Resolving water vapor in planet-forming disks

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Abstract

Water plays an important role in the formation of planetary systems. Where the protoplanetary disk is sufficiently cold, water freezes out onto dust grains, increasing the prospects of giant-planet formation outside this *snow line*. In those regions that are warm enough for water vapor to persist, the inner several AU of the disk and the exposed disk surface further out, water emission lines offer powerful probes of the conditions in the disk. And the presence of water, either as a vapor, an ice, or locked up in hydrous minerals, offers clues to the origin of terrestrial oceans. Essentially blocked out by the Earth's atmosphere, thermal emission lines of water require space-based instruments to be detected. A large and sensitive single-aperture instrument can detect water emission lines at far-infrared wavelengths (50–500 μ m) in many disks; and spatially resolved imaging requires a far-infrared interferometer array operating at these same wavelengths.

1. Water in planet-forming disks

Measurements with the SWAS satellite (e.g, Bergin et al. 2000) have shown that water is an interstellar chameleon. On the one hand, in warm (>200 K) regions of interstellar molecular clouds its abundance relative to H₂ can rise $\sim 10^{-4}$ when all oxygen is driven into water by gas-phase reactions. On the other hand, in dense regions colder than ~ 90 K, water rapidly freezes out onto dust grains and its abundance drops by four orders of magnitude or more.

The conditions in the disks that surrounds newly formed stars – the likely birth sites of future planetary systems – run through an even more extreme range of temperatures and densities than can be found in interstellar clouds. From the dense and cold mid-planes, temperatures rise and densities drop with increasing height in these flared disks. With decreasing distance to the central star, temperature also increases from $\sim 10-20$ K at a few hundred AU to hundreds of K with 1 AU. The ultraviolet and X-ray radiation from the young star or from neighboring young stars also strongly affects the chemistry of the disk gas, evaporating or desorbing molecules from the ice mantles of dust grains into the gas phase, but also dissociating many species.

These complex environments in protoplanetary disks suggest that water is likely to be present at abundances that show a similar large range in relative abundance (four orders of magnitude or more) within each disk as encountered throughout the interstellar medium of the Galaxy. Detecting and studying the spectral lines of water in these disks therefore is likely to provide us significant insight into the conditions in the disk.

Furthermore, the presence of water in itself is highly relevant for the formation of planetary systems. A favored theory for the formation of gas-giant planets involves the presence of water ice

on dust particles: as planetesimals grow, the increased weight of the solids with their water ice content adds sufficient gravity to capture a large molecular hydrogen envelope (Hayashi 1981). Closer to the star, where temperatures are higher and water is expected to be in the gas phase, the reduced gravitational pull allows only smaller, rocky planets to form. However, in these regions (~1 AU) the presence of water lays a crucial role in the possible formation of oceans of terrestrial planets, either through direct accretion, or, perhaps more likely, through the later bombardment with comets (Raymond et al. 2004). The latter consist for a large fraction of water ice, and their location of origin can be investigated through present-day cometary appearance in the Solar System (Festou, Keller, & Weaver 2004). Directly observing the water content of disks on 1 AU scales will provide the necessary corroboration of such hypotheses. Alternatively, or, more likely, in addition, terrestrial oceans may originate from the impact of planetesimals containing hydrous minerals.

There is an additional aspect why resolving the spectral lines of water with high velocity and angular resolution is important. Naively, one expects water to be largely frozen out throughout most of the disk, except for regions of a couple of hundred of K where the H₂O abundance is expected to be large. However, theories of planet formation suggest that when planetary cores form, their gravitational pull can open gaps in the disk or excite spiral waves (e.g., Lin et al. 2000). These features may have a profound effect on the water gas-phase abundance, leaving an imprint also on the shape of any spectral lines, and would directly pinpoint the location of active planet formation.

2. Observations to-date and in the near future

So far, water has not been detected in disks in the environments discussed above: the relatively cool (tens to hundreds of K) regions making up the bulk of the planet-forming zones. The low-excitation thermal lines one expects from these regions are effectively blocked by the Earth's atmosphere, while sensitive space-based missions have not yet commenced. Water *has* been detected in disks, but in regions very close to the young star, where abundant *hot* water vapor resides and is observable through mid-infrared lines observed with the Spitzer Space Telescope (Carr & Najita 2008). This shows that water is present in disks, but does not address its abundance, state (frozen or gaseous), or role in the planet-forming zone.

The launch of the Herschel Space Observatory, foreseen for April 2009, will alter this situation. Two instruments on board Herschel will be able to access the thermal water lines in the farinfrared: the PACS instrument will be able to detect many water lines throughout the FIR, albeit at limited spectral resolution. The HIFI instrument will cover a more limited wavelength range, but provide excellent spectral resolution (of the order of a fraction of a km s⁻¹, the expected width of these lines). Several approved key programs will capitalize on these capabilities. The program 'Water in Star-Forming Regions with Herschel' (WISH) will, among other goals, survey a welldefined sample of a dozen or so disks, searching for the two ground state-lines of ortho-, respectively, para-H₂O with HIFI. Their aim is to detect, spectrally resolve, and characterize the water emission from these disks. The program 'Dust, Ice, and Gas In Time' (DIGIT) will obtains PACS scans of a large sample of disks. While these observations will not resolve the lines spectrally (or spatially), they will provide essential insight into the presence of strong lines of water and of other species, such as oxygen and carbon. Finally, the program 'Gas in Protoplanetary Systems' (GASPS) focusses on oxygen and carbon lines of disks, probing the major atomic gas constituents and cooling lines. Taking into account the beam size of Herschel, none of these observations will spatially resolve the disk emission.

Although water is difficult to observe from the ground, the Atacama Large Millimeter / Submillimeter Array (ALMA) will be equipped with a number of receivers covering the 183 GHz (1.6 mm; 3_{13} - 2_{20}) transition of water. Under good observing conditions, and using appropriate Doppler-shifts due to the Earth's orbit, this line can be detected from Galactic sources on the shoulder of the atmospheric absorption zone (e.g., Cernicharo et al. 1990); similarly, isotopic lines of species like H₂¹⁸O can be (and have been successfully) attempted from the ground under favorable conditions (Phillips et al. 1978; Jacq et al. 1988). Unlike the space-based observations sketched above, ALMA will be able to resolve the emission toward typical disks in nearby starforming regions. However, the capabilities will be somewhat limited by the Earth's atmosphere and only a single line will be available, limiting the diagnostic power. Furthermore, the 3_{13} - 2_{20} line can be inverted, leading to maser emission which, although strong, is more difficult to interpret quantitatively.

3. Resolving water in disks

With Herschel about to be launched and ALMA coming on-line in the next few years, there is great hope that luke-warm water (as opposed to hot water vapor) in protoplanetary disks will be detected toward several objects by the early years of the next decade. Only ALMA observations of the 183 GHz line have the capability of resolving the disks, but this line is difficult to interpret quantitatively. The Herschel observations will be unresolved, and the size of the Herschel beam at the frequency of the water ground-state lines is in fact so large (30 arcsec) that the emission of the disks, several arcsec in size, will suffer from severe beam dilution. Signal strengths of several mK only are predicted (see below), and only lengthy (multiple hours) integrations will yield detections. Obviously, this is only feasible for a small number of well chosen targets.

Two clear ways forward present themselves, which will allow further study of the water emission from disks. First, a large cooled single-dish far-infrared telescope in space can detect the water lines with more favorable beam coupling and higher sensitivity than Herschel. This would greatly increase the accessible source sample. Note that lines above 1 THz suffer from continuum opacity, unless the lines originate from above the dust disk photosphere. In the former case, absorption against the disk's dust continuum may be detectable in higher excitation lines; in the latter case, bright emission lines from hot gas in the surface of the disk may be present.

To spatially resolve the lines, and directly access the inner several tens of AU where the bulk of the lukewarm H_2O gas is expected to reside, and where planet-formation is expected to occur, requires either a very large single-dish (unfeasible) or an interferometer. Within the small beam that such an instrument would provide, the limited collecting area and therefore sensitivity, is not foreseen to be a limitation. The brightness temperature is sufficiently high to be detected, as the

example in the next section shows. Table 1 summarizes some of the typical wavelengths, line strengths, and line widths that instruments should cover in order to successfully exploit water.

| Table 1. Requirements to exploit far-infrared observations of planet-forming disks | | |
|--|---|----------------------|
| Capability | Science Driver | Specification |
| Wavelength coverage | H ₂ O lines | 100–538 μm |
| | O, C, C ⁺ lines | 63–609 μm |
| | Solid-state features | 62–150 μm |
| Sensitivity | Conservative estimate of H ₂ O line strength in 100 mas beam (section 4) | 10 K |
| Spectral resolution | H ₂ O line widths | 1 km s ⁻¹ |
| | Solid-state features | 1 μm |
| Spatial resolution | To couple a single-dish to a typical disk at 140 pc | few arcsec |
| | To spatially resolve emission region | 20 mas |

4. Case study: Imaging low-excitation water lines from a typical T Tauri disk

All these aspects mentioned above make for a strong case for high spectral and angular resolution observations of water lines. What kind of line strengths could be expected? Obviously, too little is known at the moment to make accurate predictions. But a simple *baseline* model can be constructed starting with a disk model that fits the average disk in the Taurus star forming region (d'Alessio et al. 1998). In this model, the water abundance is set to 2×10^{-4} with respect to H₂ in those regions where the gas temperature exceeds 200 K; it is set to 0 whenever T_{kin} <90 K mimicking total freeze out; and is set to an 'intermediate' value of 10^{-8} ('high') or 10^{-10} ('low') in between. The disk is then placed at a typical distance of 140 pc (~Taurus) and the statistical equilibrium excitation and line formation calculated, using the code of Hogerheijde & van der Tak (2000). The resulting emission is convolved in beams of 1" (140 AU), 100 mas (14 AU), and 20 mas (3 AU) diameter.

The results show that the strongest lines are found among the lowest transitions (e.g., $1_{10}-1_{01}$ at 538 µm, $2_{12}-1_{01}$ at 180 µm, and $1_{11}-0_{00}$ at 269 µm). Typically, these lines are several mK in the 30" Herschel beam. In a 1" beam they will be several K. In a 100 mas beam, which will start to resolve the emission they will be tens of K. Even smaller beams, for example 20 mas, will not see any brighter emission: instead they resolve the emission over multiple pixels. The emission is also not very strongly dependent on the adopted abundance in the 'intermediate' regions ('low'

or 'high'). This indicates that the emission in these small beams is dominated by the >200 K gas where the water abundance is high, and probably also that the emission is quite optically thick. The latter matches the maximum line intensities of a ~hundred K. This means that the beam-convolved intensity depends on the relative size of the optically thick region in the beam and not on the column density.

It should be stressed that the above results are strictly for the *baseline* model that does not include any effects of gaps, spiral arms, shocks, or processes induced by the ultraviolet radiation that may penetrate the disk. For example, recent results by Ceccarelli et al. (2005) and Dominik et al. (2005) suggest that increased photodesorption may increase the water gas-phase abundance on even weak radiation fields. Any regions of enhanced density or temperature due to shocks or gaps on ~1 AU scales (the highly interesting terrestrial planet formation zone), and the resulting increased water gas-phase abundance, would of course significantly increase the line strength in 10–20 mas beams. Recent work by Meijerink et al. (2008) strongly suggests that significant emission from water emission lines will be present.

5. Supporting theoretical work

Simply detecting and imaging the H₂O emission is a goal in itself, but only reached its diagnostic potential when coupled to a sound understanding of the water chemistry, the disk structure, and the line formation mechanisms. Therefore, supporting work is necessary to profit from any such observations. This work is already ongoing, and yield results well before the middle of the coming decade.

Much work has already been done on the theoretical understanding of the structure of protoplanetary disks (see, e.g., the overview by Dullemond et al. 2008). This includes both accretion processes, which determine the mass distribution in the disk, as well as the heating and cooling balance (dominated by infrared continuum radiation, with important contributions from ultraviolet and X-ray energy input by the star) which determines the temperature distribution in the disk and the resulting vertical thickness of the disk through hydrostatic equilibrium. The disk's spectral energy distribution (SED) from near- to far-infrared wavelengths reflects the disk's structure, and has been used, together with resolved images of the disks millimeter emission and the scattered light images, to constrain such models.

The temperature structure and any external ultraviolet or X-ray field further determines what the chemical structure of the disk will be (e.g., van Zadelhoff et al. 2003; Meijerink et al. 2008). In cold and dense regions, most molecules and also water will freeze out on dust grains, while regions exposed to ultraviolet radiation will have their gas photodissociated or -ionized. Extensive models for this already exist, although still critically depend on the amount of vertical and radial mixing (turbulence) that occurs in the disk (e.g., Semenov et al. 2006; Aikawa 2007). So far, such models have been able to explain the large fractional depletion (freeze out) of molecules inferred for many disks, but detailed abundances cannot yet be interpreted.

Once the disk structure and chemical composition is known theoretically, the observation of water emission lines (and their spectral line profiles) can be interpreted quantitatively if accurate molecular collision rates, molecular excitation codes, and line formation tools are available. Good collision rates are available for water, although they often only go up to rotational *J* levels of 10 (and energies of 2000 K). In addition, effects like the different efficiencies of collisions with ortho- and para-H₂ respectively need to be taken into account, as well as collisions with electrons in those regions with large fractional ionization. Codes to solve the molecular excitation and line formation are now becoming available for complex three-dimensional structures (e.g., Brinch 2008).

The final step required for a fruitful program is the identification of suitable targets. The population of relatively nearby young stars with planet-forming disks is starting to be well characterized through observations from Spitzer. In the future Herschel will add significantly to this, while ALMA observations will increase the sample size of objects studied in detailed in molecular tracers (but not water); at the moment, interferometers like the IRAM Plateau de Bure Interferometer, the Combined Array for Research in Millimeter Astronomy, and the Submillimeter Array are not sensitive enough to allow for more than a piecemeal approach.

The developments above are currently in full swing, and well before the middle of the 2010–2020 time frame, all supporting work to quantitatively interpret resolved water-line observations from disks should be well in place.

6. Other species: atomic gas, hydrides, ices and hydrous minerals

Sensitive far-infrared space-based platforms have a usefulness for protoplanetary disk research far beyond just water lines (where single-dishes provide very sensitive observations but of limited spatial resolution and interferometers high spatial resolution imaging of the brighter features).

In the same wavelength range, important lines of atoms like oxygen ([O I] ${}^{3}P_{1}-{}^{3}P_{2}$ at 63 µm and [O I] ${}^{3}P_{0}-{}^{3}P_{1}$ at 145 µm) and carbon ([C I] ${}^{3}P_{1}-{}^{3}P_{0}$ at 609 µm and ${}^{3}P_{2}-{}^{3}P_{1}$ at 370 µm), as well as ionized carbon ([C II] ${}^{2}P_{3/2}-{}^{2}P_{1/2}$ at 157 µm), are accessible. These species trace the warmest regions of the disk, material photodissociated or -ionized by the central star or neighboring stars. They are unique probes of the gas that may be destined to leave the protoplanetary system (see, e.g., Kamp et al. 2005).

Hydrides also have lines in this wavelength range, and they uniquely probe the chemical species related to water – only by looking at the full chemical network can the true place and role of water be understood.

Finally, the far-infrared regions, just like the rest of the infrared, is rich in mineralogical features. Some of these are due to hydrous minerals (e.g., features due to hydrosilicates in the $80-110 \mu m$ range, but also carbonates at 92 and 62 μm which may have formed in the presence of liquid wa-

ter) and ices (e.g., around 62 μ m for water and 85 and 150 μ m for CO₂), the two other 'hideouts' of water and possible sources of water to be delivered to terrestrial planets.

Sensitive and spatially resolved observations in the far-infrared will open a treasure trove of probes of the protoplanetary environment.

7. Summary

This document briefly describes the great potential for discovery offered by sensitive, spatially resolved far-infrared observations in the area of protoplanetary disks. This wavelengths range is rich in tracers that address important questions about the structure and composition of disks, the potential role of water (and the location of the snowline) in the planet formation process, and the origin(s) of oceans on future terrestrial planets. All these together provide the essential framework to pose the question: what are the initial conditions for the formation of earthlike planets and the origin of life?

References

Aikawa, Y. 2007, ApJL, 656, L93 Bergin, E. A., et al. 2000, ApJL, 539, L129 Brinch, C. 2008, PhD Thesis, Leiden University Carr, J. S., & Najita, J. R. 2008, Science, 319, 1504 Cernicharo, J., Thum, C., Hein, H., John, D., Garcia, P., & Mattioco, F. 1990, A&A, 231, L15 Ceccarelli, C., Dominik, C., Caux, E., Lefloch, B., & Caselli, P. 2005, ApJL, 631, L81 D'Alessio, P., Canto, J., Calvet, N., & Lizano, S. 1998, ApJ, 500, 411 Dominik, C., Ceccarelli, C., Hollenbach, D., & Kaufman, M. 2005, ApJL, 635, L85 Dullemond, C., Pavlyuchenkov, Y., Apai, D., & Pontoppidan, K. 2008, Journal of Physics Conference Series, 131, 012018 Festou, M. C., Keller, H. U., & Weaver, H. A. 2004, Comets II (University of Arizona Press, Tucson) Hayashi, C. 1981, Proc. IAU Symp. Fundamental Problems in the Theory of Stellar Evolution, 93, 113 Hogerheijde, M.R., & van der Tak, F. F. S. 2000, A&A, 362, 697 Jacq, T., Henkel, C., Walmsley, C. M., Jewell, P. R., & Baudry, A. 1988, A&A, 199, L5 Kamp, I., Emilio Enriquez, J., & Hogerheijde, M. 2005, Proc. Nearby Resolved Debris Disks, 14 (STScI) Lin, D. N. C., Papaloizou, J. C. B., Terquem, C., Bryden, G., & Ida, S. 2000, Protostars and Planets IV, 1111 Meijerink, R., Poelman, D. R., Spaans, M., Tielens, A. G. G. M., & Glassgold, A. E. 2008, ApJL, 689, L57 Phillips, T.G., Scoville, N. Z., Kwan, J., Huggins, P. J., & Wannier, P. G. 1978, ApJL, 222, L59 Raymond et al. 2004, Icarus 168, 1 Semenov, D., Wiebe, D., & Henning, T. 2006, ApJL, 647, L57 van Zadelhoff, G.-J., Aikawa, Y., Hogerheijde, M. R., & van Dishoeck, E. F. 2003, A&A, 397, 789