Detection of OD with SOFIA

SOFIA Community Tele-Talk, December 2013

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Water formation in the ISM?

Water formation in cold gas:

\[ \text{O} + \text{H}_3^+ \rightarrow \text{OH}^+ \]
\[ \text{O}^+ + \text{H}_2 \rightarrow \text{OH}^+ \]
\[ \text{OH}^+ + \text{H}_2 \rightarrow \text{H}_2\text{O}^+ \]
\[ \text{H}_2\text{O}^+ + \text{H}_2 \rightarrow \text{H}_3\text{O}^+ \]
\[ \text{H}_3\text{O}^+ + e^- \rightarrow \text{H}_2\text{O} \]

Water formation in hot gas:

\[ \text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H} \]

Water formation on dust surfaces:

Cuppen et al. 2010
First detection of H$_2$O$_2$ in the interstellar medium with the APEX telescope, towards Oph A (Bergman, Parise, Liseau et al. 2011)
Water formation constrained in one particular environment

First detection of H\textsubscript{2}O\textsubscript{2} in the interstellar medium with the APEX telescope, towards Oph A (Bergman, Parise, Liseau et al. 2011)

Relevance to the chemistry of water.

Grain surface chemistry formation of water (Cuppen et al. 2010)
First detection of $\text{H}_2\text{O}_2$ in the interstellar medium with the APEX telescope, towards Oph A (Bergman, Parise, Liseau et al. 2011)

Relevance to the chemistry of water.

Astrochemical modeling of the abundance of $\text{H}_2\text{O}_2$, $\text{O}_2$, and other molecules predicted the abundance and detectability of a new molecule: $\text{HO}_2$ (Du, Parise & Bergman, 2012)

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Water formation constrained in one particular environment

First detection of H$_2$O$_2$ in the interstellar medium with the APEX telescope, towards Oph A (Bergman, Parise, Liseau et al. 2011)

Relevance to the chemistry of water.

Astrochemical modeling of the abundance of H$_2$O$_2$, O$_2$, and other molecules predicted the abundance and detectability of a new molecule: HO$_2$ (Du, Parise & Bergman, 2012)

First detection of HO$_2$ with the APEX and IRAM telescopes and validation of the prediction of the astrochemical model (Parise, Bergman & Du 2012)

In this environment (~20K), the O$_2$ route to water is dominant

Grain surface chemistry formation of water (Cuppen et al. 2010)
Follow-up search for H$_2$O$_2$ towards a sample of sources

Parise et al., Faraday Discussion 168, subm.

- Using the APEX telescope, search for H$_2$O$_2$ towards a sample of 10 sources, including low-mass protostars, IRDCs, massive YSOs, ...

- No detection obtained, with upper limits on H$_2$O$_2$ abundance (much) lower than abundance in Oph A

- Similarity with the O$_2$ search

- Oph A seems to be a unique example of a source where conditions are about right (~ 20-30 K) for the O$_2$ route to be dominant in the formation of water. This particularity may result from external heating by the “S1” source.

- The abundance of H$_2$O$_2$ may thus be used to constrain the physical conditions during the source evolution.

7 - 9 April 2014, Leiden, The Netherlands
Call for poster abstracts - deadline 27 January 2014
Other approach to constrain water formation: isotopic study

Measuring the deuterium fractionation of water

<table>
<thead>
<tr>
<th>Source</th>
<th>HDO/H₂O</th>
<th>HDCO/H₂CO</th>
<th>CH₂DOH/CH₃OH</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inner</td>
<td>outer (3σ)</td>
<td>–</td>
</tr>
<tr>
<td>IRAS2A</td>
<td>≥ 0.01</td>
<td>0.07 ± 0.11</td>
<td>0.17 ± 0.12</td>
</tr>
<tr>
<td>IRAS 16293</td>
<td>0.03</td>
<td>≤ 0.002</td>
<td>0.15 ± 0.07</td>
</tr>
<tr>
<td>Orion KL</td>
<td>0.02</td>
<td>0.14</td>
<td>0.04</td>
</tr>
</tbody>
</table>

- The deuterium content of water has been observed to be low compared to that of other molecules also formed on dust surfaces (e.g. CH₃OH) for over a decade now [e.g. Parise et al. 2005]

- The number of observational studies deriving HDO/H₂O has been booming with the Herschel Space Observatory, and all confirm the lower deuterium fractionation of water [e.g. Liu et al. 2011, Coutens et al. 2013]

- The HDO/H₂O directly measured in ices is also low (< 1%, Parise et al. 2003, Dartois et al. 2003)

- Apparent problem for astrochemical models, but new generation of models propose different explanations (Cazaux et al. 2011, Taquet et al. 2013, Du et al. in prep.)

- Add more observational constraints: search for OD
Search for OD in the ISM

Previous attempts:

- Allen et al. 1974 at 310 MHz towards Galactic Center
- OD recently detected towards comet C/2002 T7 (LINEAR) via coaddition of 30 lines of UV fluorescence spectrum (Hutsemekers et al. 2008) OD/OH ~ $3.5 \times 10^{-4}$, result of photodissociation of HDO and H$_2$O
- Our search: ground-state transition with SOFIA
Target: IRAS16293-2422, a low-mass protostar in the ρ Oph complex, where high levels of deuterium fractionation have been observed (up to the detection of CD$_3$OH, Parise et al. 2004)

OD ground state transition at 1391.5 GHz
Column density of OD?

<table>
<thead>
<tr>
<th>$T_{ex}$ (K)</th>
<th>$N_{OD}$ (cm$^{-2}$)</th>
<th>$N_{HDO}$ (cm$^{-2}$)</th>
<th>OD/HDO</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7</td>
<td>$(3.5 \pm 1.5) \times 10^{13}$</td>
<td>$(6.0 \pm 1.5) \times 10^{11}$</td>
<td>60 ± 30</td>
</tr>
<tr>
<td>5.0</td>
<td>$(5.0 \pm 2.0) \times 10^{13}$</td>
<td>$(1.2 \pm 0.3) \times 10^{12}$</td>
<td>45 ± 20</td>
</tr>
<tr>
<td>10.0</td>
<td>$(1.0 \pm 0.3) \times 10^{14}$</td>
<td>$(4.0 \pm 1.0) \times 10^{12}$</td>
<td>27 ± 10</td>
</tr>
</tbody>
</table>

OD/HDO ~ 17 - 90

<table>
<thead>
<tr>
<th>Molecular line</th>
<th>Fit type</th>
<th>$\int T_{mb} dv$ (K km s$^{-1}$)</th>
<th>FWHM (km s$^{-1}$)</th>
<th>$v_{lsr}$ (km s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HDO $1_{11} - 0_{00}$</td>
<td>two-Gauss</td>
<td>+4.4 ± 0.6</td>
<td>5.9 ± 1.0</td>
<td>4.5 ± 0.3</td>
</tr>
<tr>
<td>OD $5/2-3/2, -1+1$</td>
<td>one-Gauss</td>
<td>-4.1 ± 0.5</td>
<td>2.9 ± 0.3</td>
<td>-</td>
</tr>
<tr>
<td>OD $5/2-3/2, -1+1$</td>
<td>hfs</td>
<td>-</td>
<td>1.3 ± 0.6</td>
<td>4.2 ± 0.2</td>
</tr>
</tbody>
</table>
Preliminary astrochemical modelling

OH/H₂O ratio predicted by the model from Du, Parise & Bergman (2012)
More detailed astrochemical modelling including deuterium

OD/HDO >> OH/H$_2$O

because there are more fractionation routes for OH than for H$_2$O

(D + OH $\rightarrow$ OD + H)

Du et al. in prep
Perspectives

• Derive directly the OD/OH ratio observationally
  - Observation of $^{18}$OH with SOFIA (Cycle I proposal rated A, not observed)

• Observation of OD towards other star-forming regions (tracing other physical conditions and history)
  - OD detected towards SgrB2 (Parise et al. in prep)
    + Cycle I accepted SOFIA proposal by Menten et al.