Observations of cold water and ammonia vapor trace ice in planet-forming disks

Michiel Hogerheijde (Leiden Observatory)

Edwin A. Bergin, Christian Brinch, L. Ilsedore Cleeves, Jeffrey K. Fogel, Geoffrey A. Blake, José Cernicharo, Carsten Dominik, Dariusz C. Lis, Gary Melnick, David Neufeld, Olja Panić, John C. Pearson, Lars Kristensen, Umut A. Yıldız, Ewine F. van Dishoeck, Kees Dullemond, Simon Bruderer
What is the origin of water on Earth?

• In the early Solar System
  • water vapor in the inner Solar System ($T>100$ K)
  • condensed as ice on dust grains outside the snow line at $\sim 3$ AU (Hayashi et al. 1981; Abe et al. 2000)

• Comets and asteroids may have delivered large amounts of water from beyond the snow line to the early Earth (Matsui & Abe 1986; Morbidelli et al. 2000; Raymond et al. 2004)

• How large is the ice reservoir?
  • 1 ‘Earth Ocean’ = $1.5 \times 10^{24}$ g of water
What we know about H$_2$O in disks

- Freeze out in outer disk (> 3 AU)
- Evaporation in inner disk (<3 AU)
- Spitzer detection of hot water vapor from inner disks (Carr & Najita 2008; Salyk et al. 2008; Pontoppidan et al. 2010).

Molecular gas parameters and abundances derived for AA Tauri.

<table>
<thead>
<tr>
<th>Object</th>
<th>L$_K$ (mag)</th>
<th>K$_s$ (mag)</th>
<th>K$_H$ (mag)</th>
<th>H$_J$ (mag)</th>
<th>O$_3$ (K)</th>
<th>H$<em>2$O$</em>{\text{gas}}$ (K)</th>
<th>H$<em>2$O$</em>{\text{ice}}$ (K)</th>
<th>H$<em>2$O$</em>{\text{gas}}$/H$<em>2$O$</em>{\text{ice}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HR 1166</td>
<td>0.16</td>
<td>0.05</td>
<td>0.04</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>AA Tauri</td>
<td>0.09</td>
<td>0.02</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

The observed continuum-traction, and telluric correction using the IRAF packages. The wavelength calibration was performed on observations of absorption bands made with the Infrared. The wavelength calibration was performed on observations of absorption bands made with the Infrared.

Comparison of metric results are shown in Table 2. While our results for HV Tau C correspond to 14.0–10.25 in 68% confidence intervals, AA Tauri (squares) are also substantially higher than expected by the greater extinction at the shorter wavelengths.

If molecular cores are representative of the disk, the molecular emission lines we observed are consistent with the magnetorotational instability (MRI), which predicts low abundances for molecules such as H$_2$O.

The organic molecules were likely to probe only the upper disk atmosphere. Knowledge of the distribution of water (gas and ice) is important in setting the oxidation state of the gas, likely to be a sign of vertical mixing that carries molecular abundances into the protostellar disk.

The observed continuum-traction, and telluric correction using the IRAF packages. The wavelength calibration was performed on observations of absorption bands made with the Infrared.
Searching for cold water vapor with Herschel/HIFI

Total observing time: ~180 hrs (!)
Targets: TW Hya, DM Tau, LkCa15, MWC480, HD100546, AA Tau, HD163296
Detections and non-detections

Also non-detections for LkCa15 and MWC480.

(Bergin et al. 2010; Hogerheijde et al. 2011; Hogerheijde et al. in prep.)

“Ice and Planet Formation” – Lund, May 15–17 2013
A model for TW Hya

- $M_{\text{star}} = 0.6 \, M_{\odot}$; spectral type K7V; $L_{\text{star}} = 0.23 \, L_{\odot}$ (Webb et al. 1999)
- Distance 53.7±6.2 pc (van Leeuwen et al. 2007)
- $R_{\text{disk}} = 196$ AU; $i = 7^\circ$: nearly face-on
- Fiducial disk structure model: Thi et al. (2010)
  - $M_{\text{dust}} = 1.9 \times 10^{-4} \, M_{\odot} \rightarrow M_{\text{gas}} = 1.9 \times 10^{-2} \, M_{\odot}$
  - (Gorti et al. 2011, Bergin et al. 2012)

- Temperature from stellar irradiation (RADMC; Dullemond & Dominik 2004)
- UV radiative transfer into disk and resulting chemistry (Fogel et al. 2010)
- Water excitation and line formation (LIME; Brinch & Hogerheijde 2010)

(Thi et al. 2004)
This over produces the emission by factor 3–5

- Remove 88% of ice from UV-affected layers
- Settling of larger, icy grains relative to the small grains which dominate the UV absorption
- Only 12% of original ice content remains in upper disk
  - Gives rise to 0.005 Earth Oceans of water vapor
- Underlying ice reservoir of at least several thousands of Earth Oceans
  - Key assumption: elemental oxygen efficiently forms water on grains
A low $\text{H}_2\text{O}$ ortho/para in TW Hya

- Observations yield $\text{OPR}=0.77\pm0.07$

- $\text{H}_2\text{O}$ OPR in TW Hya’s disk $\ll$ Solar System comets (1.5–3): long range mixing?

Figure 10. Ortho-para ratios and nuclear spin temperatures for $\text{H}_2\text{O}$ and $\text{NH}_3$ in comets.

A. (upper left) OPR for $\text{H}_2\text{O}$ (Bonev et al. 2007, Dello Russo et al. 2007; Woodward et al. 2007; Bonev et al. 2008). The measured values are placed on a theoretical curve that connects them to the corresponding nuclear spin temperature (Mumma et al. 1987).

B. (upper right) The 6.5 $\mu m$ $\text{H}_2\text{O}$ band in C/2003 K4, both fully resolved and also convolved to the resolution of Spitzer (Woodward et al. 2007). Ortho and para lines are indicated.

C. (lower left) Ortho-para ratios and spin temperatures for $\text{NH}_3$ and $\text{H}_2\text{O}$ in eight comets ($\text{H}_2\text{O}$ from references cited in panel ‘A’, $\text{NH}_3$ measurements from Shinnaka et al. 2011).

D. (lower right) A comparison of $T_{\text{spin}}$ for $\text{NH}_3$ and $\text{H}_2\text{O}$ in the eight comets of Fig. 9C. The spin temperatures for these primary volatiles agree within a given comet. Six Oort Cloud comets show relaxed spin temperatures near 29K. However, ortho-para ratios in two fragments of a Jupiter family comet (73P/SW 3) are consistent with statistical equilibrium (left). The lower bounds to their spin temperatures are shown as 95% confidence limits (right). Similar measurements are beginning to emerge for methane. The spin temperature measured for $\text{CH}_4$ in C/2001 Q4 (33K $\pm$ 2) agrees with that found for $\text{NH}_3$ and $\text{H}_2\text{O}$ in that comet (Kawakita et al. 2006).

Bonev et al. 2007; Mumma & Charnley (2011)
**NH$_3$/H$_2$O in TW Hya**

- Line strength of NH$_3$ consistent with NH$_3$/H$_2$O $\sim 4\%$
- Comparable to Solar System comets and low-mass protostellar cores
- Released when water photodesorbs
An alternative model for TW Hya

• CAVEAT: An alternative model for TW Hya
• Andrews et al. 2011: millimeter-sized grains have drifted inward to <60 AU in TW Hya’s disk
• H₂O line width suggests that emission originates from radii up to ~115 AU
• Smaller emitting area ➔ larger beam dilution ➔ weaker lines ➔ no settling of icy grains needed (but radial drift necessary)
• This *may* make the lines optically thick ➔ o/p can no longer be derived (to be confirmed)
HD 100546: H$_2$O but no NH$_3$

- Line profile suggests emission from $\sim$70 to $\sim$300 AU
- Line strength suggests photodesorbed water is *not* present
- May explain lack of NH$_3$
- All water from $T>200$ K gas-phase chemistry in disk surface
- Where is the water inside $\sim$70 AU?
Conclusions and further work

- Ground-state transitions of water trace the ices via photodesorption in TW Hya
- Vertical settling (or radial drift?)
- o/p << comets (to be confirmed)
- Non-detection to other disks ~consistent with settling/drift
- HD 100546 appears dominated by water formed in warm surface layer, and photodesorption needs to be suppressed strongly.
- A different story for every disk?
- Diversity of location & evolution of icy grains