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

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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
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The astrochemical heritage of the Solar System

1- PRE- STELLAR PHASE: cold and dense gas
FORMATION OF SIMPLE AND COMPLEX MOLECULES, THICK ICY MANTLES.

2- PROTOSTELLAR PHASE: collapsing, warm dense gas
PARTIAL ICE SUBLIMATION, HOT/SHOCK CHEMISTRY.

3- PROTOPLANETARY DISK PHASE:
DUST COAGULATION, GAS/ICE PROCESSING.

4- PLANETESIMAL FORMATION: grains agglomeration

5- PLANET FORMATION AND THE "COMET/ASTEROID RAIN"
DELIVERY OF PROCESSED AND PRISTINE MATERIAL (?) + LIFE

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

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

\[ (D/H)_{\text{cosmic}} \sim 1.5 \times 10^{-5} \]

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

(Oliveira et al. 2003)
The first two steps

1. Formation of $H_2$ onto dust grain particles

2. Formation of $H_3^+$

$$H_2 + \text{cosmic ray} \rightarrow H_2^+ + e^- + \text{cosmic ray}$$

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$
- Freeze-out of neutrals boosts D-fractionation (Dalgarno & Lepp 1986)
- D-fractionation slows down if ortho-\(\text{H}_2/\text{para-\(\text{H}_2\)} > 0.001\) (Flower et al. 2006)
- Importance of \(\text{H}_2\) tunneling reactions on surface (Sipila et al. 2013)
1) On the surface of cold grains

2) D-H exchange in the gas
   2a) cold (T<30K) gas
       Key species: H₂D⁺
   2b) warm (30<T<100 K) gas
       Key species: CH₂D⁺
   2c) hot (T>100 K) gas
       Key species: OD
   2d) very hot (T>500 K) gas
       reaction: HDO + H₂

3) D-H exchange in the ice
   3a) thermal (T_{grain}>100K)
      Example:
      HDO + CH₃OH -> H₂O + CH₃OD
      or
      H₂O + CH₃OD -> HDO + CH₃OH
   3b) photolysis
      Example:
      HDO + CH₄ -> H₂O + CH₃D
      or
      H₂O + CH₃D -> HDO + CH₄

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: $\text{N}_2\text{H}^+(1-0)$; contour: $\text{N}_2\text{D}^+(2-1)$

$\text{N}_2\text{D}^+/\text{N}_2\text{H}^+ \sim 0.03-0.7$ (Crapsi et al. 2005; Pagani et al. 2007)
$\text{NH}_2\text{D}/\text{NH}_3 \sim 0.06-0.4$ (Shah & Wootten 2001; Crapsi et al. 2007)
$\text{D}_2\text{CO}/\text{H}_2\text{CO} \sim 0.01-0.1$ (Bacmann et al. 2003)
$\text{DCN}/\text{HCN} \sim 0.01-0.04$ (Turner 2001)
$\text{DNC}/\text{HNC} \sim 0.02-0.09$ (Hirota et al. 2003)
$\text{DCO}^+/\text{HCO}^+ \sim 0.04$ (Butner et al. 1995; Caselli et al. 2002)
c-$\text{C}_3\text{D}_2$/c-$\text{C}_3\text{H}_2 \sim 0.01-0.02$ (Spezzano et al. 2013)
orthogonal-H$_2$D$^+$

The o-H$_2$D$^+$ line is strong and its emission is extended $\sim$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)

Caselli et al. 2003, 2008

Vastel et al. 2006

- o-H$_2$D$^+$
- CS$^+$
- N$_2$H$^+$(1-0)
- IRAM
- N$_2$D$^+$(2-1)
- IRAM
para-$\text{D}_2\text{H}^+$

Extended para-$\text{D}_2\text{H}^+$ emission (~40'' ~5000 AU) toward L1688/H-MM1 (APEX-CHAMP+)

[Para-$\text{D}_2\text{H}^+$ was first detected by Vastel et al. (2004) toward another pre-stellar core]
1.3mm dust continuum map

outer edge

Deuteration zone

$A_v \approx 10 \text{ mag}$

Dark-cloud zone

$3 \leq A_v \leq 10 \text{ mag}$
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


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 (ND₃); Magnus Persson poster (1B070)]]
H$_2$O: Coutens et al. 2012
Persson et al. 2013
Taquet et al. 2013
Butner et al. 2007
Vastel et al. 2010
H$_2$S: Vastel et al. 2003
NH$_3$: Loinard et al. 2001
van der Tak et al. 2002
H$_2$CS: Marcelino et al. 2005
H$_2$CO: Ceccarelli et al. 1998
Parise et al. 2006
CH$_3$OH: Parise et al. 2002
Parise et al. 2004
Parise et al. 2006
Deuterium fractionation in protoplanetary disks

http://www.spacetelescope.org/images/opo9545c/

Deuteration in TW Hya
Öberg et al. 2012

TW Hya with ALMA (SV)+ SMA: DCN/HCN \approx DCO^+/HCO^+ \sim 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.

Hartogh et al. (2011)

D/H in Hartley 2 = D/H in oceans (Hartogh et al. 2011);
Deuteration of organic molecules in COMETS

DCN/HCN ~ 10 times HDO/H₂O (Meier et al. 1998)

\[
\begin{align*}
\text{HDCO/H₂CO} & < 0.05 \\
\text{CH₃OD/CH₃OH} & < 0.04 \\
\text{CH₂DOH/CH₃OH} & < 0.008 \\
\text{CH₃D/CH₄} & < 0.04 \text{ (Kawakita et al. 2005)}
\end{align*}
\]

\{ Crovisier et al. 2004 \}
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 ~ 1.2-2.2×10^{-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)
(Reusat et al. 2005; Cody & Alexander 2005)

Soluble Organic Matter (SOM)
(Pizzarello et al. 2006)
Robert (2013)
D/H in IOM

Remusat et al. 2009
SUMMARY: UNROLLING THE THREAD

D/H in water vs. D/H in organics

- CC
- Enceladus
- Oort cloud
- Jupiter family
- DISKS
- PROTOSTARS
- PRESTELLAR CORES
- Ice
- EARTH
- PROTO SOLAR NEBULA
(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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