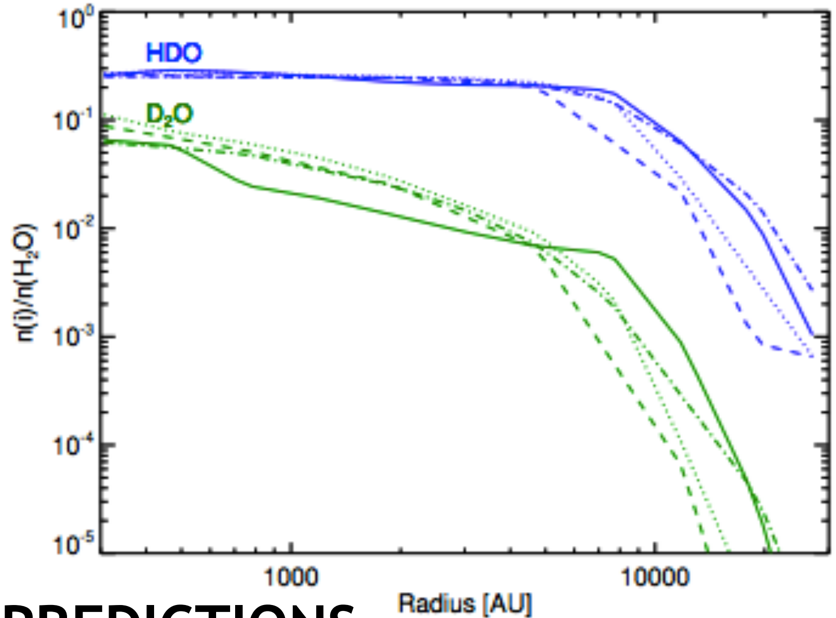
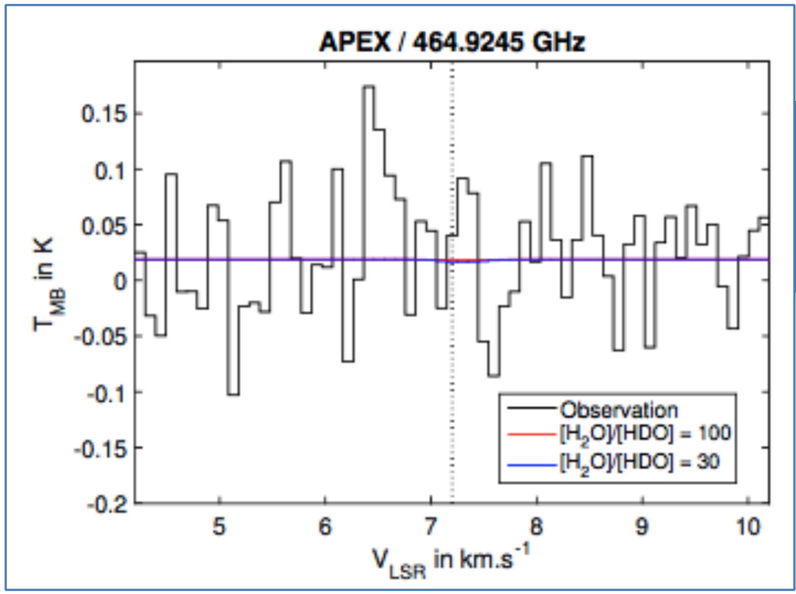
2.3 Super-deuteration





MODEL PREDICTIONS



HDO IN PSCs UNDETECTABLE WITH PRESENT FACILITIES

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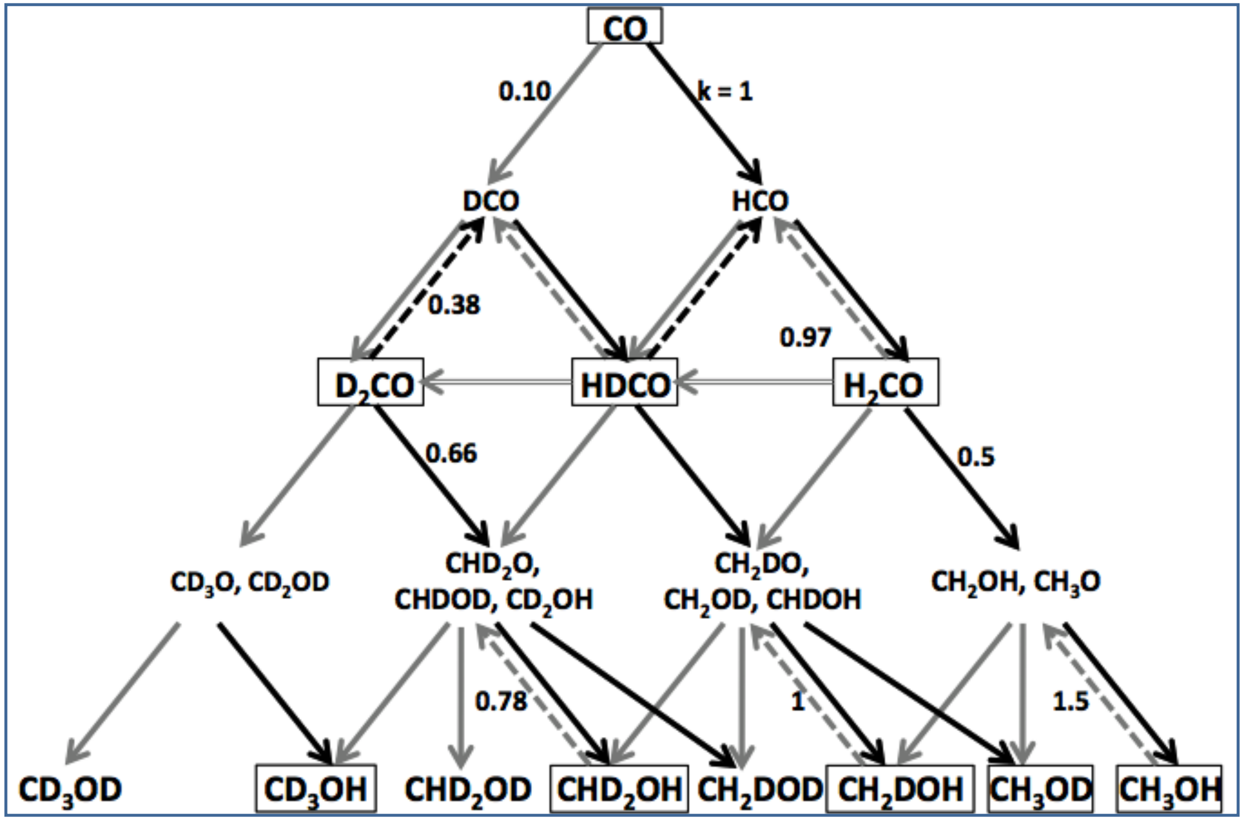
DEUTERATION OF METHANOL



Watanabe et al. 2010

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THE DEUTERATION OF THE SPECIES FORMED ON THE GRAIN SURFACES DEPEND IN FIRST INSTANCE ON THE GAS ATOMIC D/H ABUNDANCE RATIO

WITH POSSIBLE EXTRACTION/EXCHANGE REACTIONS

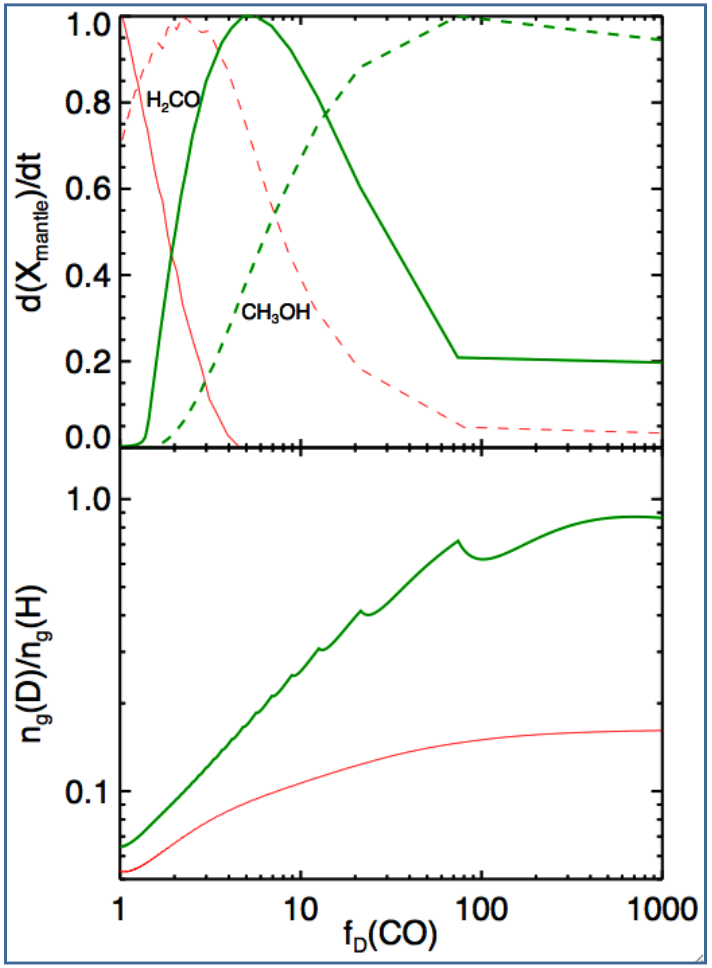
DEUTERATION OF WATER, FORMALDEHYDE AND METHANOL

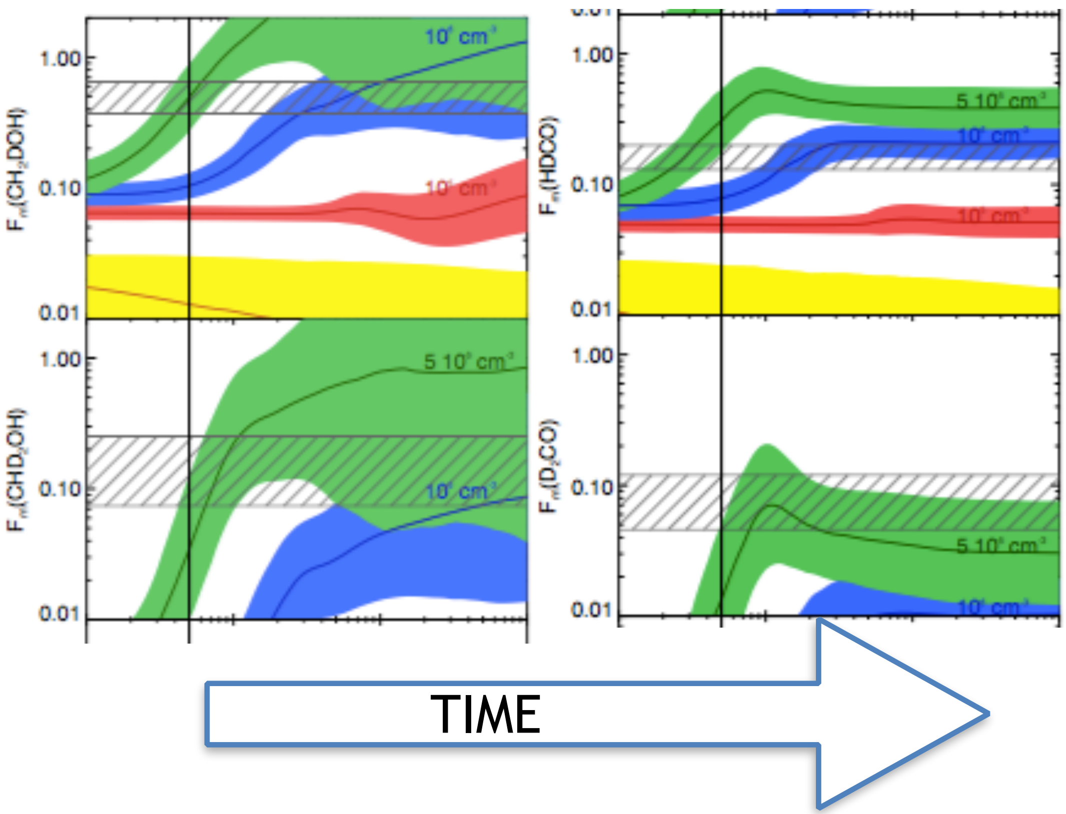
Taquet et al. 2013

2. Time for planting

2.3 Super-deuteration

C.Ceccarelli





THE DEUTERATION OF THE SPECIES FORMED ON THE GRAIN SURFACES DEPEND IN FIRST INSTANCE ON THE GAS ATOMIC D/H ABUNDANCE RATIO

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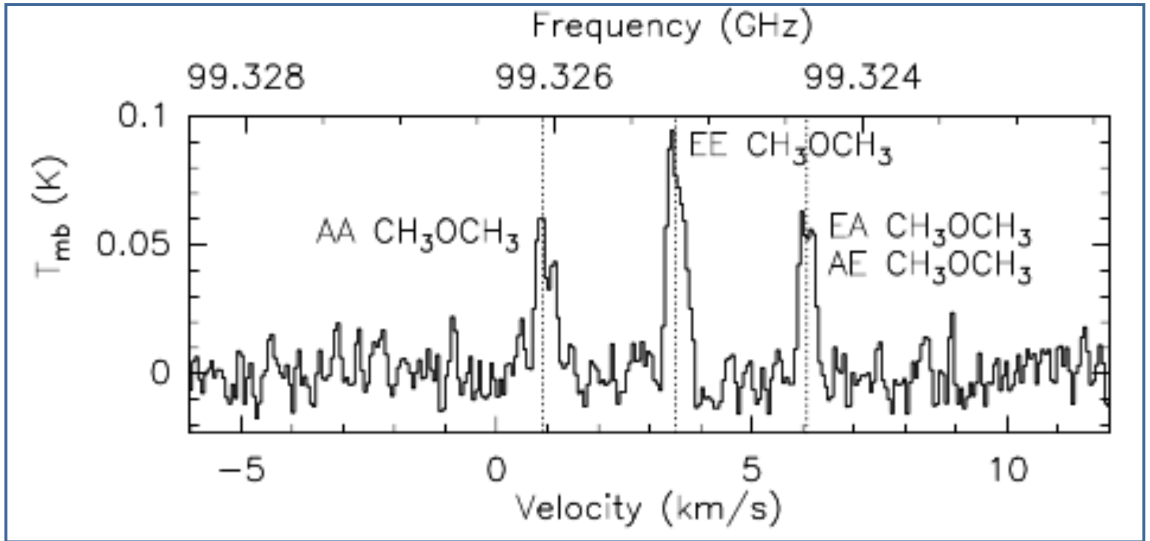
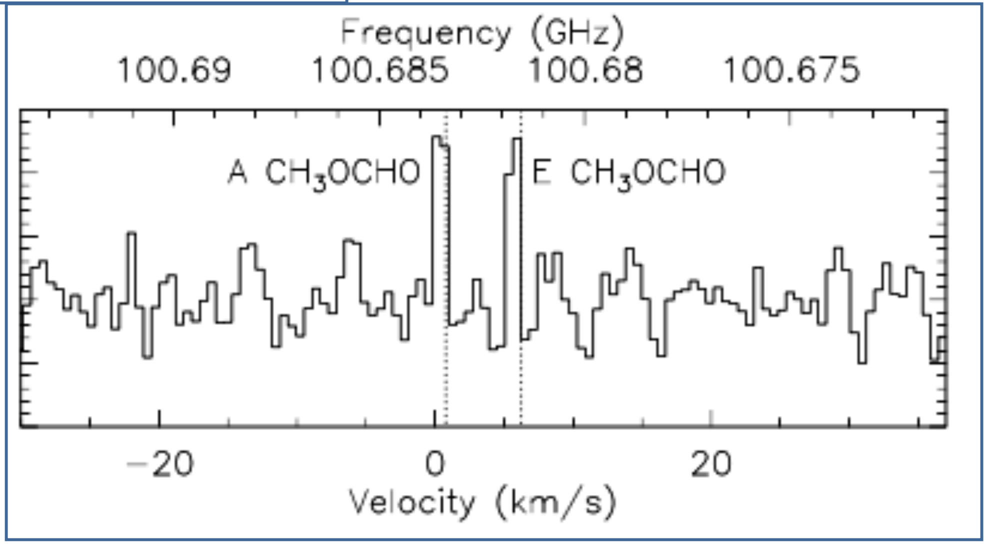
2.4 ORGANIC MOLECULES IN PSCS

C.Ceccarelli

OBSERVATIONS OF ORGANIC MOLECULES



Bacmann, Taquet, Faure et al. 2012; Cernicharo, Marcelino, Roueff et al. 2012; Vastel, Ceccarelli, Lefloch et al. 2014



QUESTIONS:
+ HOW THESE COMs ARE FORMED? WHERE?
+ IF ON THE GRAIN SURFACES, WHY ARE THEY IN THE GAS?

C.Ceccarelli

PREDICTIONS OF ORGANIC MOLECULES

Balucani, Ceccarelli, Taquet 2015

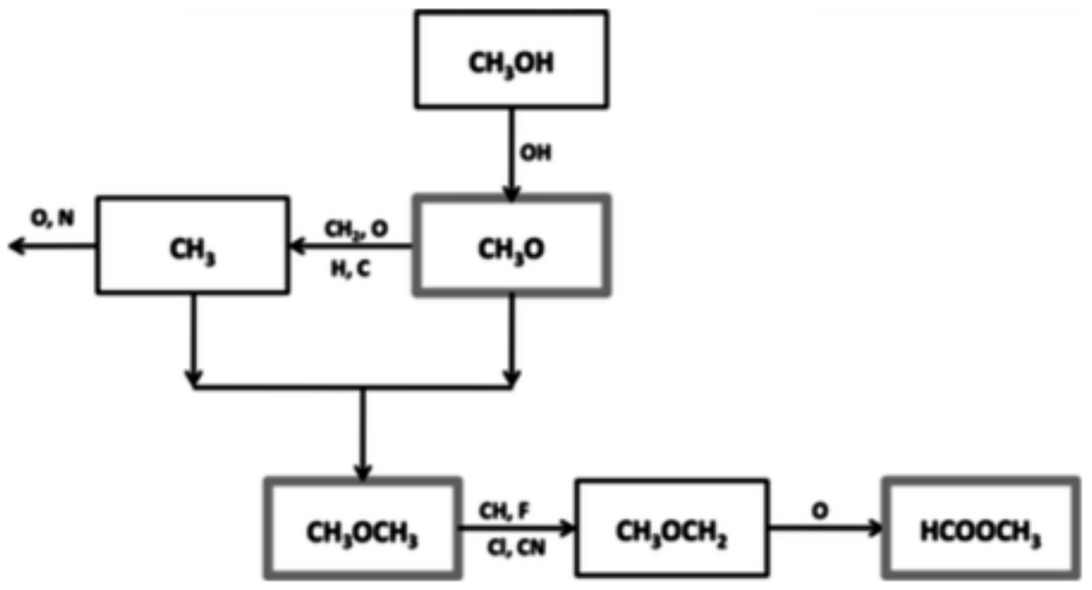
1) METHANOL IS FORMED ON THE GRAIN SURFACES
2) IT IS PHOTO-DESORBED AT THE BORDER OF THE PSC
3) REACTIONS IN THE GAS PHASE FORM COMs

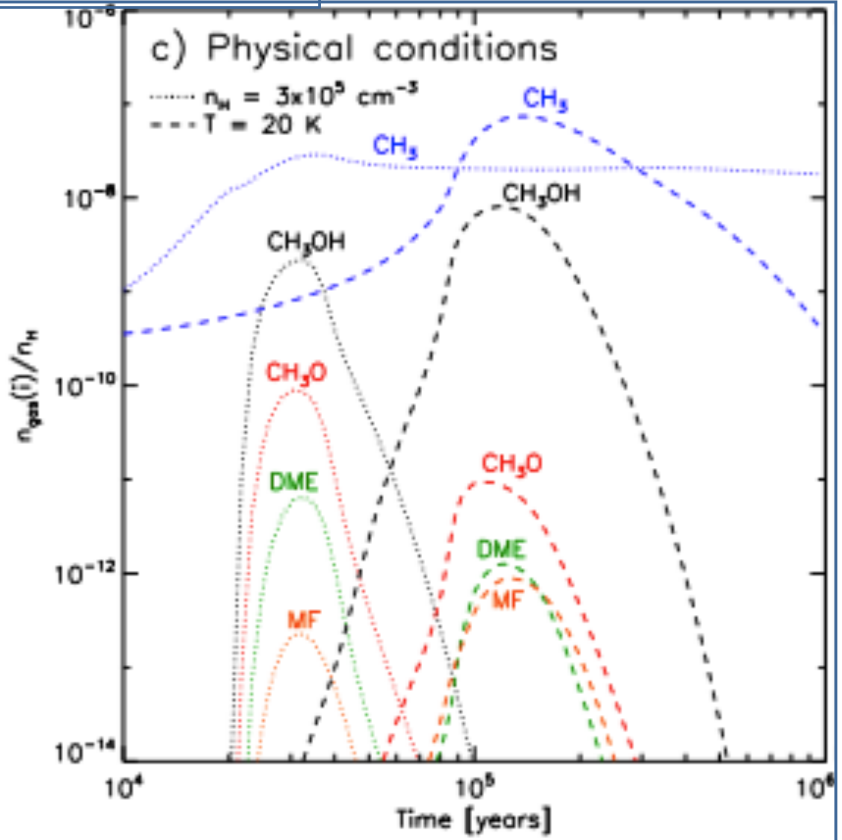
2. Time for planting

Example of DME and MF formation

2.

C.





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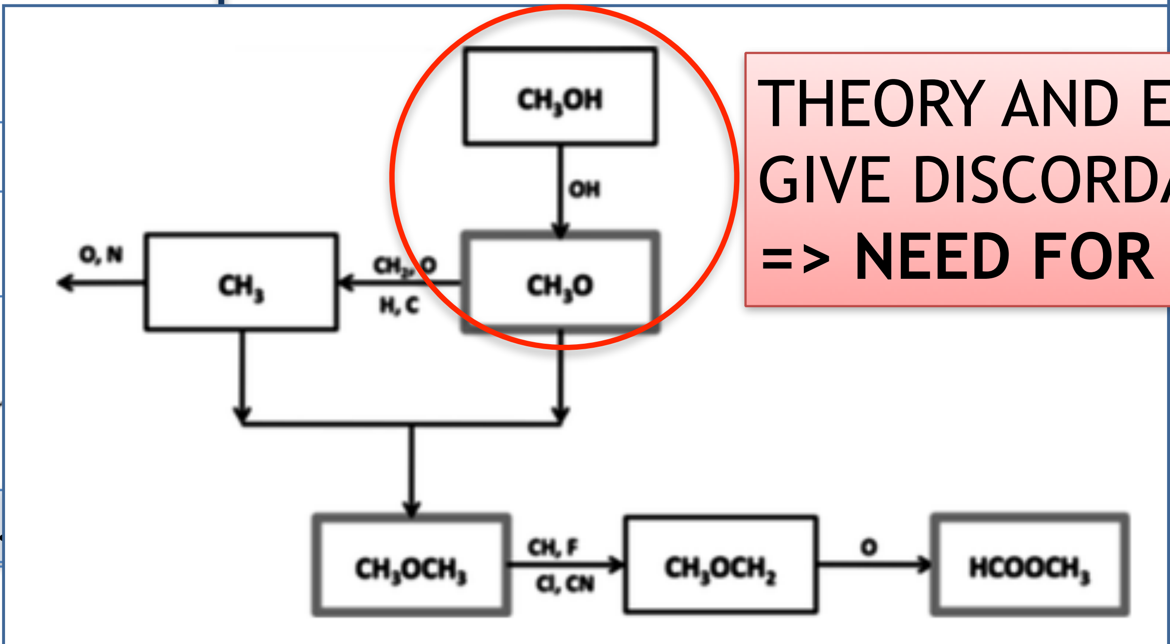

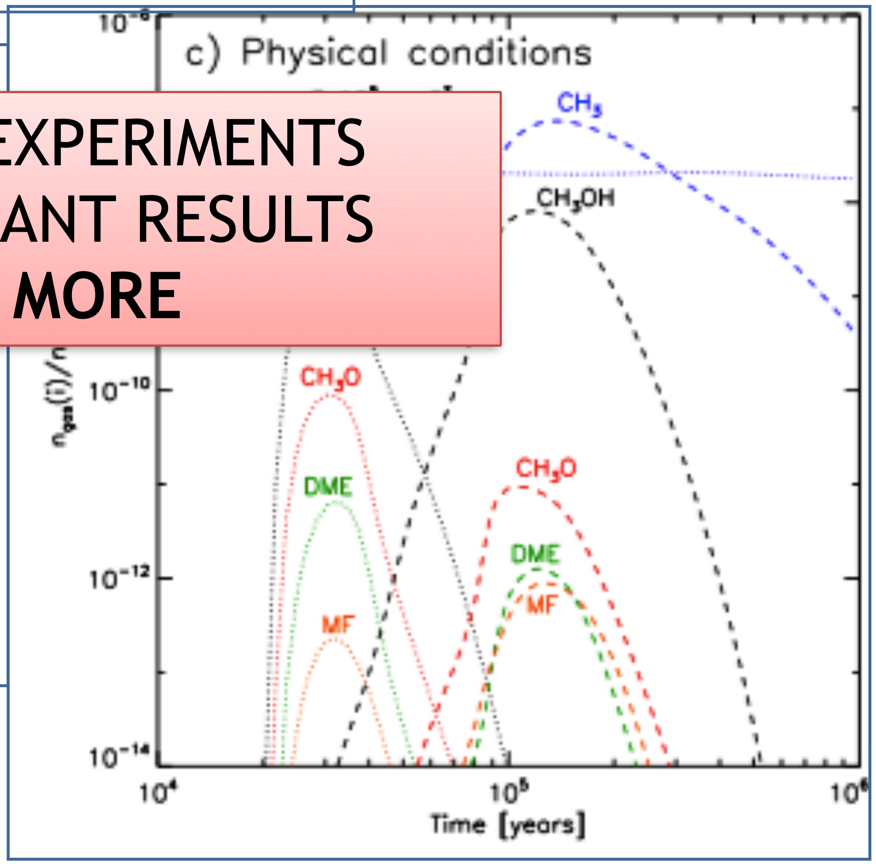

THEORY AND EXPERIMENTS GIVE DISCORDANT RESULTS
=> **NEED FOR MORE**

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ORGANIC MOLECULES

2. Time for planting

2.4 Organics

THE "RETAIL SHOPS" OF ORGANIC MOLECULES ARE THE HOT CORINOS
STAY TUNED FOR THE NEXT LECTURE

C.Ceccarelli