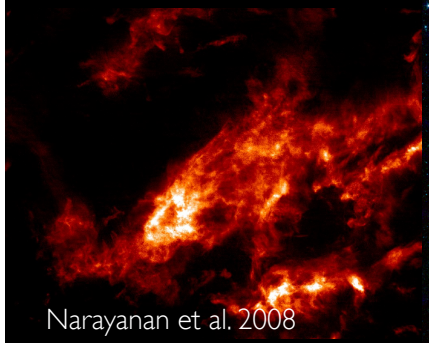
Deuterium Fractionation

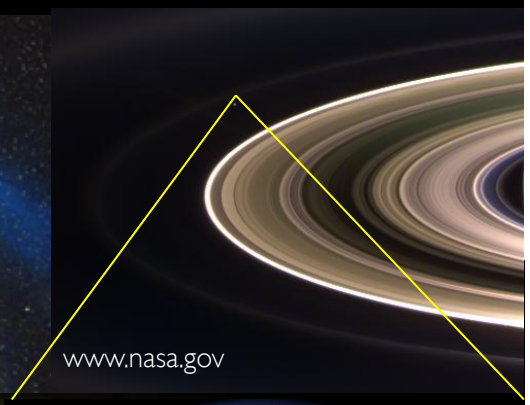
the Ariane thread from the pre-collapse phase to meteorites and comets today

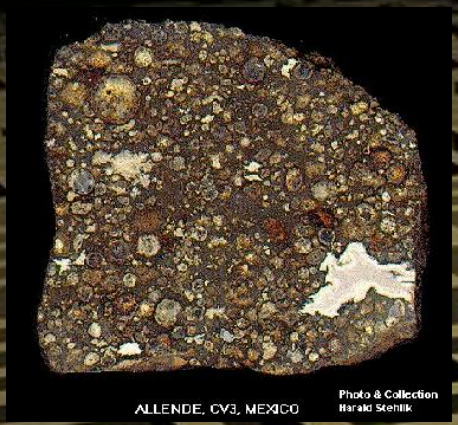

Narayanan et al. 2008

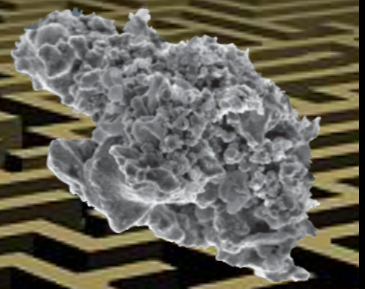

Gutermuth et al. 2008


Miotello et al. 2012


www.nasa.gov


www.nasa.gov



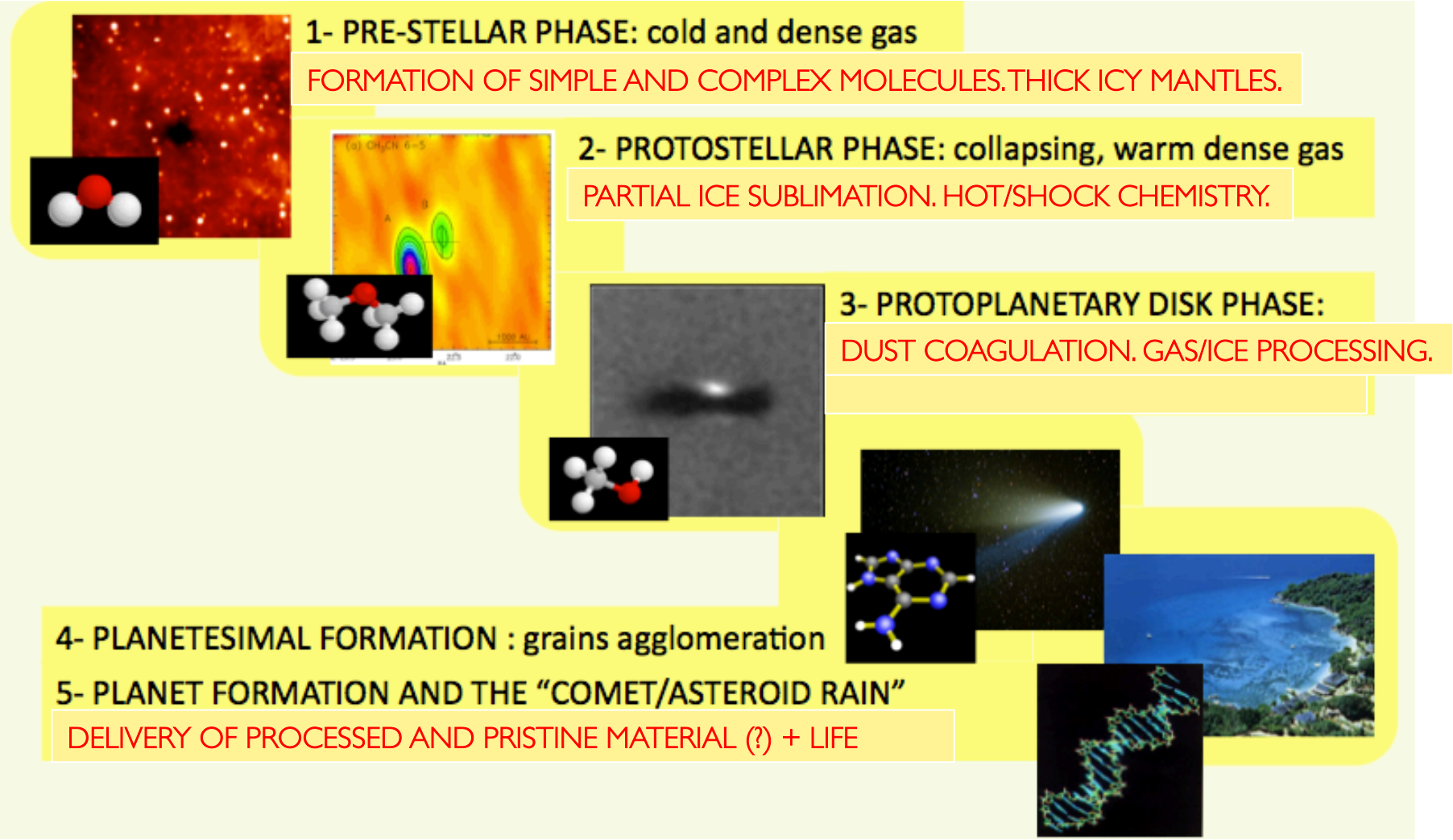


Cecilia Ceccarelli, Paola Caselli, Dominique Bocklelèe-Morvan, Olivier Mousis, Sandra Pizzarello, Francois Robert, Dimitry Semenov

STRUCTURE OF THE CHAPTER

1. Introduction: the Ariane thread and our history
2. Setting the stage
    - 2.1 Chemical processes of deuterium fractionation
    - 2.2 Deuterium fractionation of water
    - 2.3 Towards a common language
3. A brief history of the Solar-type System formation
4. Pre-stellar cores
5. Protostars
6. Protoplanetary disks
7. Comets
8. Carbonaceous Chondrites and Interplanetary Dust Particles
    - 8.1 Clays minerals
    - 8.2 Insoluble Organic Matter
    - 8.3 Soluble Organic Matter
9. The ^{15}N enrichement
10. Unrolling the thread: summary of the deuterium fractionation
11. The Proto-Solar Nebula models
12. Where does the terrestrial water come from?
12. Conclusions

The astrochemical heritage of the Solar System



Caselli & Ceccarelli 2012, ARA&A, 20, 56

Basic questions

- Are there clear links between our Solar System and star/planet forming regions?

- Can such links help us to better understand our origins?

- Can such links help us to better understand the chemical and physical processes in star/planet forming regions?

We have two treasures: our studies of the Solar System and our studies of star and planet forming regions. It is now time to work together for a full exploitation of such treasures!

Outline

- Deuterium fractionation processes
- Pre-stellar cores
- Protostars
- Disks
- Comets
- Meteorites & IDPs
- Summary: unrolling the thread
- (Some of the) Things to do

Deuterium Fractionation
processes

The Star Formation – Solar System Dictionary

$$\delta D = \frac{(D/H)_{measured} - (D/H)_{VSMOW}}{(D/H)_{VSMOW}} \times 1000$$

$$(D/H)_{VSMOW} = (1.554 \pm 0.001) \times 10^{-4}$$

$$(D/H)_{\text{cosmic}} \sim 1.5 \times 10^{-5}$$ *(Oliveira et al. 2003)*

VSMOW=Vienna Standard Mean Ocean Water
(refers to evaporated ocean water)

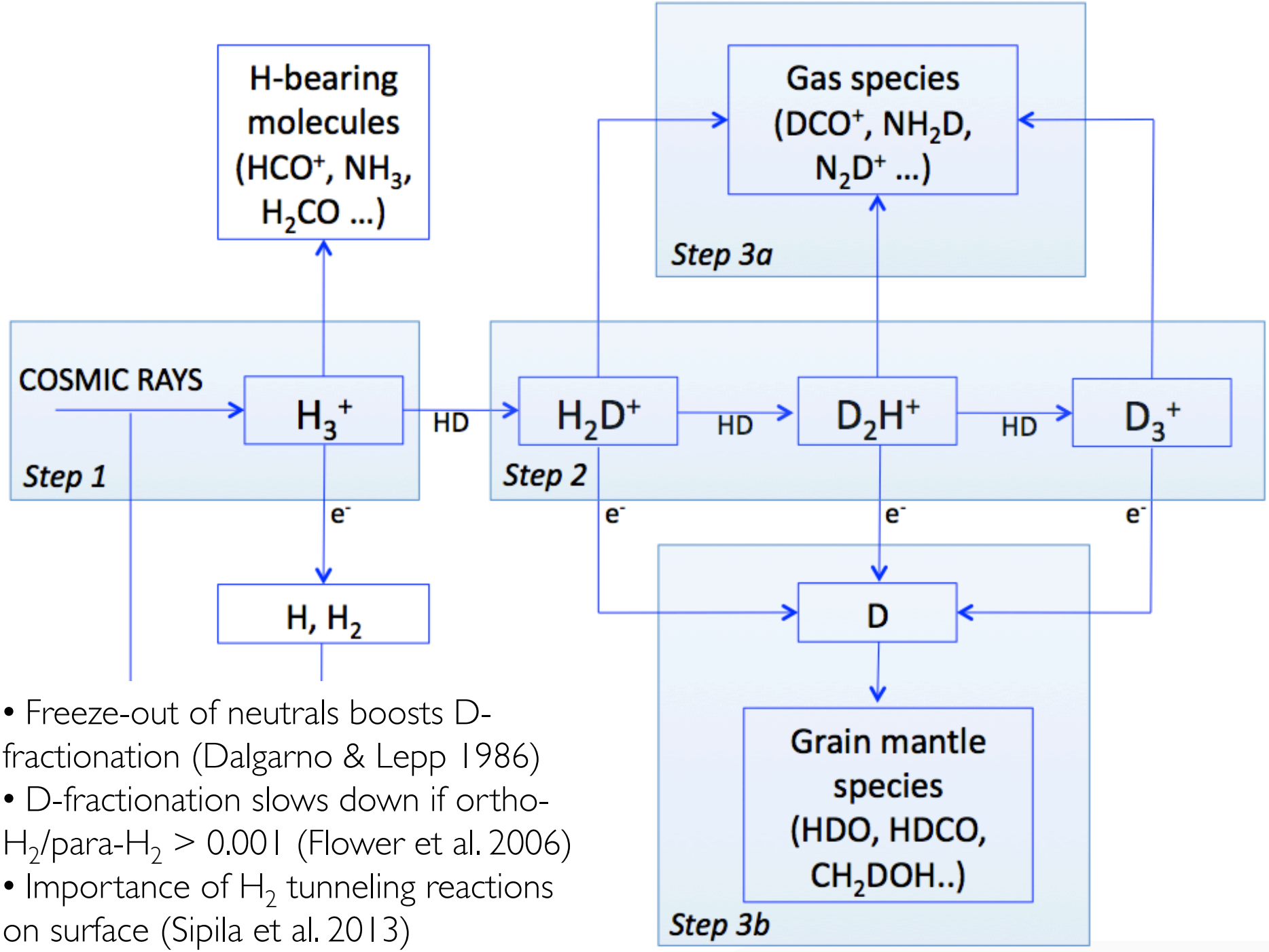
The first two steps

1. Formation of H_2 onto dust grain particles

2. Formation of H_3^+

$$H_2 + \text{cosmic ray} \xrightarrow{97\%} H_2^+ + e^- + \text{cosmic ray}$$

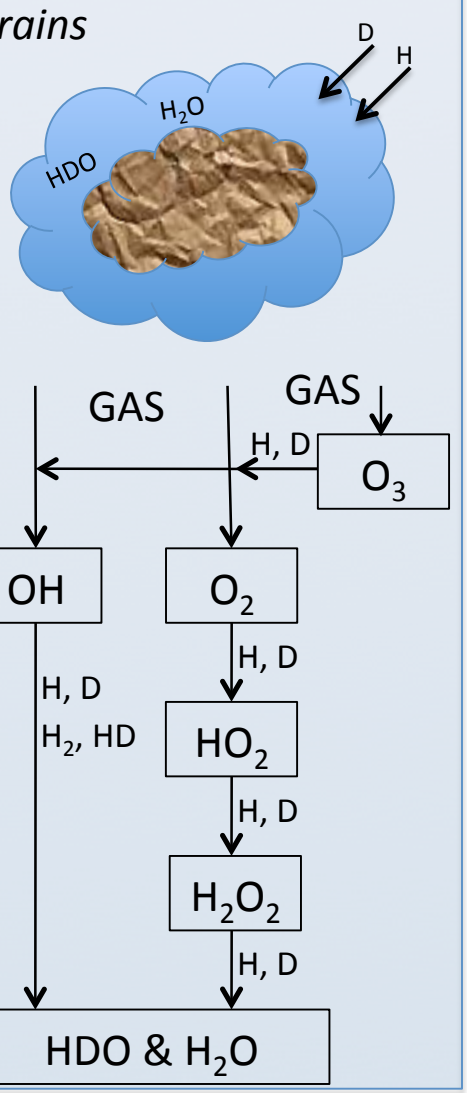
$$H_2^+ + H_2 \rightarrow H_3^+ + H$$



- Freeze-out of neutrals boosts D-fractionation (Dalgarno & Lepp 1986)
- D-fractionation slows down if ortho-H_2/para-H_2 > 0.001 (Flower et al. 2006)
- Importance of H_2 tunneling reactions on surface (Sipila et al. 2013)

ROUTES TO WATER DEUTERATION

1) On the surface of cold grains



Hiraoka+1998, Dulieu+2011, 2013, Miyauchi +2008, Ioppolo+2010, Mokrane+2009, Romanzin+2011, Oba 2011, 2012

2) D-H exchange in the gas

2a) cold (T<30K) gas

Key species: H_2D^+

2b) warm (30<T<100 K) gas

Key species: CH_2D^+

2c) hot (T>100 K) gas

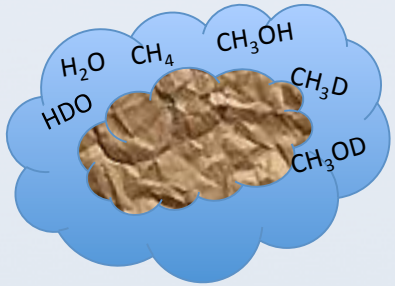
Key species: OD

2d)very hot (T>500 K) gas

reaction: HDO + H_2

Herbst & Klemperer 1973, Geiss & Reeves 1981, Lécluse & Robert 1994, Drouart +1999, Thi+2010

3) D-H exchange in the ice



3a) thermal (T_{grain}>100K)

Example:

HDO + CH_3OH -> H_2O + CH_3OD

or

H_2O + CH_3OD -> HDO + CH_3OH

3b) photolysis

Example:

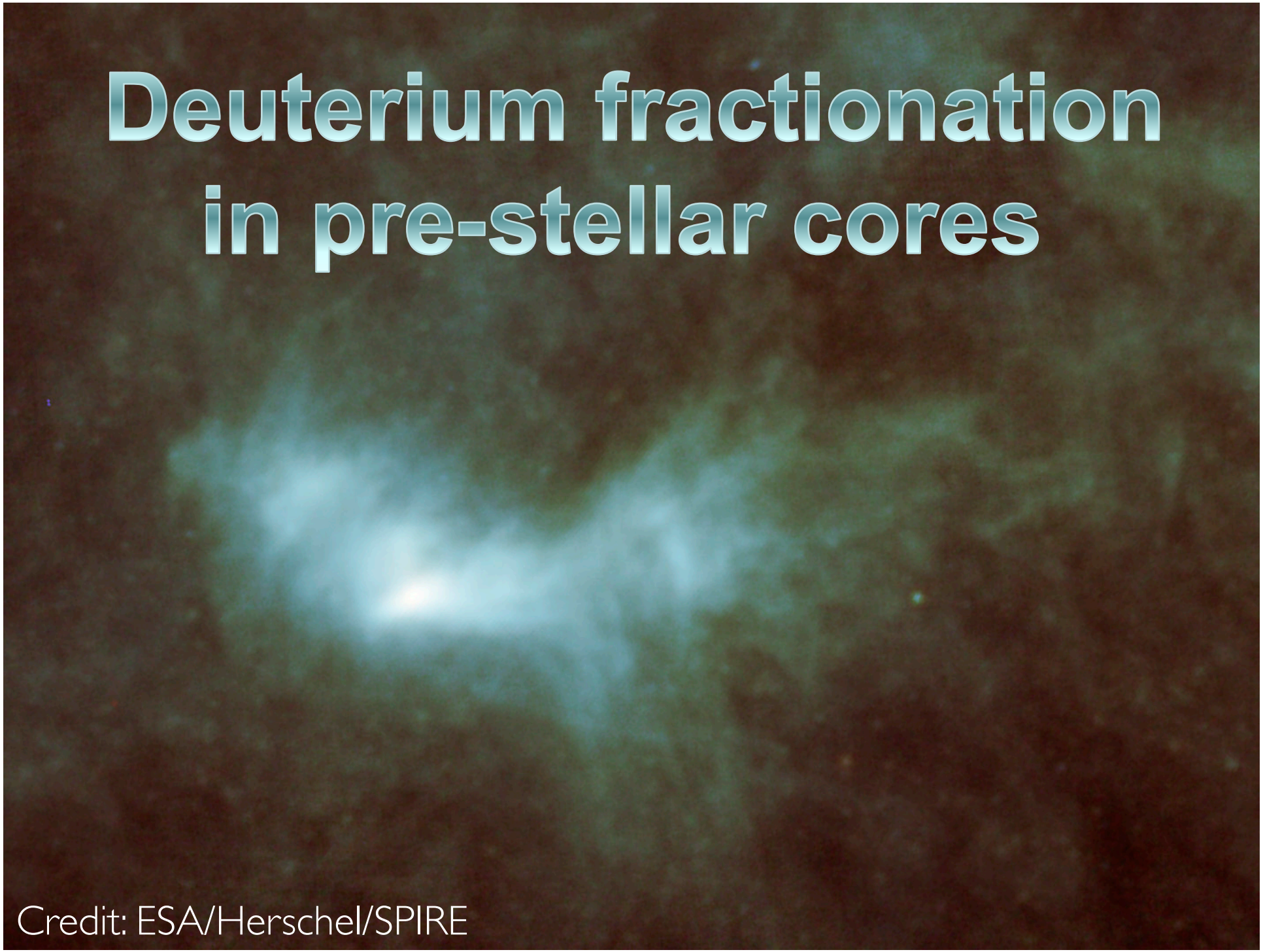
HDO + CH_4 -> H_2O + CH_3D

or

H_2O + CH_3D -> HDO + CH_4

Ratajczak+2009, Gàlvez+2011, Weber+2009

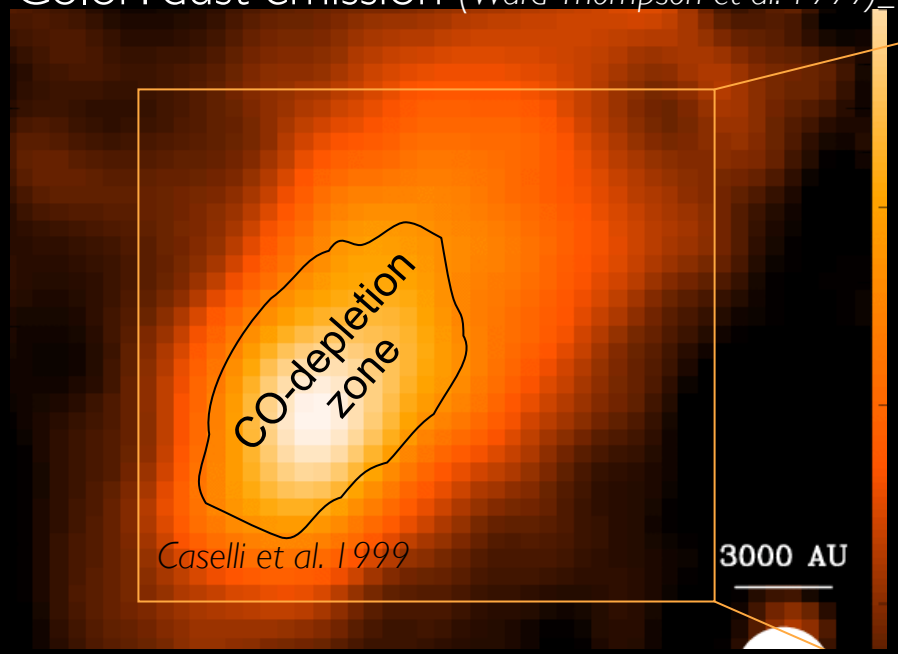
Deuterium fractionation in pre-stellar cores



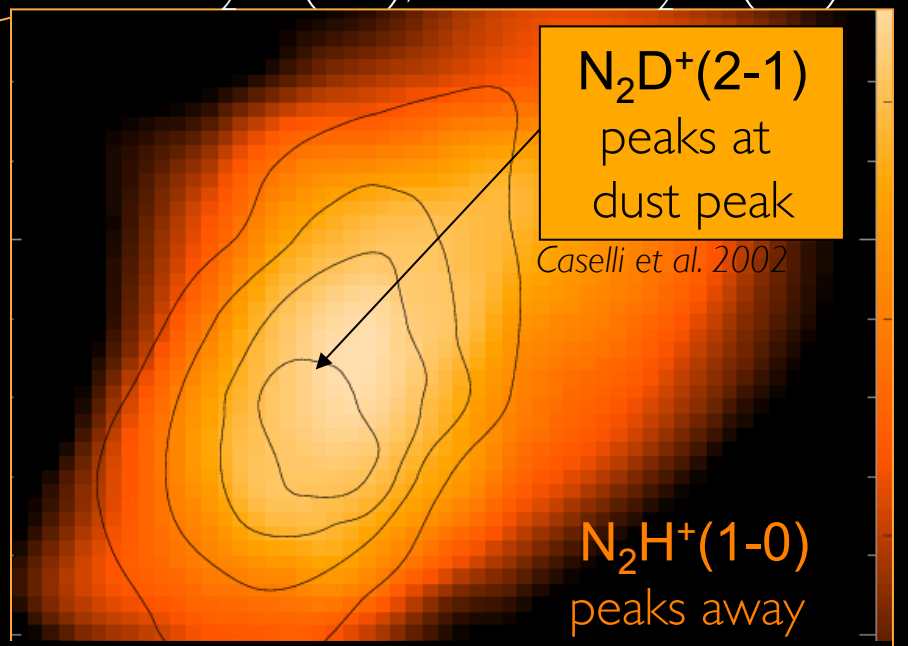
Credit: ESA/Herschel/SPIRE

Pre-stellar cores: freeze-out & deuterium fractionation

Color: dust emission *(Ward-Thompson et al. 1999)*



Color: N_2H^+(1-0); contour: N_2D^+(2-1)

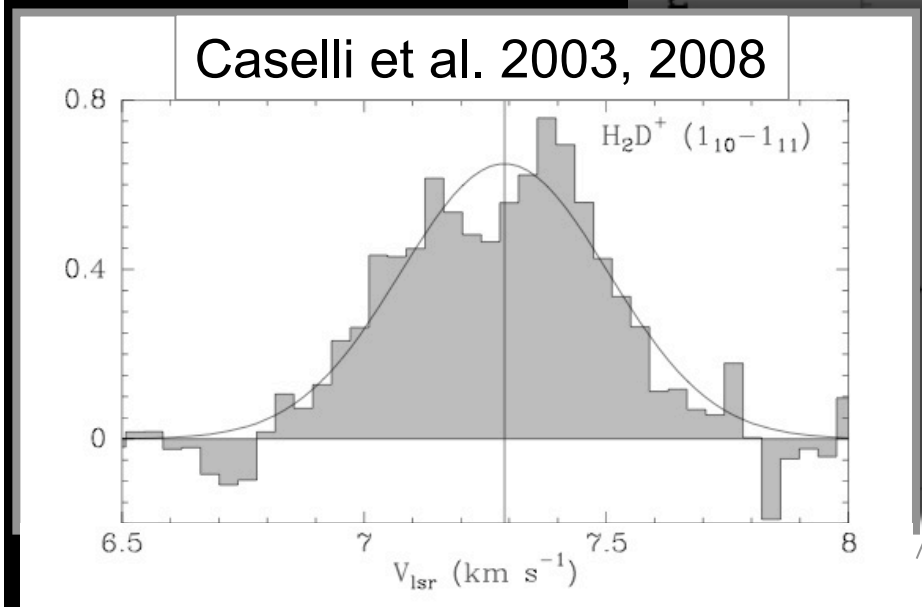


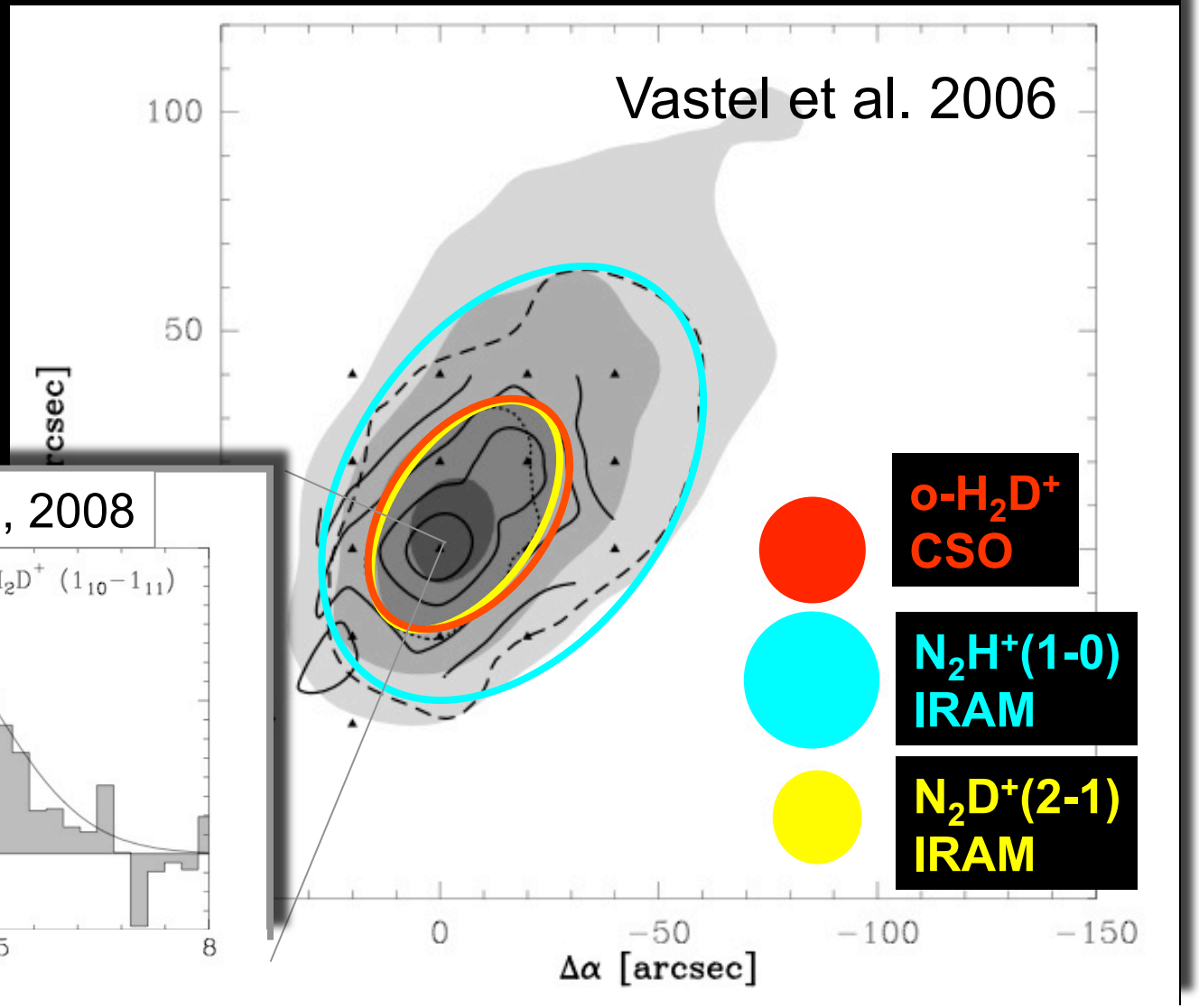
N_2D^+/N_2H^+ ~ 0.03-0.7 (Crapsi et al. 2005; Pagani et al. 2007)
NH_2D/NH_3 ~ 0.06-0.4 (Shah & Wootten 2001; Crapsi et al. 2007)
D_2CO/H_2CO ~ 0.01-0.1 (Bacmann et al. 2003)
DCN/HCN ~ 0.01-0.04 (Turner 2001)
DNC/HNC ~ 0.02-0.09 (Hirota et al. 2003)
DCO^+/HCO^+ ~ 0.04 (Butner et al. 1995; Caselli et al. 2002)
c-C_3D_2/c-C_3H_2 ~ 0.01-0.02 (Spezzano et al. 2013)

ortho-H_2D^+

The o-H_2D^+ line is strong and its emission is extended ~5000 AU

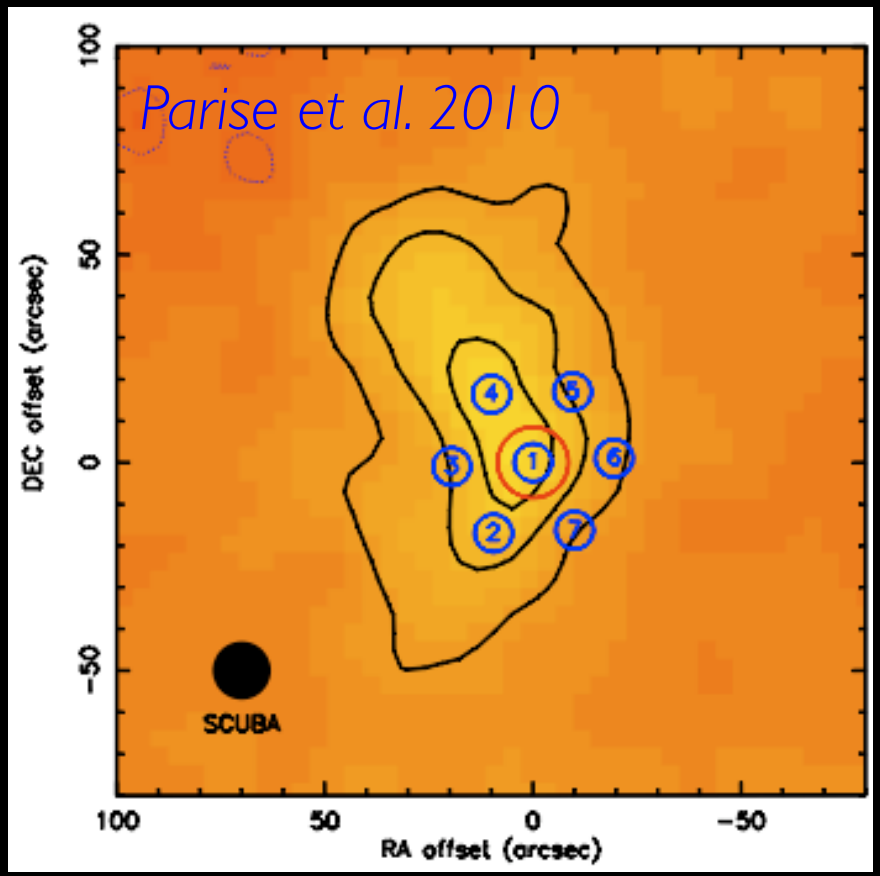
Only models including all multiply deuterated forms of H_3^+ can reproduce these data
(Roberts et al. 2003; Walmsley et al. 2004; Aikawa et al. 2005)

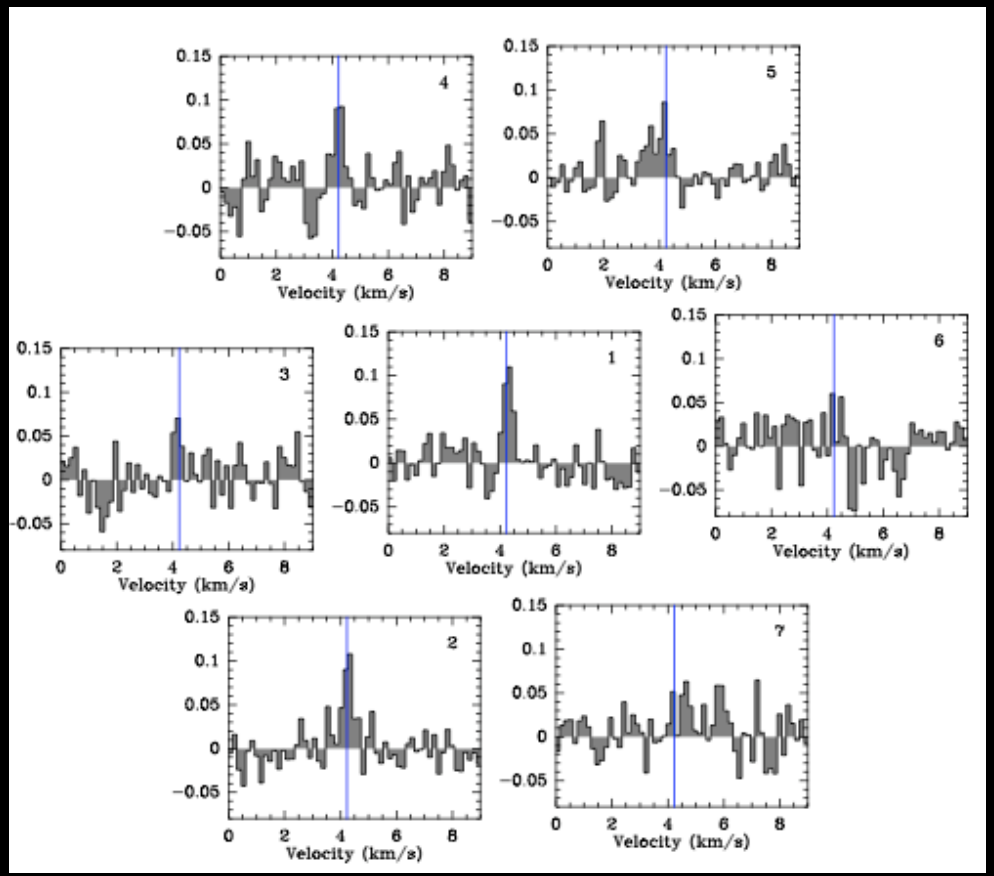




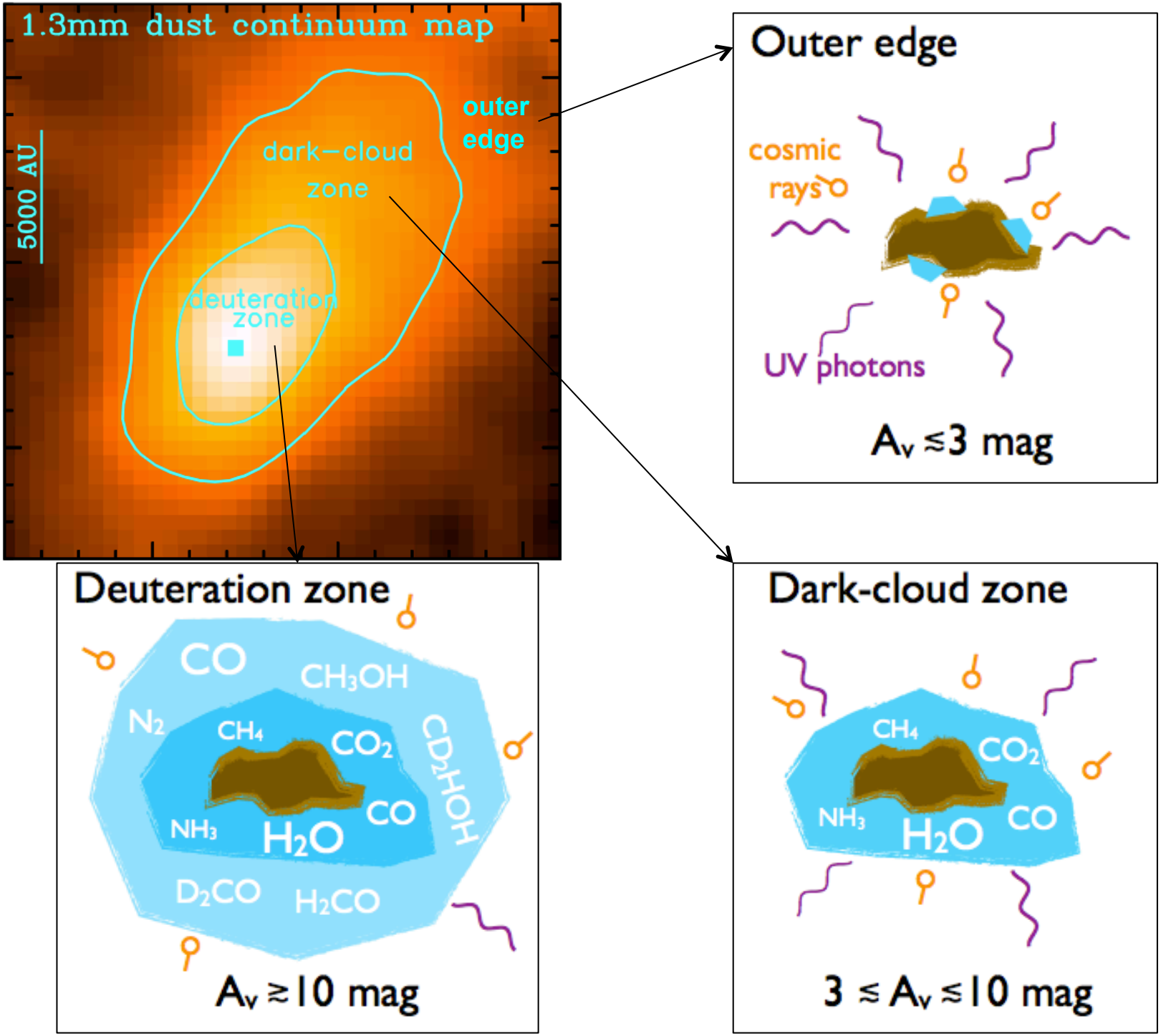
para-D_2H^+

Extended para-D_2H^+ emission (~40" ~5000 AU) toward L1688/H-MM1 (APEX-CHAMP+)

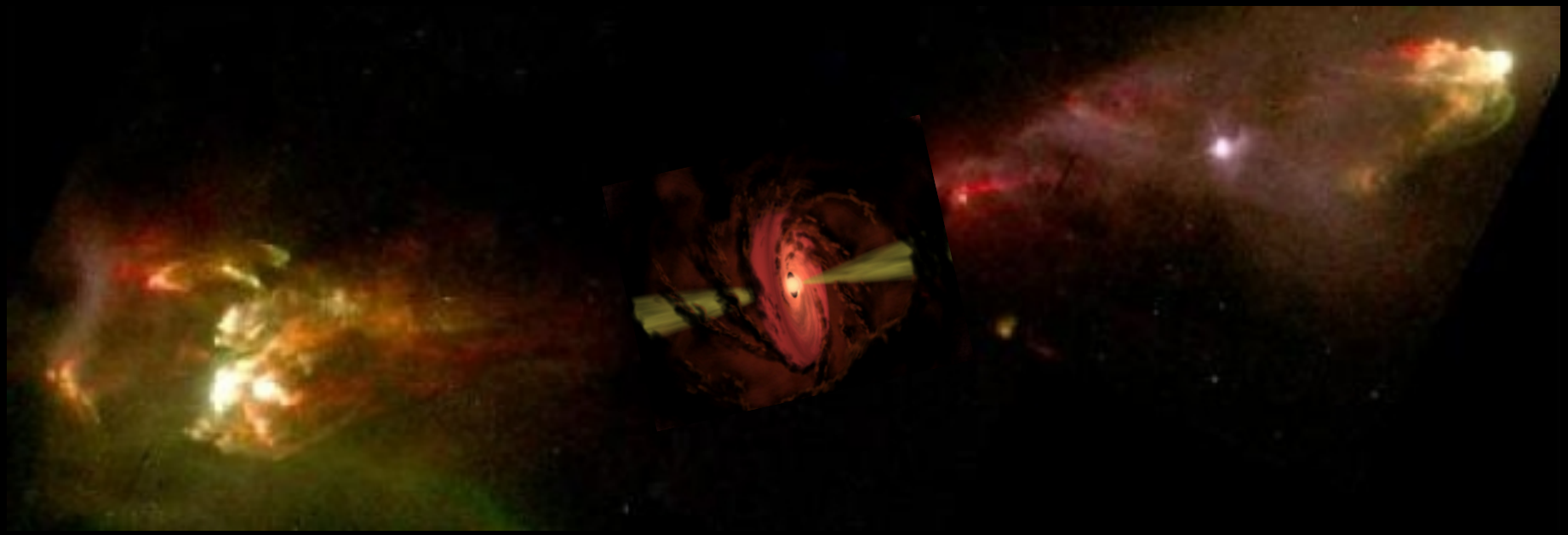




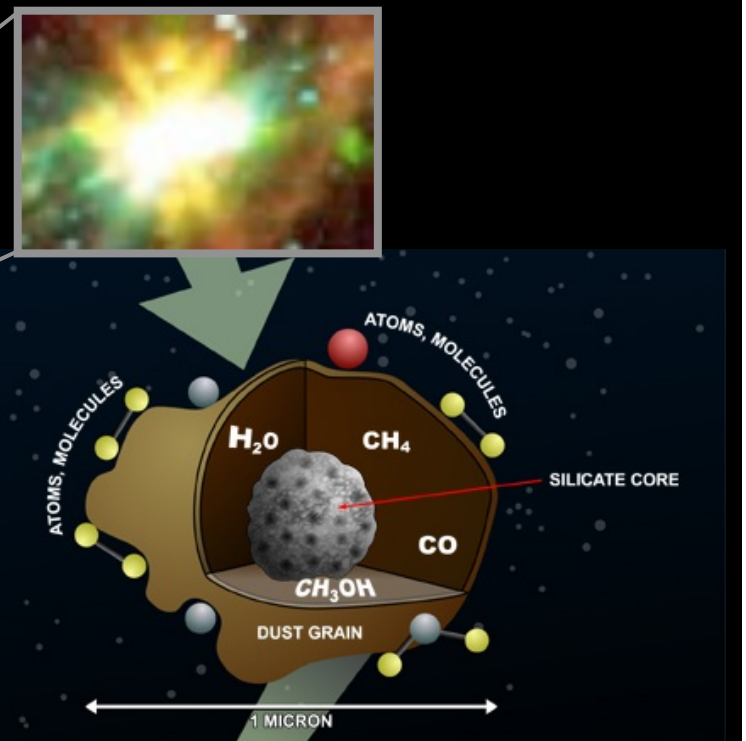
[Para-D_2H^+ was first detected by Vastel et al. (2004) toward another pre-stellar core]

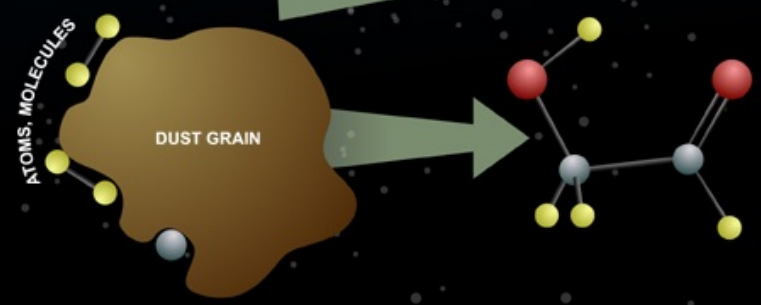

1.3mm dust continuum map
5000 AU
outer edge
dark-cloud zone
deuteration zone
Outer edge
cosmic rays
UV photons
$A_V \lesssim 3$ mag
Deuteration zone
CO
CH_3OH
N_2
CH_4
CO_2
CD_2HOH
CO
NH_3
H_2O
D_2CO
H_2CO
$A_V \gtrsim 10$ mag
Dark-cloud zone
CH_4
CO_2
NH_3
H_2O
CO
$3 \lesssim A_V \lesssim 10$ mag

Deuterium fractionation around protostars



Hubble/WFPC2 – http://hubblesite.org/gallery/album/entire/pr1995024c/web/npp/16/





- dust heating, X-rays nearby protostars (mantle processing and evaporation)

- dust (mantles and cores) sputtering + vaporization along protostellar outflows

MODELS:

Taquet et al. 2012a,b
(see also Cazaux et al. 2011)

OBSERVATIONS:

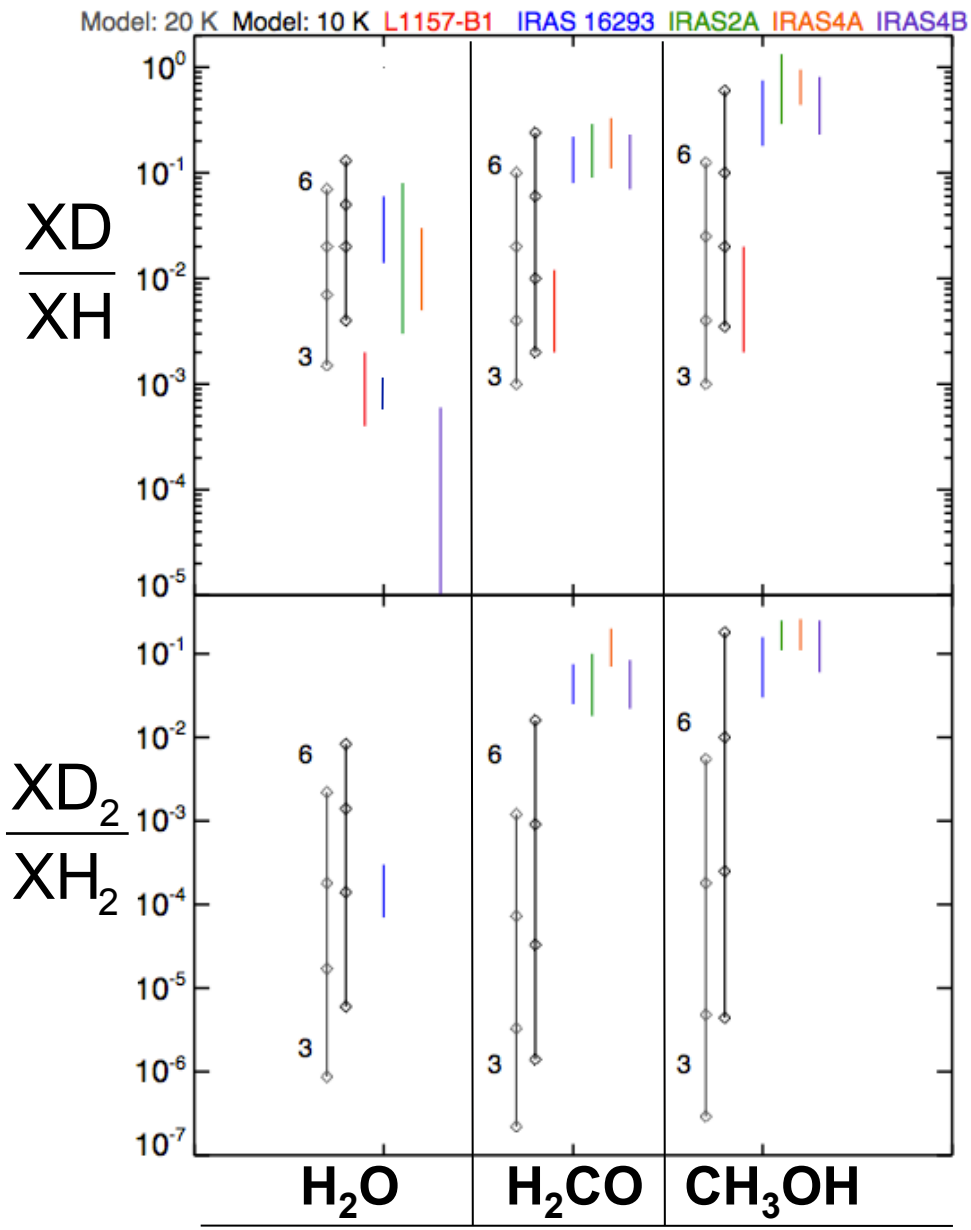
L1157-B1 *Codella et al. 2012*

IRAS 16293 *Loinard et al. 2001; Parise et al. 2002, 2004; Vastel et al. 2010; Coutens et al. 2012; Persson et al. 2013*

IRAS2A *Taquet et al. 2013; Parise et al. 2006*

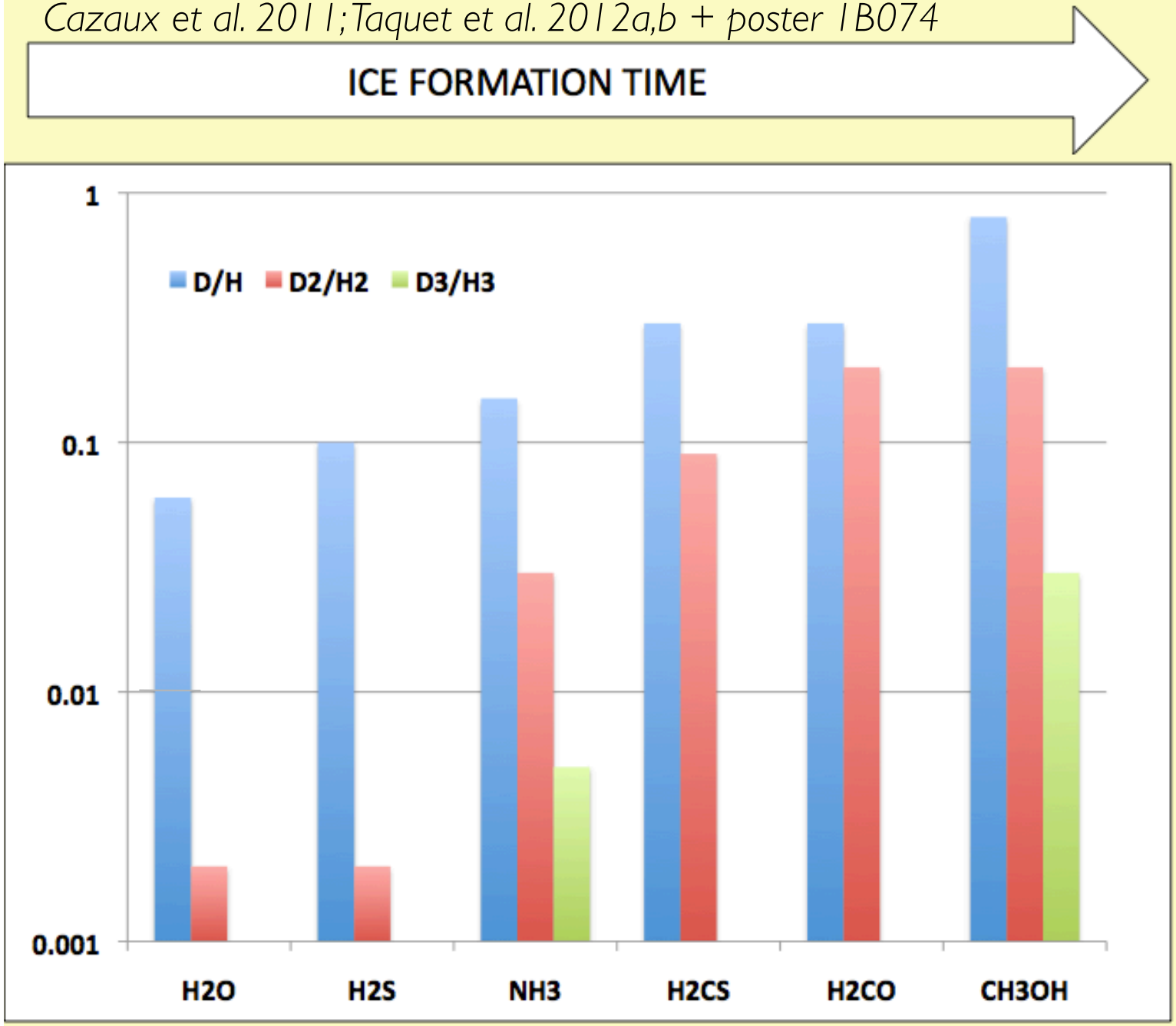
IRAS4A *Taquet et al. 2013; Parise et al. 2006*

IRAS4B *Jørgensen & van Dishoeck 2010, Parise et al. 2006*



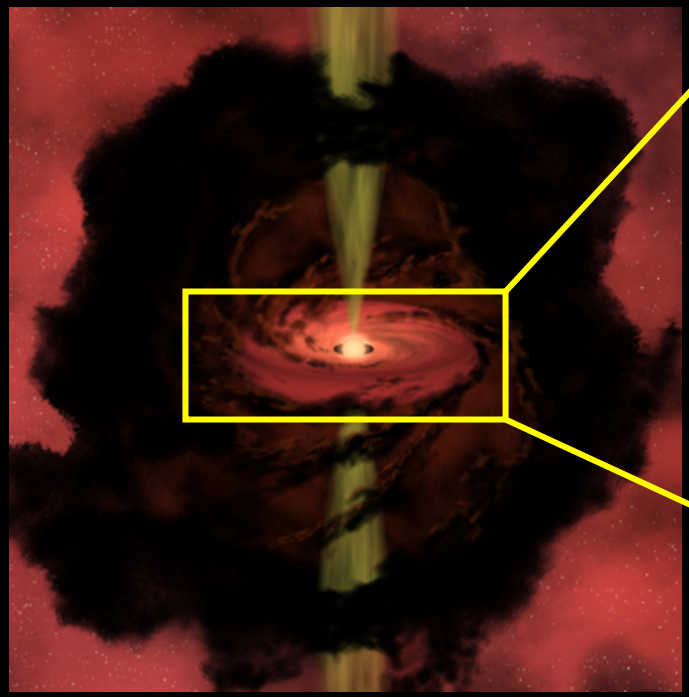
[See also Lis et al. 2002 + van der Tak et al. 2002 (ND_3); Magnus Persson poster (1B070)]

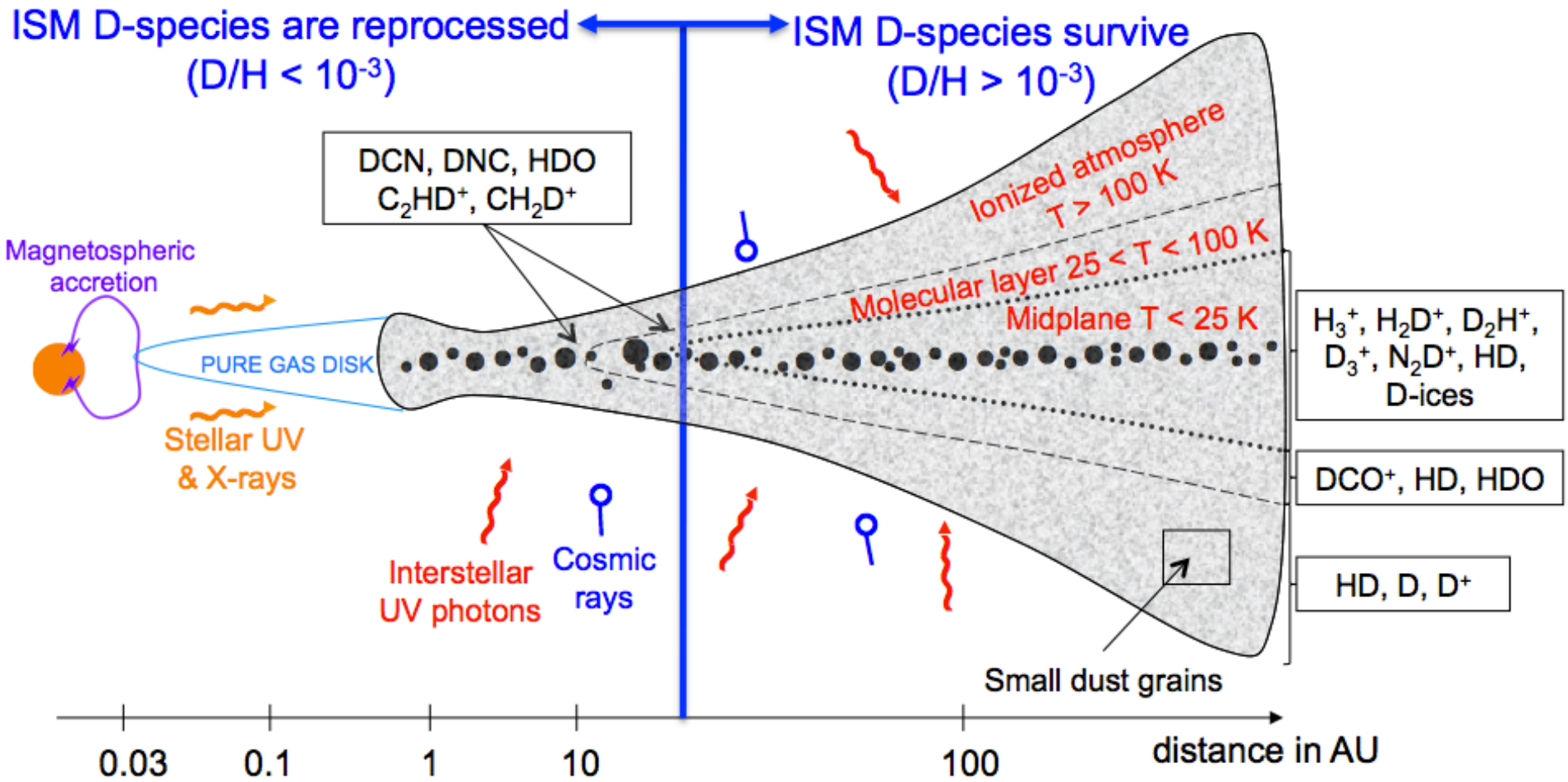
Cazaux et al. 2011; Taquet et al. 2012a,b + poster 1B074



H_2O:
Coutens et al. 2012
Persson et al. 2013
Taquet et al. 2013
Butner et al. 2007
Vastel et al. 2010
H_2S:
Vastel et al. 2003
NH_3:
Loinard et al. 2001
van der Tak et al. 2002
H_2CS:
Marcelino et al. 2005
H_2CO:
Ceccarelli et al. 1998
Parise et al. 2006
CH_3OH:
Parise et al. 2002
Parise et al. 2004
Parise et al. 2006

Deuterium fractionation in protoplanetary disks



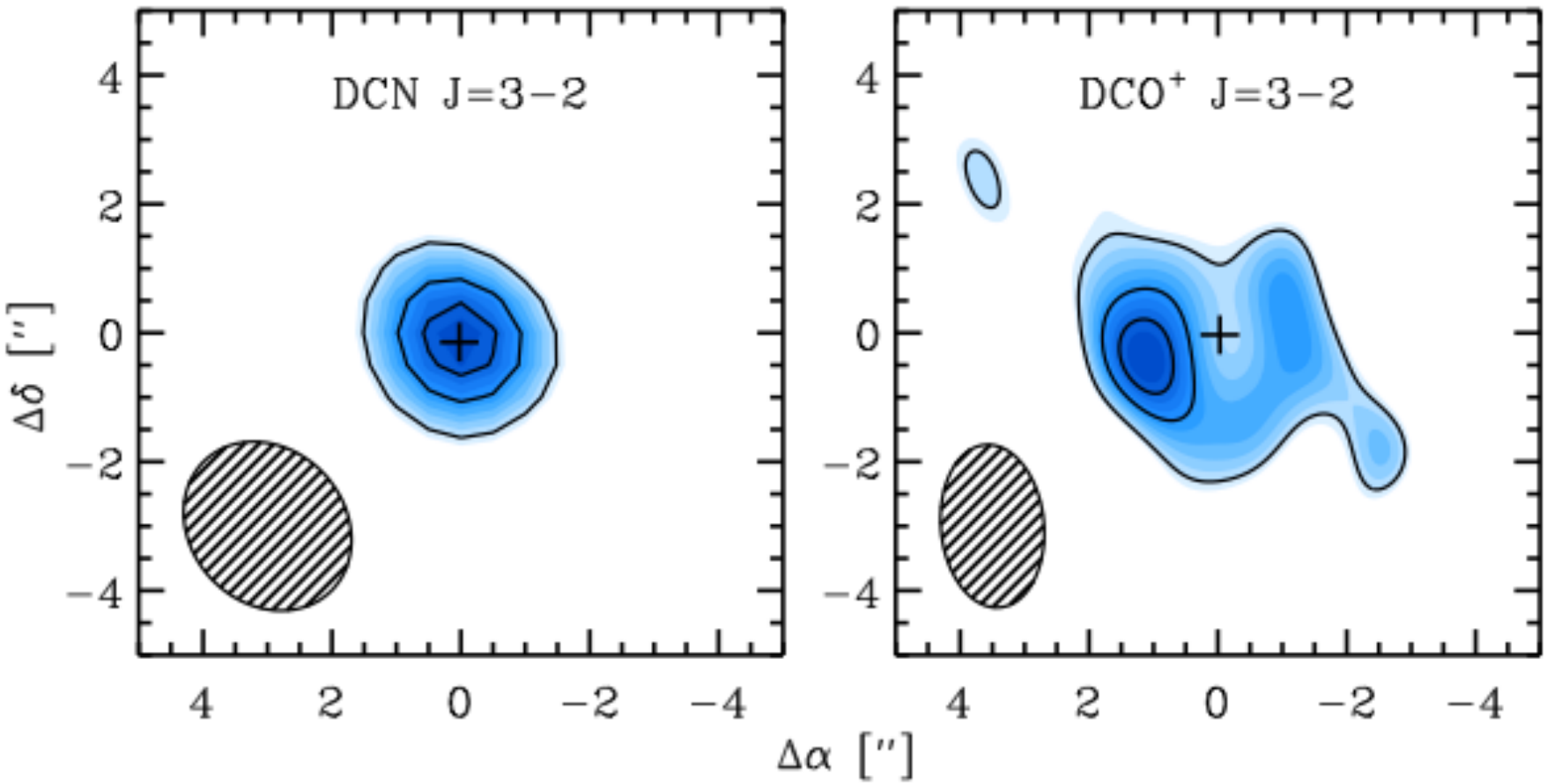


Adapted from: Bergin et al. 2007 + Caselli & Ceccarelli 2012 + Dullemond et al. 2007 + 2010 + Öberg et al. 2011 + Semenov 2011

See also, e.g., Willacy et al. 1998, 2000; Aikawa et al. 2006; Vasyunin et al. 2008, 2011; Woitke et al. 2010; Kamp et al. 2011; Walsh et al. 2012, 2013; poster 2K091 (Albertsson)

Deuteration in TW Hya

Öberg et al. 2012

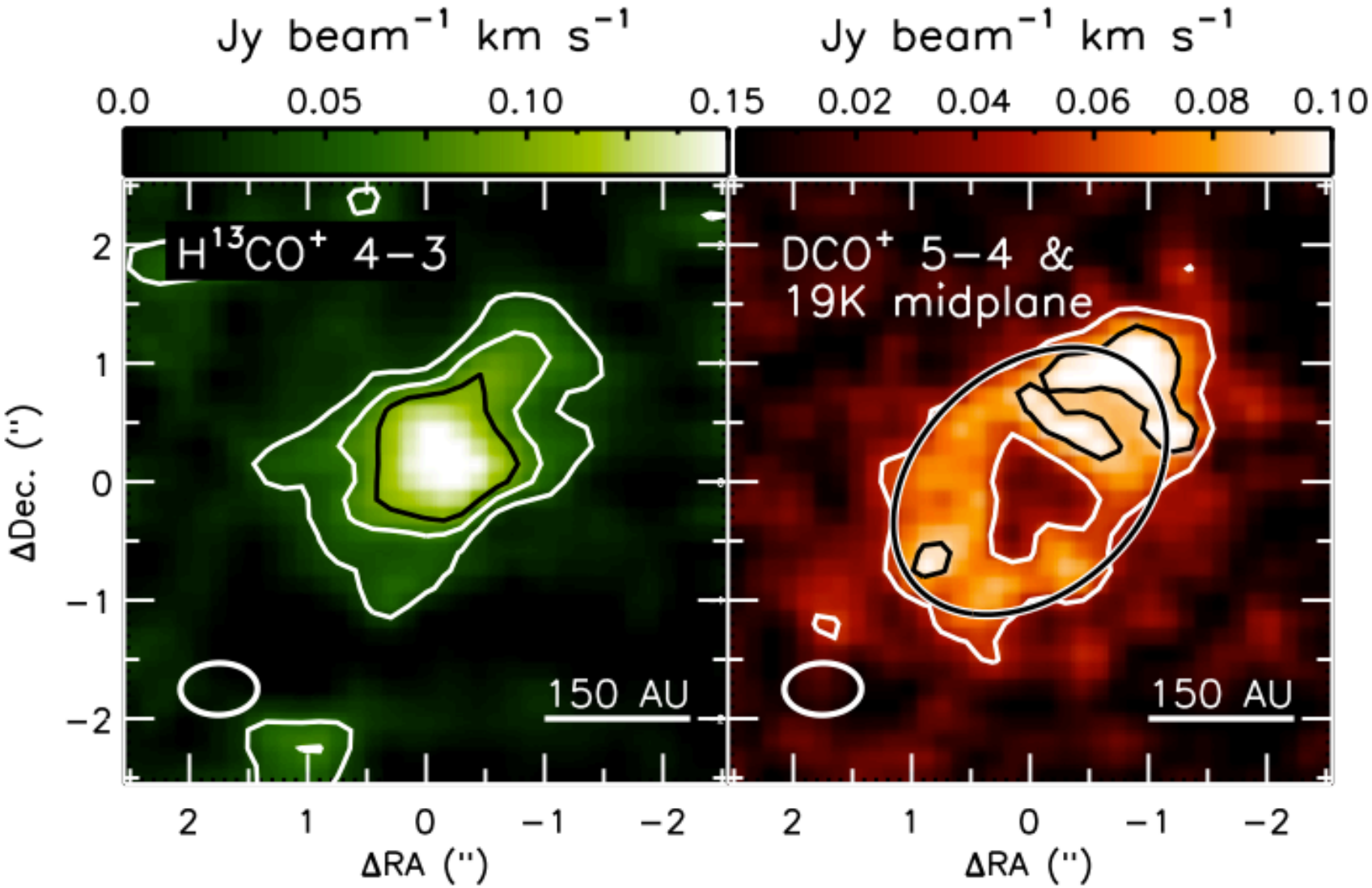


TW Hya with ALMA (SV)+ SMA : DCN/HCN ≈ DCO^+/HCO^+ ~ 0.02

(see also van Dishoeck et al. 2003; Qi et al. 2008)

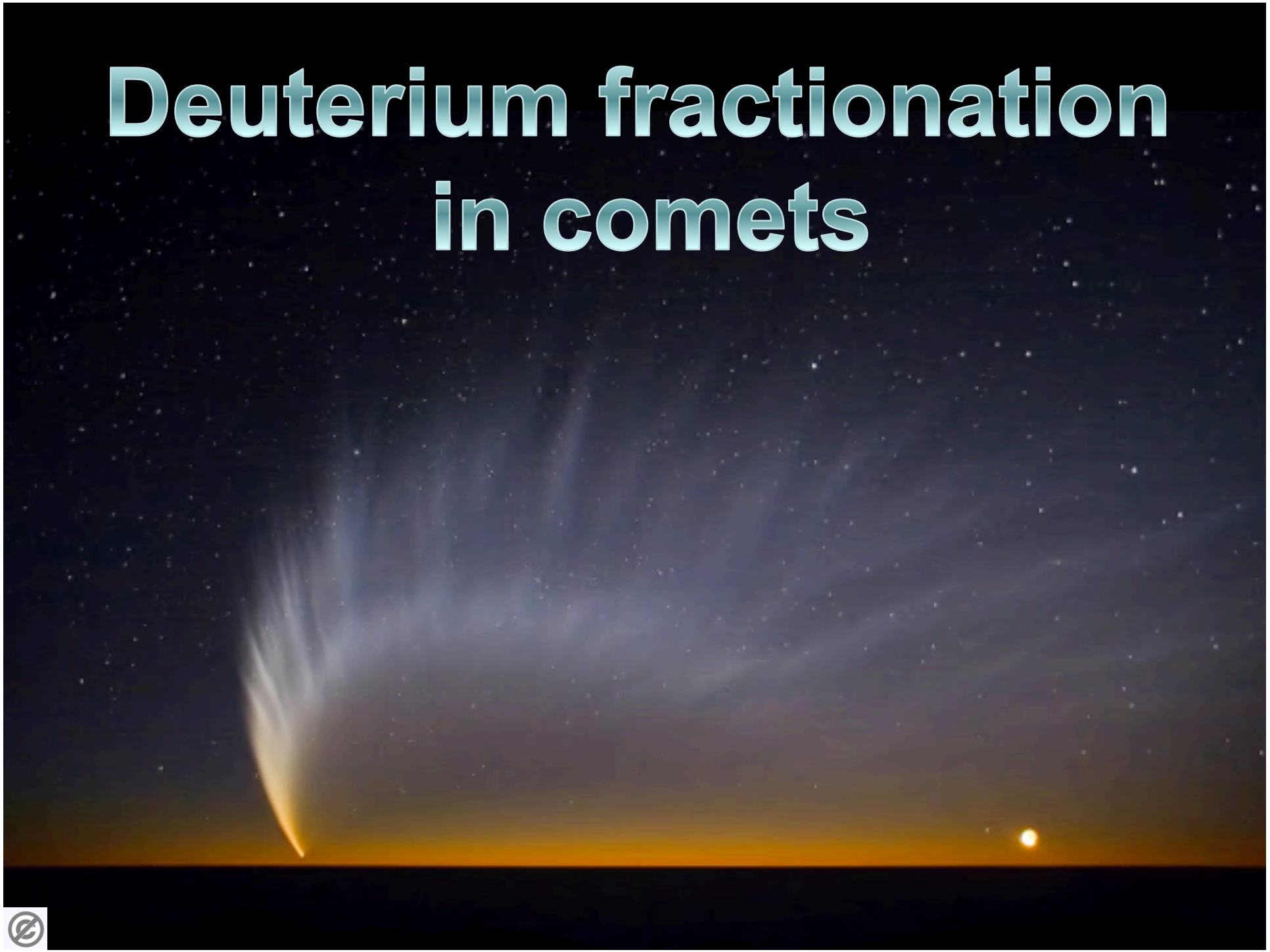
ALMA imaging of the CO snowline of HD163296

(Mathews, Klaassen et al. 2013, in press)

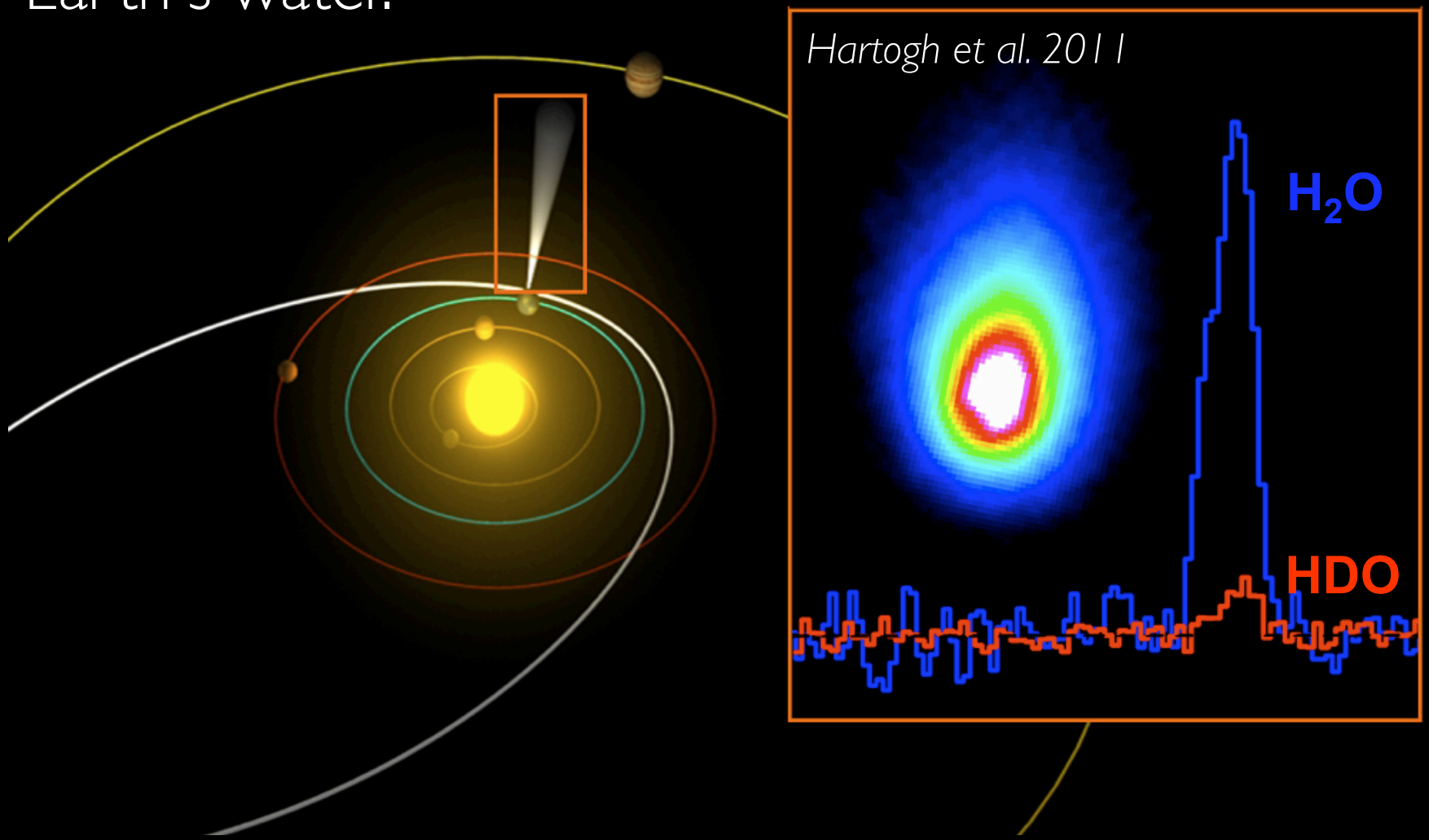


$DCO^+/HCO^+ \sim 0.3$; DCO^+ in a 110-160 AU ring (T = 19-21 K)

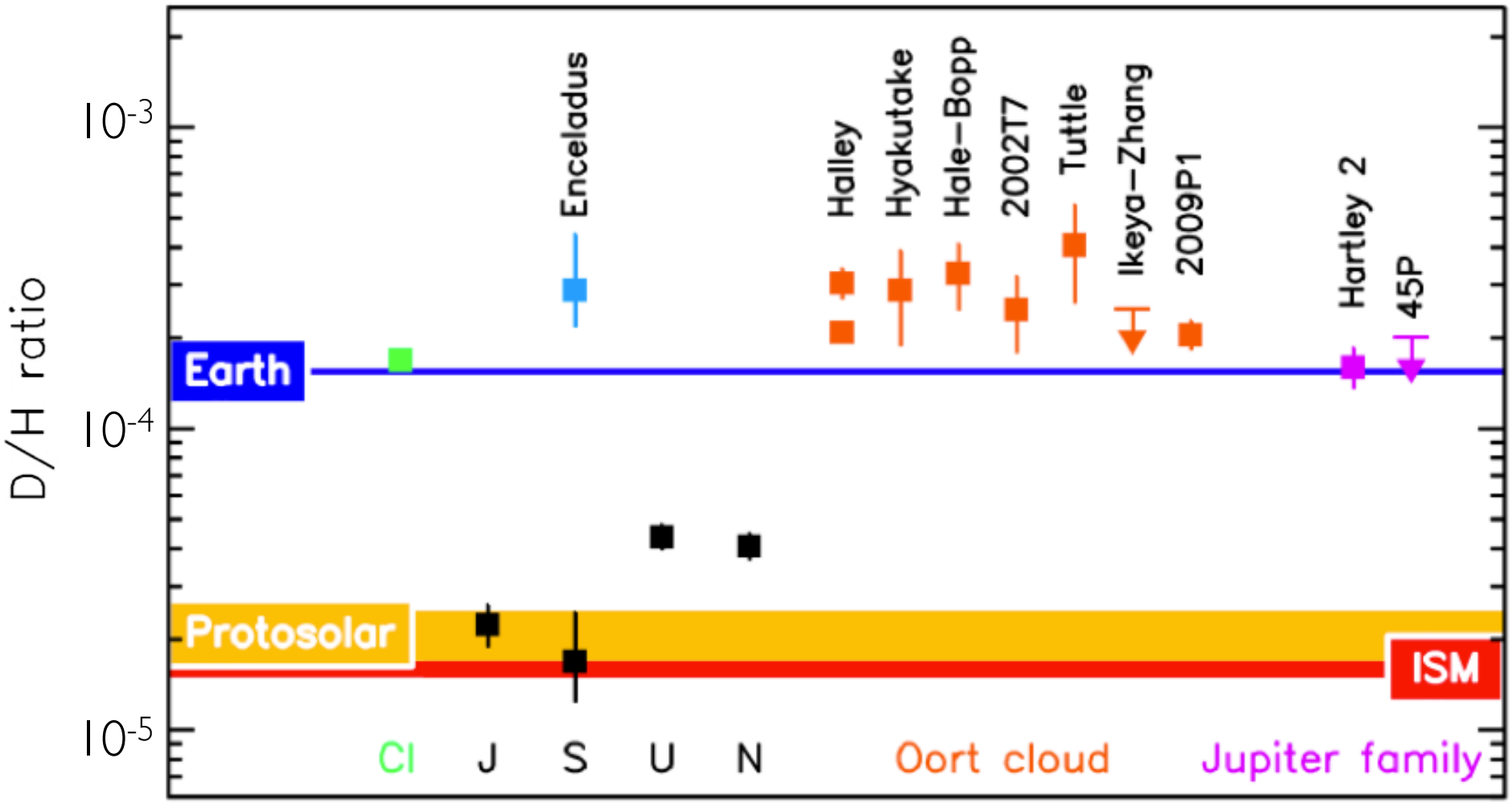
Deuterium fractionation in comets



Herschel observes water and heavy water in a comet and fuels the controversy of the origin of Earth's water.



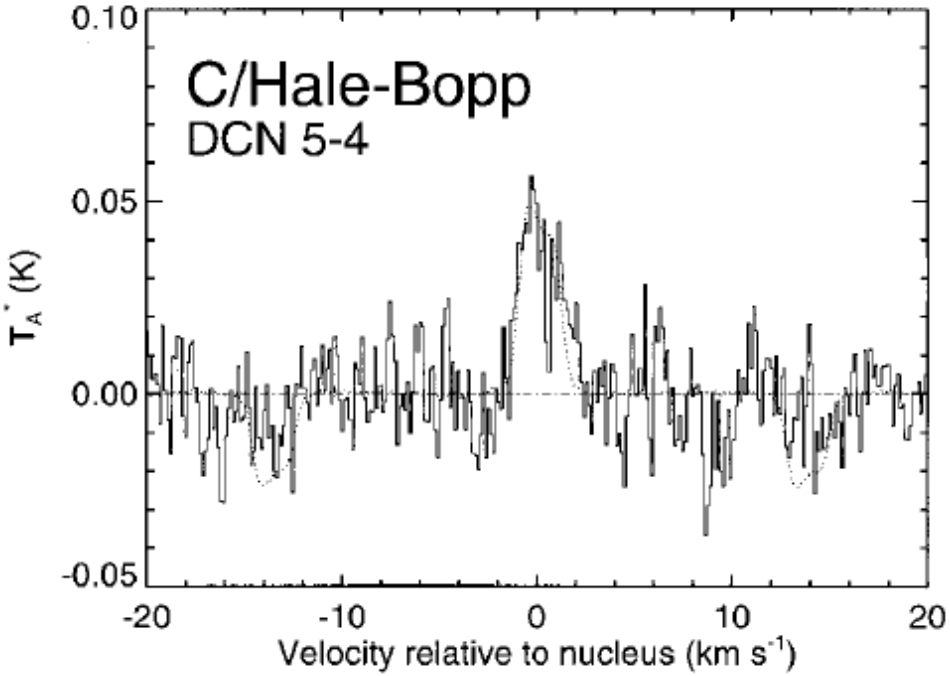
http://sci.esa.int/herschel/49386-herschel-finds-first-evidence-of-earth-like-water-in-a-comet/

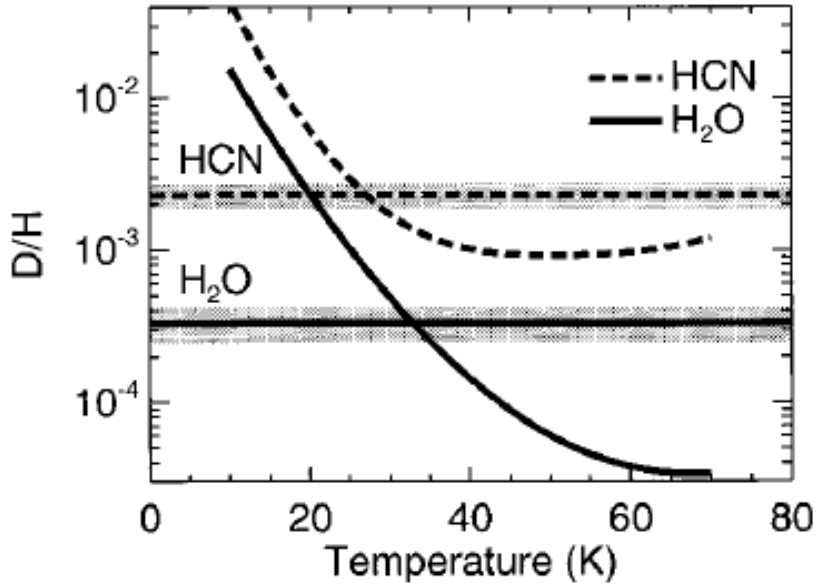


Adapted from Hartogh et al. (2011)

D/H in Hartley 2 = D/H in oceans (Hartogh et al. 2011);
D/H in C/2009 PI = 2×10^{-4} (Bockelée-Morvan et al. 2012).

Deuteration of organic molecules in COMETS





DCN/HCN ~ 10 times HDO/H_2O (Meier et al. 1998)

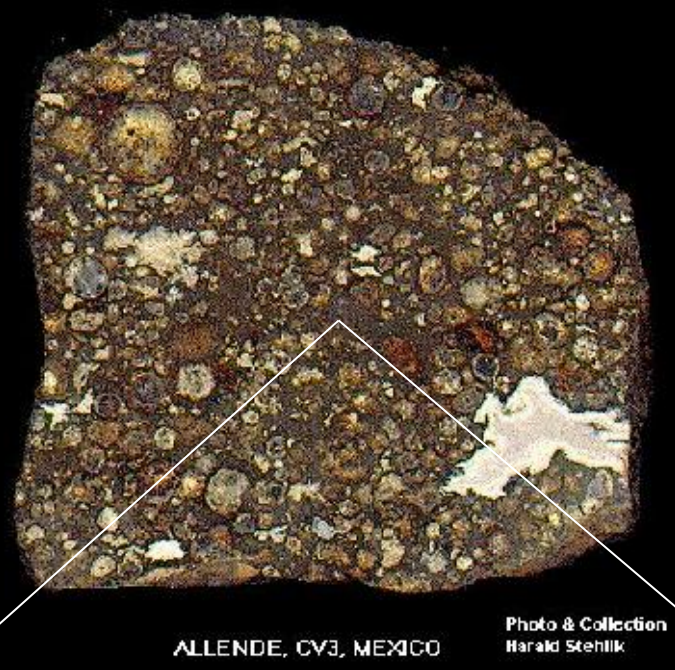
$HDCO/H_2CO < 0.05$
$CH_3OD/CH_3OH < 0.04$
$CH_2DOH/CH_3OH < 0.008$
} Crovisier et al. 2004

$CH_3D/CH_4 < 0.04$ (Kawakita et al. 2005)

Deuterium fractionation in meteorites

http://www.arizonaskiesmeteorites.com/AZ_Skies_Links/NWA_2364/

Carbonaceous Chondrites

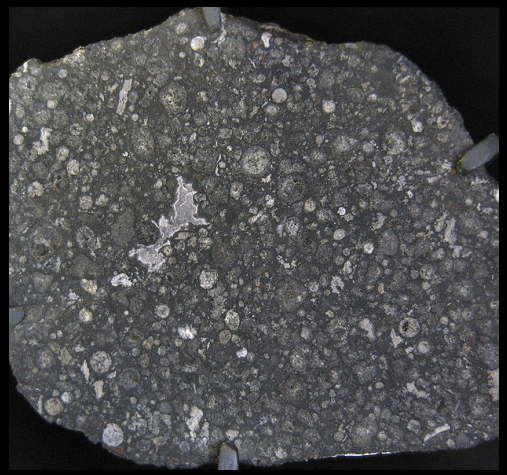


CLAY MINERALS

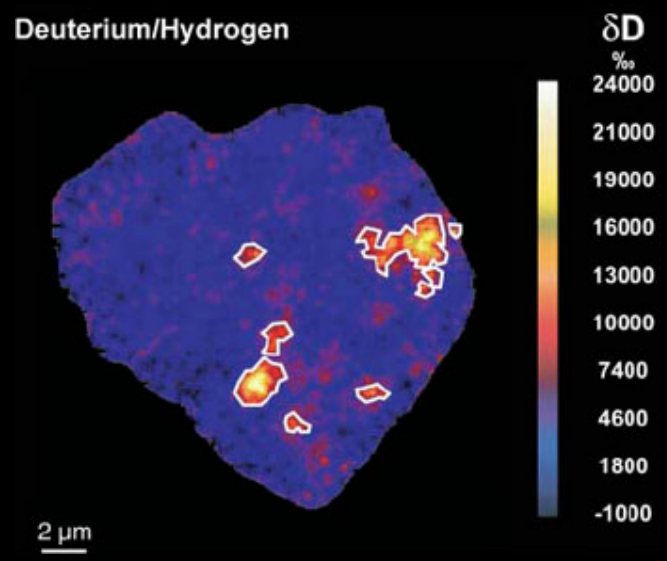
ORGANIC MATTER

(e.g. Alexander 2011)

D/H in carbonaceous chondrites and IDPs



Hydrated silicates and hydrous carbon:
D/H ~ $1.2\text{-}2.2\times10^{-4}$ (Robert 2003), similar to terrestrial oceans.



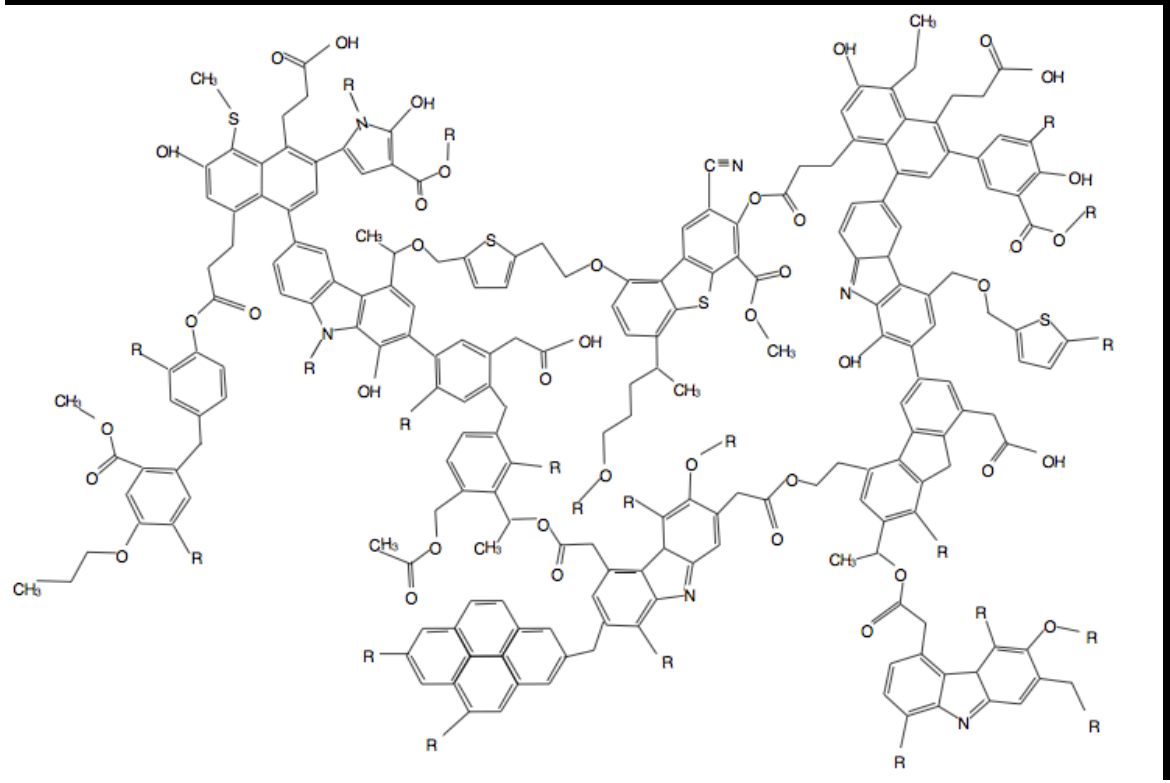
Micrometer-sized "hot spots" in organic matter within chondrites and IDPs:
D/H up to 0.01 (e.g. Alexander et al. 2007; Remusat et al. 2009).

http://www.psrd.hawaii.edu/May06meteoriteOrganics.html

ORGANIC MATTER

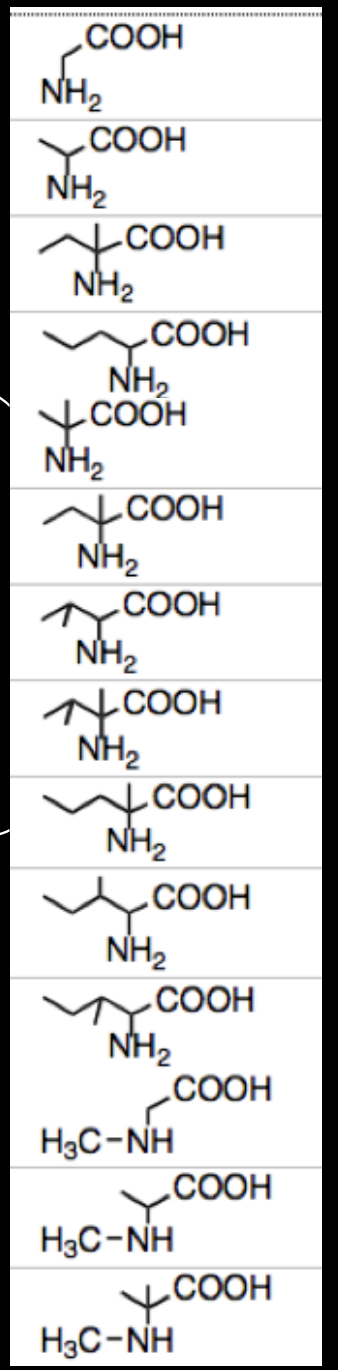
Insoluble Organic Matter (IOM)

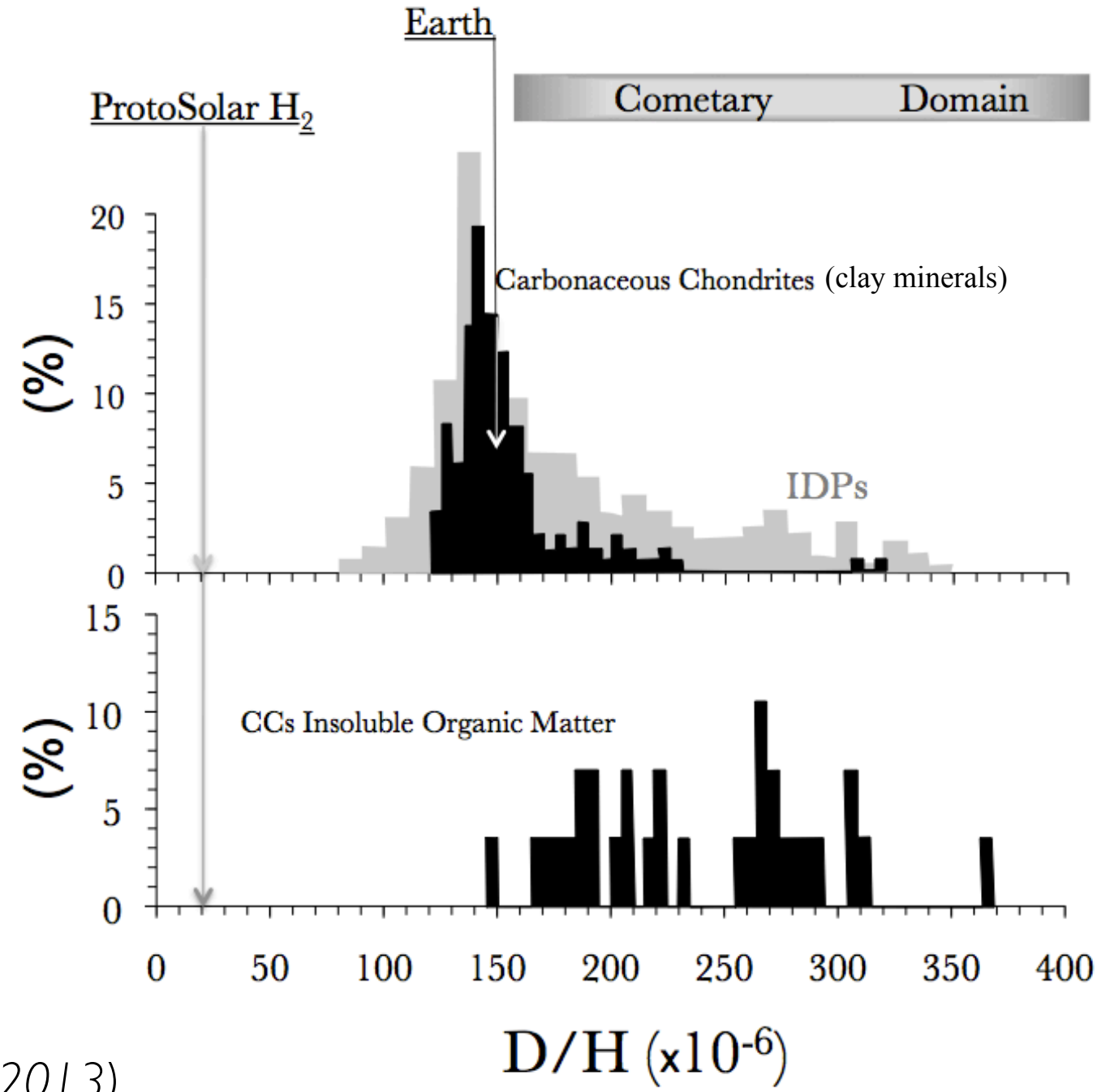
(Remusat et al. 2005; Cody & Alexander 2005)



Soluble Organic Matter (SOM)

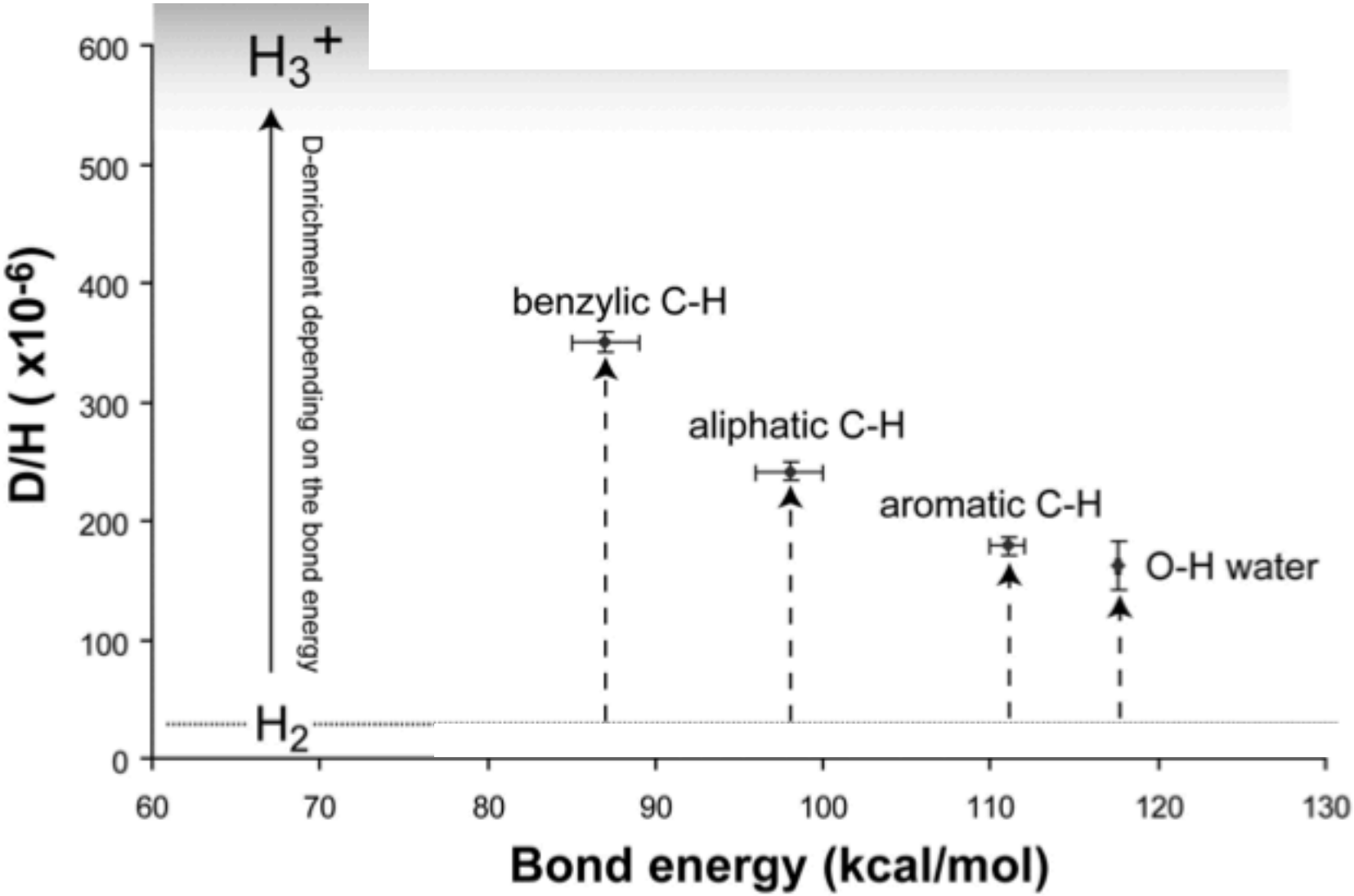
(Pizzarello et al. 2006)




Earth
ProtoSolar H_2
Cometary Domain
Carbonaceous Chondrites (clay minerals)
IDPs
CCs Insoluble Organic Matter
(%)
(%)
20
15
10
5
0
15
10
5
0
0
50
100
150
200
250
300
350
400
D/H ($\times 10^{-6}$)

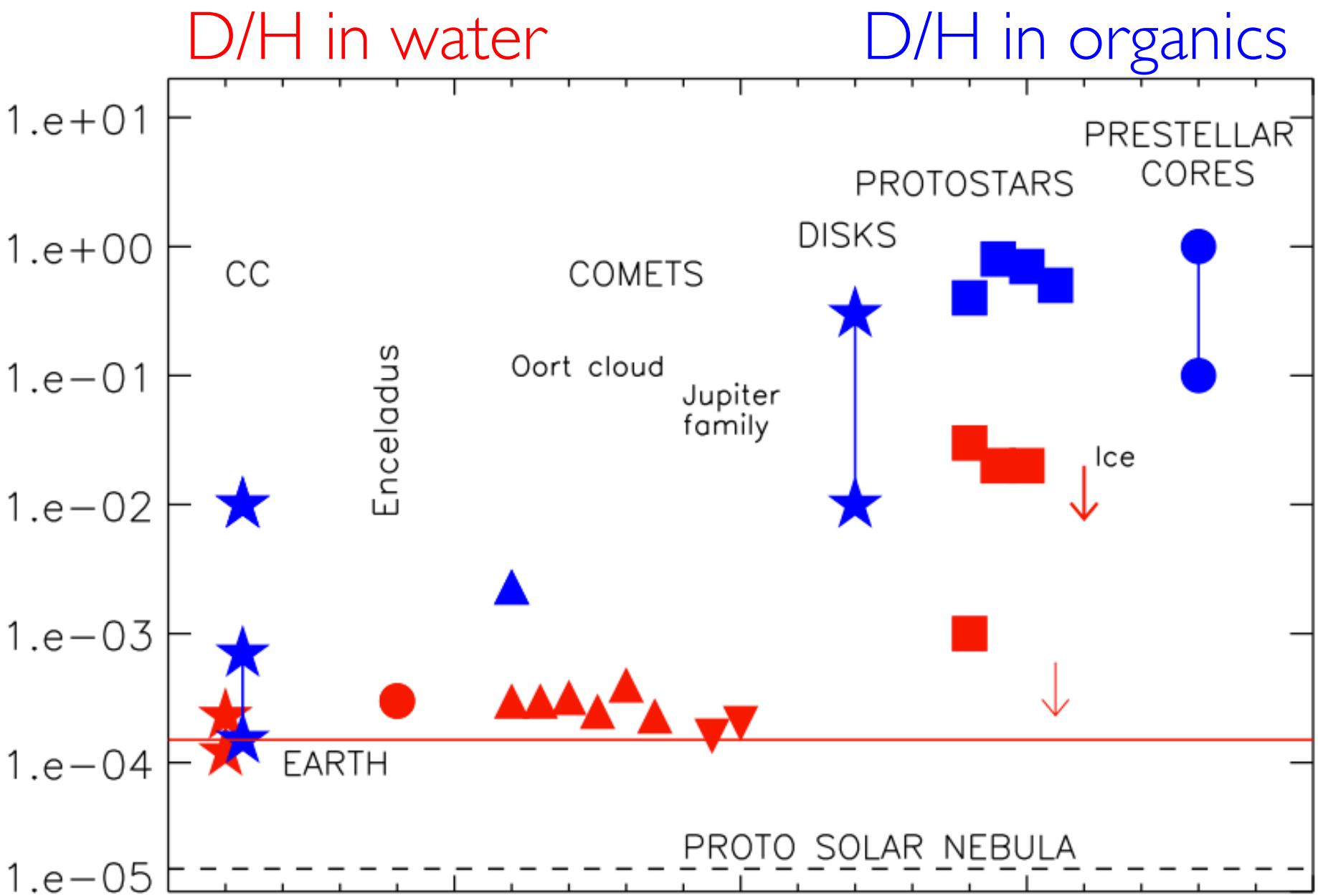
Robert (2013)

D/H in IOM



Remusat et al. 2009

SUMMARY: UNROLLING THE THREAD



(Some of the) Things to do

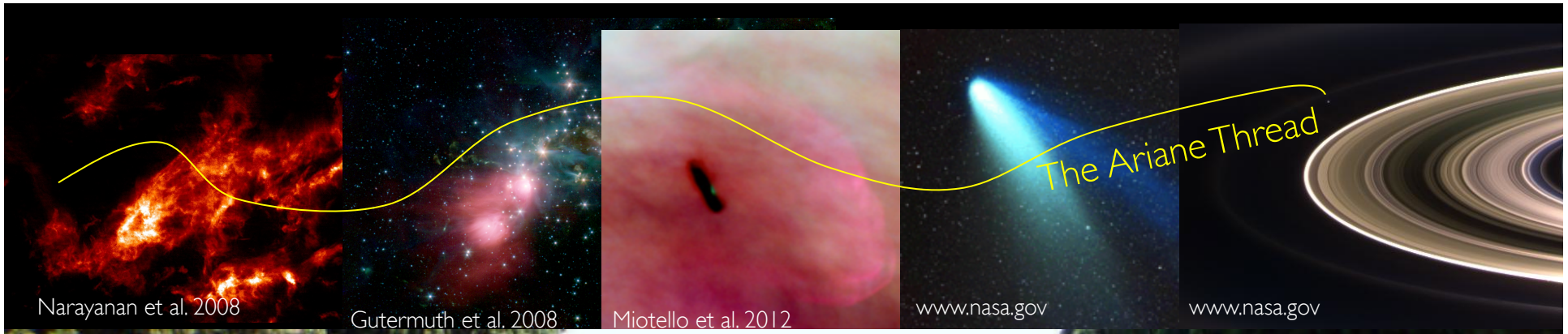
- Bridge the gap between pre-stellar cores and protoplanetary disks *(e.g. how important are the initial conditions in the physical and chemical evolution of PPDs?).*

- Study the reprocessing of material during the early stages of protoplanetary disks *(e.g. can self-gravitating accretion disks help in understanding some of the observed chemical & physical features of more evolved PPDs?).*

- Study the reprocessing of material (including dust coagulation and chemical evolution of trapped ices) throughout the PPD evolution *(e.g. which conditions favor the production of the organic material observed in pristine bodies of our Solar-System?).*

- Compare PPD models with Solar Nebula models.

- More observations (ALMA, NOEMA, …), theoretical chemistry and laboratory work!



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