Deuteration and fractionation in prestellar cores and IRDCs from an observational point of view

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Florence, October 11th, 2016
Elemental abundances

<table>
<thead>
<tr>
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<th>Solar system</th>
<th>local ISM</th>
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<tbody>
<tr>
<td>D/H</td>
<td>1.94 $10^{-5}$ (a)</td>
<td>1.6 $10^{-5}$ (c)</td>
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<tr>
<td>$^{12}$C/$^{13}$C</td>
<td>89.3 (a)</td>
<td>69±6 (c)</td>
</tr>
<tr>
<td>$^{14}$N/$^{15}$N</td>
<td>441±6 (b)</td>
<td>338±32 (c)</td>
</tr>
<tr>
<td>$^{16}$O/$^{18}$O</td>
<td>499 (a)</td>
<td>557±30 (c)</td>
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<tr>
<td>$^{18}$O/$^{17}$O</td>
<td>5.4 (a)</td>
<td>3.6±0.2 (c)</td>
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<tr>
<td>$^{32}$S/$^{34}$S</td>
<td>22.5 (a)</td>
<td>24±5 (d)</td>
</tr>
<tr>
<td>$^{34}$S/$^{33}$S</td>
<td>5.6 (a)</td>
<td>6.3±1.0 (d)</td>
</tr>
<tr>
<td>$^{28}$Si/$^{29}$Si</td>
<td>19.7 (a)</td>
<td></td>
</tr>
<tr>
<td>$^{29}$Si/$^{30}$Si</td>
<td>1.5 (a)</td>
<td>1.5 (c)</td>
</tr>
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(b) Marty et al. 2011, Science 332, 1533  
(c) Wilson, 1999 Rep. Progress Phys. 62, 143  

Gradient of $^{12}$C/$^{13}$C, $^{16}$O/$^{18}$O, $^{14}$N/$^{15}$N as a function of distance from the Galactic Center, $D_{GC}$
Detected Deuterated species

HD, ND, HDO, D₂O, NH₂D, ¹⁵NH₂D, ND₂H, ND₃, DCN, DNC, C₂D, HD₃O, D₂CO, CH₂DOH, CH₃OD, CHD₂OH, CD₃OH, c-C₃HD, c-C₃D₂, CH₃C₂D, CH₂DC₂H, CH₂DCN, HDS, HDCS, D₂CS, C₄D, l-C₄HD, DC₃N, DC₅N
H₂D⁺, D₂H⁺, DCO⁺, D¹³CO⁺, CH₂D⁺, NH₃D⁺, N₂D⁺

Detected ¹³C species

¹³CO, ¹³CN, ¹³CS, H¹³CN, HN¹³C, H₂¹³CO, ¹³CH₃OH, H¹³COOH, ¹³CCH, C¹³CH, c-H¹³CC₂H, c-HCC¹³CH, ¹³CC₃H, C¹³CC₂H, C₂¹³CCH, C₃¹³CH, ¹³CC₂N, C¹³CCN, C₂¹³CN, H¹³CC₂N, HC¹³CCN, HC₂¹³CN, ¹³CH₂NH, NH₂¹³CHO, H₂¹³CHCHCN, H₂C¹³CHCN, H₂C₂H¹³CN, ¹³CH₃CN, CH₃¹³CN, C₂H₅¹³CN, ¹³CH₃CH₂CN, CH₃¹³CH₂CN, H₂¹³CS, O¹³CS, C¹³CCS, ¹³CH⁺, H¹³CO⁺

Detected ¹⁵N species

C¹⁵N, HC¹⁵N, H¹⁵NC, ¹⁵NH₃, CH₃C¹⁵N, HC₃¹⁵N, C₂H₅C¹⁵N, ¹⁵NNH⁺, ¹⁵NNH⁺
Detected $^{18}$O species

$c^{18}$O, $^{13}c^{18}$O, $^{18}$OH, $H_2^{18}$O, $H_2c^{18}$O, $CH_3^{18}$OH, $Si^{18}$O, $S^{18}$O, $^{18}$OCS, $HC^{18}$O$^+$

Detected $^{17}$O species

$c^{17}$O, $^{13}c^{17}$O, $S^{17}$O, $HC^{17}$O$^+$

Detected $^{34}$S and $^{33}$S species

$c^{34}$S, $^{34}$SO, $H_2^{34}$S, $H_2c^{34}$S, $C_3^{34}$S, $^{34}$SO$_2$, $OC^{34}$S, $Si^{34}$S, $^{30}Si^{34}$S, $^{29}Si^{34}$S, $C^{33}$S, $^{33}$SO, $^{33}$SO$_2$, $H_2^{33}$S, $OC^{33}$S, $Si^{33}$S, $H_2c^{33}$S

Detected $^{30}$Si and $^{29}$Si species

$^{30}$SiO, $^{30}$Si$C_2$, $^{30}$SiS, $^{29}$SiS
Deuterated molecules are useful diagnostic tools for studying the cold and dense environments where stars are born.

**Low-mass:** Caselli+ 2002, Crapsi+ 2007

**High-mass:** Fontani+ 06,09,11; Pillai+ 07,12

\[ \text{T} \leq 20 \text{ K} \]

\[ \begin{align*}
H_3^+ + O & \rightarrow H_3O^+ \\
H_3^+ + N & \rightarrow NH^+ + H_2 \\
\text{highly endothermic! Slower neutral-neutral reactions}
\end{align*} \]
Prestellar cores provide the original reservoir of material from which future planetary systems are built.

- Low $T_{\text{gas}}$ and $T_{\text{dust}}$ (< 10 K)
- High density ($\geq 10^5$ cm$^{-3}$)
- Typical lifetime $\sim 10^5$ years
- Strong mm emissivity; absorption NIR, MIR
- High deuterium fractionation
Prestellar cores

1.3mm dust continuum map

Dark-cloud zone
- c.r., H₂, C, ²H₂, O, e⁻
- H₂ → H₂⁺ → H₃⁺ → CH⁺ → CH₄⁺ → HCO⁺ → CO
- C → N₂H⁺
- N → CN → NH → NH⁺ → NH₄⁺ → NH₃

Deuteration zone
- H₃⁺ → HD⁺ → D₂⁺ → D⁺ (gas deuteration)
- freeze-out of neutral species
- D/H increases → surface deuteration

Caselli et al. 2011, Keto & Caselli 2010
Deuteration as a chemical clock?

\[ \text{D}_{\text{frac}}(\text{N}_2\text{H}^+) = 0.2 \]

3-5 \(10^5\) years (6-10 x \(t_{\text{ff}}\))

(depending on \(H_2\) OPR)

Very slow contraction

(ambipolar diffusion)

Kong+2015

Many first detections:

- \(H_2D^+\) (Caselli et al. 2004)
- \(H_2O\) (Caselli et al. 2010, 2012)
- \(c-C_3D_2\) (Spezzano et al. 2013)
- \(HDCCC\) (Spezzano et al. 2016)
Deuterated water in prestellar cores

- Detection limits!
- ALMA: extended emission
- Need of a detailed benchmark among different radiative transfer codes for this particular problem of water in prestellar cores.

Quénard, Taquet, Vastel et al. 2016
High spatial resolution of H$_2$D$^+$

Friesen et al. 2014:

Integrated H$_2$D$^+$ 1$_{10}$-1$_{11}$ intensity (black contours) toward the SM1N core (grayscale) at 1.3″ (FWHM) resolution. White contours show the continuum emission ALMA (black) and JCMT (gray) H$_2$D$^+$ spectra toward SM1N.

These data observationally reveal the earliest stages of the formation of circumstellar accretion regions and agree with theoretical predictions that disk formation can occur very early in the star formation process, coeval with or just after the formation of a first hydrostatic core or protostar.
Nitrogen fractionation in L1544

Nitrile-bearing species (molecule carrying the -CN group or its isomer) have been found to be considerably enriched in $^{15}$N (Ikeda+2002; Milam & Charnley 2012; Hily-Blant+2013):

Low $^{14}$N/$^{15}$N ~ 260 (HCN)

whereas ammonia derivatives show no $^{15}$N enhancements or even a substantial depletion:

High $^{14}$N/$^{15}$N > 700 (NH$_2$D: Gérin+09; N$_2$H$^+$: Bizzocchi+2013)

Nitriles derive from atomic nitrogen, while ammonia is formed via N$^+$, which in turns come from N$_2$. The chemical networks responsible for their $^{15}$N enrichment are thus well separated.
$^{15}\text{N}$-enrichment of ammonia is highly sensitive to the H$_2$ ortho-to-para (OPR) ratio, while the fractionation evolution of nitriles is not significantly affected (Wirstrom+12).

The production of NH$_3$ is initiated by the ion-neutral reaction:

$$\text{N}^+ + \text{H}_2 \rightarrow \text{NH}^+ + \text{H}$$

whose activation energy barrier of $\sim 200$ K can be efficiently overcome by the o-H$_2$ internal energy.

On the other hand, ammonia fractionation gets much less efficient as the OPR decreases, and then an increasing quantity of $^{15}\text{N}^+$ is circulated back into molecular nitrogen by the equilibrium:

$$^{15}\text{N}^+ +^{14}\text{N}_2 \rightleftharpoons ^{14}\text{N}^+ + ^{15}\text{N}^{14}\text{N}$$
Nitrogen fractionation in L1544

Bizzocchi+10: $^{14}\text{N}/^{15}\text{N} \sim 446\pm71$
(N$^{15}\text{NH}$+, LTE)

Bizzocchi+13: $^{14}\text{N}/^{15}\text{N} \sim 1000\pm200$
($^{15}\text{N}_2\text{H}$+, non LTE)
Gérin+09: $^{14}\text{N}/^{15}\text{N} > 700$
(NH$_2$D)

Common fractionation pathway for the two molecules: not consistent with chemical models, which predicted small or no $^{15}\text{N}$ fractionation of $\text{N}_2\text{H}^+$. Depletion?

$\text{N}_2\text{H}^+$: N$_2$ + H$_3^+$ $\rightarrow$ N$_2\text{H}^+$ + H$_2$
NH$_3$: N$^+$ + H$_2$ $\rightarrow$ NH$^+$ + H
depends on the H$_2$ OPR

A way to reconcile our observational results with chemical modelling is to allow selective freeze-out of $^{15}\text{N}$ in some molecular form (possibly $^{15}\text{N}^{14}\text{N}$) on the surface of dust grains, something that needs to be tested in future models that include $^{15}\text{N}$-bearing species and surface chemistry, as well with laboratory work.
Influence of the environment: 16293E

D-ammonia:
Lis+ 2002, 2006, Roueff+ 2015

H$_2$D$^+$, D$_2$H$^+$:
Vastel+ 2004, 2012

ND:
Bacman+ 2016

Interferometric ND$_3$, N$_2$D$^+$:
Lis+ 2016

Daniel+ 16: N$_2$H$^+$ / N$^{15}$NH$^+$ ~ 330 comparable to the elemental isotope ratio inferred for the local ISM: no chemical fractionation.

Indeed, the most recent gas-phase network of Roueff+ 15 suggests that the fractionation reaction of $^{15}$N with N$_2$H$^+$ is inefficient due to the presence of an activation barrier. However, cannot explain the L1544 observations.

Temperature dependance?
Massive vs low-mass prestellar core?

The sites of initial conditions of massive star birth are difficult to study. Infrared dark clouds (IRDCs) are dense ($n_{\text{H}_2} \sim 10^5 \text{ cm}^{-3}$), cold molecular clouds (T<20K), with masses 100-1000 $M_\odot$, seen in silhouette against 8µm Galactic plane emission.

Pillai et al. (2007) detected high deuteration in IRDC clumps, evidence of very low temperatures.
$D^{N_{2}H^+}_{\text{frac}}$ as an evolutionary indicator in the low and high-mass star formation process?

- Evolutionary state of prestellar cores: Crapsi+05
- Evolutionary state of Class 0 protostars: Emprechtinger+09
- Evolutionary state for high-mass star forming regions: Chen+11
Massive vs low-mass prestellar core?

Differences: widespread NH$_3$ and N$_2$H$^+$ emission, presence of large scale SiO emission (shocks across the whole length of filament), higher pressure (larger line widths). But high deuteration.

Caselli 2014
Fontani+11,15
Crapsi+2005
1) Some low D-frac found in some IRDCs (Gerner+15, Barnes+16) might be due to some unresolved evolved object (24 µm sources) since the average D-frac to similar to the values observed towards HMPO candidates (0.04; Fontani+11).

2) $N_2D^+$ more spatially concentrated in cores than $N_2H^+$ which is also present in the clump envelope. Therefore, measurement of the D-frac in massive star forming region could be limited by low spatial resolution (beam dilution).

**Need for high spatial resolution of $N_2H^+$, $N_2D^+$ and $H_2D^+$ observations**
A distant dark cloud?

W51
d~5 kpc

Flagey+2013

Mookerjea+2013

Vastel+2016
Herschel pointed position

Large scale filament ([62-70] km/s)

Towards the telescope
A distant dark cloud?

Herschel position

Result from the collision of the filament with W51

HDO/H$_2$O=0.001
DCO$^+$/HCO$^+=0.2$
DNC/HNC=0.14
T$\sim 10$K
n$_{H_2}\sim 2.5\times 10^4$ cm$^{-3}$

Dark cloud conditions (TMC1)

NH$_2$D
IRAM/NOEMA

Vastel+2016
Relative abundances of HDO and H$_2$O

Persson+ (2014)

Cosmic D/H

Earth’s oceans

Protosolar

From prestellar, to protostar and planet

Protostars

Prestellar

Comets

Protostars

Jupiter family comets

Oort Cloud comets

Protostars

L1544

Protosolar

ISM

Earth (SMOW)
Thanks for your attention!