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Observations of planet-forming volatiles

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Abstract. Water is observed to be a major constituent of planet-forming disks around young stars and its presence likely plays a major role in formation of planets and their atmospheres, including those destined to orbit in a habitable zone. Yet, the path from disks to planets is one fraught with complexity, making it difficult to derive precise theoretical predictions for planetary chemistry. Planet-forming disks are no longer considered uniform well-mixed structures; rather, they are complex worlds with many different heterogenous environments, most of which play some part in determining the composition of planetesimals and planets. Direct observations of atomic and molecular abundances on all size scales are therefore needed for understanding planet formation at a very fundamental level, and for answering the question of how chemically common the Earth is among exoplanets. In the past years, great progress has been made in observing protoplanetary chemistry, in particular in measuring the molecular composition in protoplanetary disks across the planet-forming regions from 1 to 10s of AU. We will present recent observations of water with Herschel, the VLT and Gemini in disks, and we will demonstrate how we retrieve the local abundances and radial distribution of water vapor and ice using detailed radiative transfer models. We find that most of the oxygen is likely bound in water near 1 AU in disks around solar-mass stars and that the disk surface composition at these radii is likely dominated by local gas-phase chemistry rather than by primordial material delivered from the interstellar medium. We discuss how these observations relate to complementary constraints from the solar system. We further discuss the implications for the observed composition of exoplanetary atmospheres.

Keywords. planetary systems: protoplanetary disks, planetary systems: formation, ISM: molecules

1. Introduction

Volatile molecular species play a central role in the formation of planets, both in terms of their composition, their final mass, and the rate by which they form. In their solid form, they are known as *ices*, and prominently include water, but also other abundant, simple molecules such as carbon monoxide, carbon dioxide, methane, ammonia and methanol. It is thought that their combined mass is similar to, or even dominates that of the refractory species – silicates and other minerals – as well as refractory carbon, by factors of 2–4 (Lodders 2003, Dodson-Robinson *et al.* 2009). In the solar system, the bulk composition of the outer planets, the Kuiper belt population and comets generally indicate that the ice/rock ratio was at least unity in the solar nebula, beyond the snowline. The presence of a large reservoir of volatile molecules affect the process of planet formation in many ways, and likely lead to the dichotomy between the rapid formation of giant planets through core accretion beyond the snow line and the slower formation of terrestrial planets inside the snow line.

However, unambiguous measurements of the composition and mass of bulk volatiles in protoplanetary disks, and in exoplanetary systems, are still very limited. To ascertain whether volatiles and ices play an important role in the formation of exoplanets, it is critical to observe them during the process of planet formation. While the importance of ices in the Solar Nebula has been recognized for decades, systematic observations of them in planet-forming regions around present-day young stars have only been underway in the few years (Pontoppidan & Blevins 2014).

2. The importance of ices for planet formation

Volatiles have their greatest impact for the formation of planets as ice. In the gas phase, they only contribute a fraction of a percent to the initial gas mass. In the classical core accretion scenario by Pollack *et al.* (1996), a difference in solid mass available for the formation of cores of a factor of a few can lead to differences in the time scale for giant planet formation of up to a factor 30. Given the short lifetimes of gas-rich protoplanetary disks, the presence of a large mass reservoir of ice may directly lead to the formation of giant planets beyond a few AU. However, static models of core accretion, which do not include advection (radial dynamical migration) of solids, fail to reproduce the complete architecture of the solar system (Levison *et al.* 2010). Recently, more quantitative models have reinforced the importance of ices for planet formation, albeit by invoking different mechanisms. In the "pebble-accretion" model of Lambrechts & Johansen (2012), giant planet cores grow by accreting small objects (cm-sized icy pebbles), which drift through their orbits by gas-pressure-driven migration. Since such pebble migration is strongly size-dependent, it becomes much less efficient inside the snow line as the pebbles break up due to the evaporation of their ices (Morbidelli *et al.* 2015). Further, the loss of ice leads to a decrease in their fragmentation velocity (Banzatti *et al.* 2015), which also acts to further decrease the ability of the solids to grow planetary cores inside of the snow line, leading to the preferred formation of stunted Mars-sized planetary embryos.

3. Observational tracers of protoplanetary volatiles

While the theoretical expectation is that protoplanetary disks contain large amounts of volatiles, either as ices beyond the snow line, or in the gas-phase inside the snow line, and in their warm surfaces, observing and characterizing them requires special techniques. The gas temperatures in the planet-forming regions of disks are similar to the $\sim$300 K of our own atmosphere, and many of the most common disk volatiles are also abundant on the Earth. As a consequence, strong telluric absorption due to gas-phase volatiles in the atmosphere generally precludes, or greatly complicates, ground-based observations of the most common disk volatiles, even though the disks may produce strong intrinsic line signatures. Common examples of such species include water and CO_2, with the former being observable from the ground from hot gas with temperatures $\gtrsim 1000$ K, while the latter cannot be observed from the ground under any known circumstance.

With a combination of ground- and space-based observations across the infrared to millimeter spectral range, we have recently dramatically improved our knowledge and understanding of planet-forming volatiles from an observational perspective. Figure 1 summarizes the observations, and illustrates how the *combination* of multi-wavelength spectroscopic observations now reveal aspects of the volatile composition at all disk radii. Mid-infrared spectroscopy reveals the composition and structure of the terrestrial planet-forming regions at $\sim$1 AU, far-infrared spectroscopy roughly traces the giant planet-formation region at a few AU, while submillimeter spectro-imaging traces the ice-giant and cometary region of disks beyond 10 AU.

4. Discussion

Using and combining multiwavelength observations of volatiles in disks have led to a number of recent findings: 1) Observations generally confirm that gas-phase emission lines

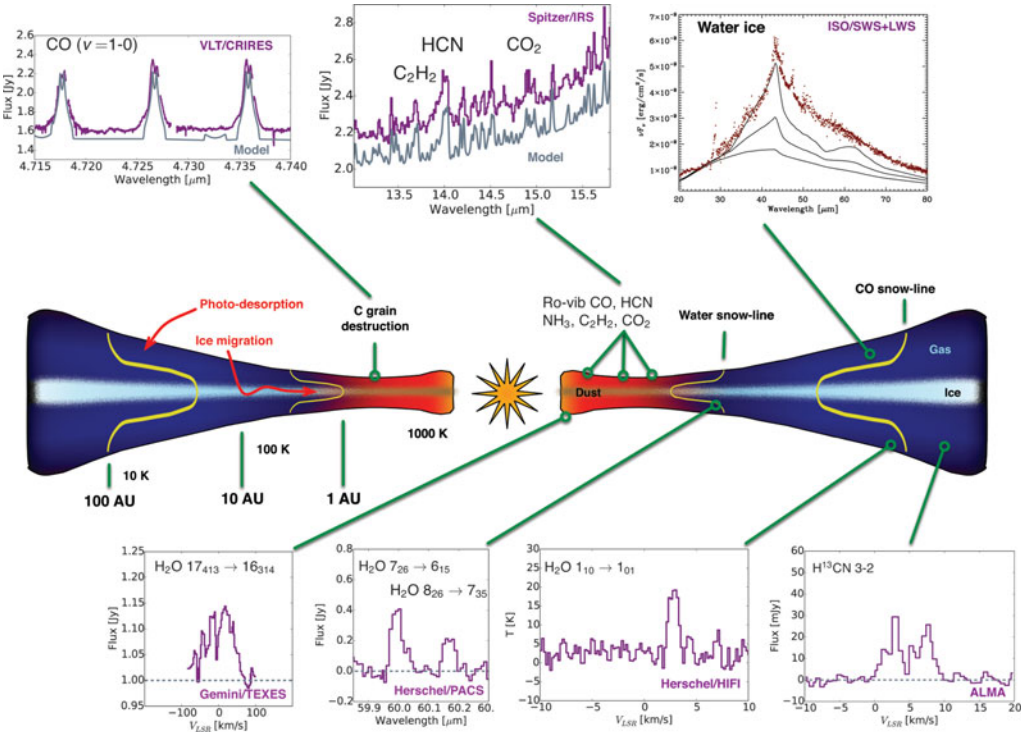

Figure 1. The disk regions traced by different volatile lines and bands. From inside-out, CO ro-vibrational lines trace the 0.1-1.0 AU region (Banzatti & Pontoppidan 2015), as mid-infrared lines from water, HCN, C_2H_2 and CO_2, as observed by Spitzer (Carr & Najita 2008). The hottest rotational water lines are observable from the ground at high resolution with VLT/VISIR and Gemini/TEXES (Pontoppidan *et al.* 2010, Salyk *et al.* 2015). Water vapor out the the snow line is traced by far-infrared lines, here illustrated by lines near 60 μm, as observed with Herschel/PACS. Beyond the snow line, cold water vapor, retained by non-thermal desorption processes, is traced by the strong ground-state lines at 269.5 and 538.7 μm. Bulk water ice is traced by its strong far-infrared band at 42-45 μm (Malfait *et al.* 1999) as well as the weaker band near 62 μm (McClure *et al.* 2015). The outer disk, extending from the CO snow line and outwards, is traced by ALMA, which can reach a wide range of species, including relatively complex organics. The spectra are all from different protoplanetary disks: TW Hya, MWV 430, RNO 90, HD 142527 and DoAr 44. The data plotted in are from Pontoppidan & Blevins (2014), Salyk *et al.* (2015), Blevins *et al.* (2015), Hogerheijde *et al.* (2011), Öberg *et al.* (2015) and the Infrared Space Observatory archive at ESA.

due to water and other volatiles generally trace disk surfaces, and will not directly trace the midplane where planetesimals and planets form (Bergin *et al.* 2013, Pontoppidan & Blevins 2014). 2) Disk surfaces have highly abundant water vapor within a critical radius at distances of 4-10 AU, depending on the luminosity of the central star and accretion region. Beyond this radius, the abundance of water vapor drops by many orders of magnitude (Blevins *et al.* 2015). It is not clear whether this drop in abundance is a freeze-out or chemical effect (Kamp *et al.* 2013). 3) In inner disks, the surface volatile abundances are consistent with most of the elemental oxygen being bound in water and CO. This is also consistent with an ice/rock ratio of 1-2 if the chemistry does not change in deeper disk layers where the volatiles freeze out. Radiative transfer models of observations of far-infrared emission from water ice in the outer disk suggest ice/rock ratios of ~2 (McClure *et al.* 2015). 4) There is observational evidence that the inner disk chemistry is very different from that of comets and the dense interstellar medium (ISM) (Pontoppidan & Blevins 2014), while the outer disk chemistry is much more ISM-like (Öberg *et al.* 2015).

Of particular note is the impressive ALMA image of dust ring structure in the young, massive disk around HL Tau (ALMA Partnership *et al.* 2015), which has generated several interpretations directly linked to the disks' volatile content. While the observed dust gaps in HL Tau are evocative of direct dynamical carving by planets (Picogna & Kley 2015, Dipierro *et al.* 2015), detailed hydrodynamical modeling including dust aggregation, fragmentation and drift demonstrate that other options exist (Lorén-Aguilar & Bate 2015, Gonzalez *et al.* 2015). A key additional constraint from the ALMA images is the finding that the submillimeter spectral index changes across the dust gaps. This has been used to suggest that the rings in HL Tau may be due to local grain growth due to volatile condensation at the condensation fronts of water, ammonia and chlathrate hydrates (Zhang *et al.* 2015). Similarly, the observed dust structures have also been suggested to be the result of strongly temperature-dependent "sintering" of icy dust grains (Okuzumi *et al.* 2015).

5. Future observations

In the nearest future, ALMA is likely to shed new light on the chemistry of volatiles in the outer regions of protoplanetary disks through gas line imaging of increasingly high fidelity. Inside 10-20 AU, the ability of ALMA to measure grain size distributions using spectral index mapping may prove to be uniquely powerful for constraining ices and their role in disk evolution and planet formation. In roughly 3 years, the James Webb Space Telescope will launch, and will produce detailed observations of the mid-infrared molecular forest from 1 AU in protoplanetary at very high signal-to-noise and fidelity, opening up a large new discovery space. Ultimately, it will still be the combination of data from mid-infrared, far-infrared and submillimeter observatories that will produce a full understanding of the role of volatiles in planet formation.

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