Cold water and ammonia vapor in protoplanetary disks

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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 ~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

**Theory**

- Equilibrium between photodesorption and dissociation in outer disk (Dominik et al. 2005):
  \[ \text{H}_2\text{O}_{\text{gas}} \sim \text{fraction} \times \text{H}_2\text{O}_{\text{ice}} \]

- Freeze out in outer disk (> 3 AU)

- Evaporation in inner disk (<3 AU)

**Observations**

- Spitzer detection of hot water vapor from inner disks (Carr & Najita 2008; Salyk et al. 2008; Pontoppidan et al. 2010).

- Subaru detection of 3μm water ice absorption (Terada et al. 2007)

See also Honda et al. (2009)
Herschel/HIFI: Cold water vapor in TW Hya

Total observing time: 6.6 hrs on o-H$_2$O and 14 hrs on p-H$_2$O (!)

Hogerheijde, Bergin, et al. (2011)
Disk origin of the H$_2$O emission

- $M_{\text{star}}$=0.6 M$_\odot$ (Webb et al. 1999)
- Distance 53.7±6.2 pc (Akeson et al. 2011)
- $R_{\text{disk}}$=196 AU; $i$=7°: nearly face-on
- Narrow line width confirms H$_2$O emission extends out to >115 AU

\[\text{(Hughes et al. (2011))}\]

\[\text{(Thi et al. 2004)}\]

\[\text{TW Hya H$_2$O $1_{10}-1_{01}$ Herschel/HIFI}\]

\[\text{CO 3–2 (JCMT, scaled)}\]
TW Hya’s disk

- $R_{\text{disk}}=196$ AU; $i=7^\circ$: nearly face-on
- Millimeter-sized dust grains confined to $<60$ AU (Andrews et al. 2011)
- $M_{\text{disk}}=2-6 \times 10^{-4}$ $M_\odot$ in dust
- $M_{\text{disk}}=5 \times 10^{-4} ... 5 \times 10^{-2}$ $M_\odot$ in gas
- (Calvet et al. 2002; Thi et al. 2010; Hughes et al. 2011)
Our model approach

• Starting point: Thi et al. (2010)
  
  • $M_{\text{dust}} = 1.9 \times 10^{-4} \, M_\odot$
  
  • $\rightarrow M_{\text{gas}} = 1.9 \times 10^{-2} \, M_\odot$

• $R_{\text{out}} = 196 \, \text{AU}$, $R_{\text{in}} = 4 \, \text{AU}$ (neglect inner disk)

• Vertical exponential scale height

• *Temperature structure* calculated from stellar irradiation (RADMC; Dullemond & Dominik 2004)

• Calculate radiative transfer of UV into disk, and calculate *resulting chemistry* (Fogel et al. 2010)

• Calculate resulting *water excitation and line formation* (LIME; Brinch & Hogerheijde 2010)
How much water?

- Ice reservoir: 6300 Earth Oceans
- Water vapor content: 0.04 Earth Oceans

This overestimates the line intensities by factors 3.3–5.3
Differential settling of icy grains

- 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 ice remains in upper disk
  - Gives rise to 0.005 Earth Oceans of water vapor
  - Underlying ice reservoir unchanged: > thousands of Earth Oceans
  - key assumption: elemental oxygen efficiently forms water on grains

![Diagram of differential settling of icy grains](image)
Lines yield H$_2$O ortho/para

- Lines are optically thin
  - ...because only 12% of water vapor remains compared to standard model
  - ...because sub-thermal excitation leads to resonant scattering rather than absorption of line photons

- Ratio of H$_2$O $1_{10}-1_{01}/1_{11}-0_{00} \propto$ ortho-to-para ratio (OPR)

- Observations yield OPR=0.77±0.07
A low H$_2$O ortho/para in TW Hya

- H$_2$O OPR in TW Hya’s disk of 0.77 $\ll$ Solar System comets (1.5–3)

![Graph showing ortho-para ratio versus H$_2$O spin temperature](image)

Bonev et al. 2007; Mumma & Charnley (2011)
Long-range mixing of volatiles

- TW Hya OPR=0.77 ⇔ $T_{\text{spin}}=13.5$ K
- Comets OPR>1.5 ⇔ $T_{\text{spin}}>20$ K
- No radiative conversion of OPR in gas phase
- Thermal evaporation preserves OPR (➞ comets)
  - Equate $T_{\text{spin}}$ with $T_{\text{grain}}$ at ice formation (?)
- Photodesorption may preserve OPR (➞ TW Hya observations)
  - ...or drive OPR to unity, implying even lower OPR for the ice (e.g., Andersson et al. 2008; Arasa et al. 2010)
- Range of cometary OPR: heterogeneous mixture of ices from small (>50 K) and large (<15 K) radii (just like refractory component; Sandford et al. 2006)
- Long-range mixing of volatiles in the Solar Nebula
More results: cold NH₃

- In the same observation as o-H₂O, HIFI also detected emission from the groundstate transition of ortho-NH₃.
  - Line strength can be reproduced by a 3% NH₃/H₂O mixing ratio, assuming NH₃ also is released through photodesorption.
  - Comparable to ice measurements (2%–15%; e.g., Bottinelli et al. 2010) and Solar System comets (0.3–2%; e.g., Mumma & Charnley 2011).
  - Alternatively, if gas-phase chemistry forms NH₃ at a similar abundance as N₂H⁺, the emission can also be explained.
More, even deeper searches for cold water vapor

• OT1 and OT2 program to search for groundstate emission of o-H$_2$O and p-H$_2$O to HD100546, AA Tau, and DM Tau
  
  • Total integration time ~140 hrs for all three sources and both lines (!)

• Early modeling results suggest that cold water vapor in HD100546 and AA Tau is just as scarce as in TW Hya.
Summary

- We have detected emission from cold water vapor from the full extent of the planet-forming disk around TW Hya.

- The line intensities hint at a ‘hidden’ reservoir of at least several thousands of Earth Oceans of ice in the disk.

- The low ortho-to-para ratio of the water vapor in TW Hya compared to Solar System comets suggest long-range mixing of volatiles in the Solar Nebula.

- Ammonia is present in the disk of TW Hya at a mixing ratio w.r.t. to water of ~3%.

- Cold water vapor is also detected in HD100546 but not in AA Tau.

- Stay tuned...!