Astro2020 Science White Paper

D/H Ratio in Water and the Origin of Earth's Oceans

Thematic Areas: ☒ Planetary Systems ☒ Star and Planet Formation
☐Formation and Evolution of Compact Objects ☐ Cosmology and Fundamental Physics
☐Stars and Stellar Evolution ☐Resolved Stellar Populations and their Environments
☐Galaxy Evolution ☐Multi-Messenger Astronomy and Astrophysics

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Abstract:

Comets contain some of the most pristine ice-rich material left over from the formation of the solar system. Measurements of the D/H ratio in cometary water provide key constraints on the origin and history of water, and the contribution of comets to Earth's oceans. Over the past quarter of a century, a dozen D/H measurements have been painstakingly gathered, using ground-based and space facilities. A significant isotopic diversity has been shown to exist, in both Oort-Cloud and Jupiter-Family comets. However, given the small sample, any trends with physical or orbital properties have yet to be established. Measurement of the D/H ratio in a *statistically significant sample* of comets has been identified by the community as a high-priority goal for the next decade, important for understanding Earth's habitability and the distribution of volatile material during the solar system's formation.

Comets and the Origin of Earth's Water

One of the key questions of modern astrophysics and planetary science concerns the development of the conditions of habitability in planetary systems, such as the early protosolar nebula. Water, an essential ingredient for carbon-based life as we know it (Westall 2018), is formed primarily via surface reactions in icy mantles of interstellar dust grains (the gas-phase chemistry only becomes efficient at temperatures above ~ 300 K). We assume that these grains subsequently find their way to dense protostellar cores and subsequently to protoplanetary disks, where they are partially processed thermally in the inner disk, before being locked up in small bodies, such as comets or asteroids (van Dishoeck et al. 2014), although this aspect remains to be unequivocally confirmed by observations.

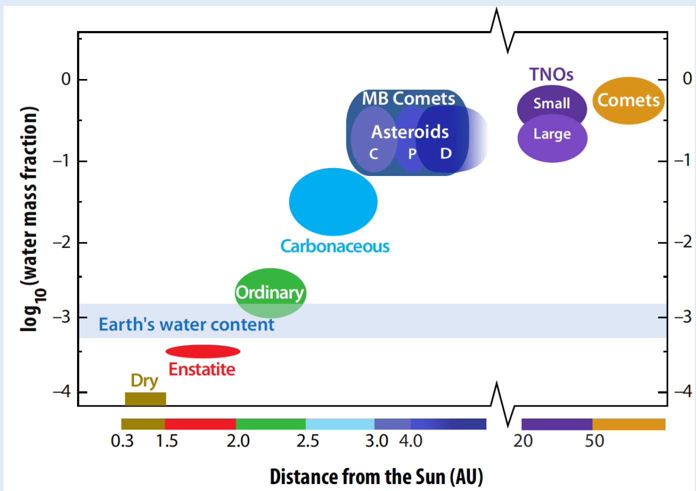

Figure 1. Water content in the Solar System bodies at the time of Earth's growth as a function of heliocentric distance (from van Dishoeck et al. 2015, adapted from Morbidelli et al. 2012).

In the standard model of the protosolar nebula, the temperature in the terrestrial planet forming zone was too high for water ices to survive (O'Brien et al. 2018). The snow line separating the inner dry and outer wet part of the disk was outside of the terrestrial plane zone (see Fig. 1 for the water content in the present-day solar system). In this simple scenario, any water ice that might have been initially present in the inner disk would have evaporated and escaped. Consequently, the Earth accreted dry and the present-day water would have been delivered in a later phase, together with organics, from external sources such as impacts of comets or asteroids (O'Brien et al. 2018).

Comets are small, icy bodies with radii less than 20 km that have formed and remained for most of their lifetimes at large heliocentric distances. Therefore, they contain some of the least-processed, pristine ices from the solar nebula disk. They have often been described as 'dirty snowballs', following the model of Whipple (1950), in which the nucleus is visualized as a conglomerate of ices, such as water, ammonia, methane, carbon dioxide, and carbon monoxide, combined with meteoritic materials. Numerous complex molecules have now been identified in comets by *Rosetta*. The composition of cometary ices is very similar to that of low-mass star-forming regions, suggesting synthesis in the pre-solar cloud or in the cold outskirts of the solar nebula (Drozdovskaya et al. 2018).

Dynamically, comets can be separated into two general groups: short-period, Jupiter-family comets and long-period comets. Short-period comets are thought to originate from the Kuiper belt, or the associated scattered disk, beyond the orbit of Neptune, while long-period comets formed in the Jupiter-Neptune region and were subsequently ejected into the Oort cloud by gravitational interactions with the giant planets. In reality, the picture is significantly more complex due to migration of the giant planets in the early solar system (Raymond et al. 2018). In fact, recent evidence suggests that the formation zones of the two families largely overlapped and extended over a broad range of heliocentric distances (Brasser et al. 2013). In addition, the Sun may have captured comets from other stars in its birth cluster (Levison et al. 2010). Consequently, there is increasing emphasis on classifying comets based on their chemical and isotopic composition rather than orbital dynamics (Mumma & Charnley 2011).

Deuterium-to-Hydrogen Ratio

Measurements of the D/H ratio in cometary water provide key constraints on the origin and history of water molecules, and the contribution of comets to Earth's oceans. Deuterium was produced in the Big Bang, with an abundance of about 2.5×10^{-5} with respect to hydrogen (Cooke et al. 2014). The reference protosolar D/H ratio in hydrogen is 2.1×10^{-5}, close to the Big Bang value (Geiss et al. 1998). However, in the cold, dense, CO-depleted interstellar medium, deuterium atoms are preferentially sequestered in heavy molecules due to differences in zero-point vibrational energies (Ceccarelli et al. 2014). Consequently, the D/H ratio in heavy molecules may be enhanced by orders of magnitude, and doubly or even triply deuterated species have been detected (Lis et al. 2002; Parise et al. 2004). Deuteration in water is less extreme than in other molecules, with water D/H ratios of order 0.001—0.01 typically measured in low-mass protostars similar to our Sun (Ceccarelli et al. 2014). This can be taken as the initial value for the protosolar nebula water. Subsequent isotopic exchanges between water molecules and molecular hydrogen in the warm inner disk will drive the ratio back toward the protosolar value (Drouart et al. 1999). The highest solar system D/H ratios in water, about 7.3×10^{-4} measured in LL3 matrix clays or R chondrites (Deloule et al. 1998; Alexander et al. 2012; McCanta et al. 2008), are in fact close to the interstellar medium values. The D/H ratio in Earth's ocean water, the Vienna Standard Mean Ocean Water (VSMOW), is significantly lower, $(1.5576 \pm 0.0001) \times 10^{-4}$, although still enhanced with respect to the protosolar ratio in hydrogen. How representative this value is for the bulk of Earth's water is a subject of discussion in the light of recent measurements of a low D/H ratio in deep mantle materials (Hallis et al. 2015). Currently, carbonaceous chondrites, in particular CI and CM types, appear to best match the terrestrial D/H ratio (Alexander et al. 2012).

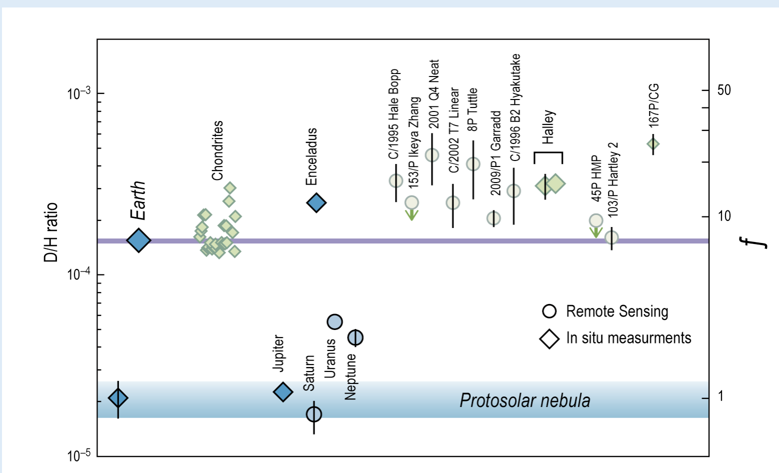

Figure 2. D/H ratio in water in the solar system bodies and planetary materials (from the Origins Report). Cometary D/H ratios vary in both dynamical groups, Oort Cloud and Jupiter Family.

The D/H ratio has been measured in a handful of Oort-Cloud comets, with typical values of about twice VSMOW (Bockelée-Morvan et al. 2015; Fig. 2). *Herschel* provided first measurements of the D/H ratio in two Jupiter-Family comets, 103P/Hartley (Hartogh et al. 2011) and 45P/Honda-Mrkos-Pajdusáková (Lis et al. 2013), both consistent with VSMOW. A relatively high D/H ratio, three times VSMOW, was subsequently measured by *Rosetta* in another Jupiter-Family comet 67P/Churyumov-Gerasimenko (Altwegg et al. 2015). The VSMOW D/H value measured in the Oort-Cloud comet C/2014 Q2 (Lovejoy) suggests that the same isotopic diversity is present in the two comet families (Biver et al. 2016).

Existing and Future Observational Capabilities

The current sample of D/H measurements in cometary water is small and no clear correlations with physical or orbital parameters have so far been identified. While rotational transitions of HDO can be observed from the ground at submillimeter or infrared wavelengths, observations of water are extremely challenging, as the low-energy rotational transitions of water are not accessible even from sub-orbital platforms. Cometary water production rates are thus traditionally inferred indirectly from radio observations of its photodissociation product, OH, at 18 cm (Crovisier et al. 2002). While often the only measurement available, OH observations are not necessarily directly comparable to many other molecular line detections due to the extended distribution and other model dependent analysis. The first direct detection of gaseous water in comet 1P/Halley, through its ν_3 vibrational band at 2.65 µm, was obtained using the KAO (Mumma et al. 1986). The 557 GHz transition of ortho-water was observed by SWAS (Neufeld et al. 2000) and *Odin* (Lecacheux et al. 2003), whereas *Herschel* provided for the first-time access to multiple rotational transitions of both ortho- and para-water (Hartogh et al. 2011).

The atmosphere at stratospheric altitudes is sufficiently transparent at the frequencies of low-energy transitions of $H_2^{18}O$. In particular, the 547 and 509 GHz $1_{10} - 1_{01}$ transitions of $H_2^{18}O$ and HDO, previously observed in several comets by *Herschel*, are now accessible using the GREAT spectrometer on SOFIA and can be used to accurately measure the D/H isotopic ratio. Given the sensitivity and operational constraints, this will approximately allow doubling the number of existing D/H measurements during the SOFIA's lifetime. Such a sample, while significant, is still insufficient to answer unequivocally the questions posed here. Moreover, such measurements require assumptions about the $^{16}O/^{18}O$ isotopic ratio, which, however, has been shown to be relatively uniform in comets, 500±50, and close to the terrestrial ratio (Bockelée-Morvan et al. 2015).

ALMA now gives access to several (sub)millimeter HDO lines. For cometary observations, the most sensitive use of ALMA would be in the autocorrelation mode, as 50 independent single-dish antennas (Cordiner et al. 2019). Such an observing mode is not currently offered, but may become available in the future. In addition, simultaneous determinations of the water production rate using other techniques will be required to accurately measure the D/H ratio based on such observations, as the excited (sub)millimeter water lines that are accessible from the ground have been often shown to be masing in astrophysical environments.

The lowest rotational lines of water and its isotopologues, $H_2^{18}O$, $H_2^{17}O$, and HDO occur at ~ 600 µm wavelengths, and the emission lines from comets are extremely narrow, ~ 1 kms^{-1} FWHM. This makes a heterodyne system, capable of resolving the lines, ideal – comparable to previous measurements conducted with *Herschel*. These systems have the advantage that they do not require a cold telescope, and hence a relatively modest Probe Class mission can devote available budget to maximizing telescope collecting area, necessary to observe a statistically significant sample of comets as discussed here. Within anticipated budget cap, we envision a mission with a dedicated 7m class FIR telescope (4 times the collecting area of Herschel), diffraction limited up to about 200 µm, and spectroscopic system covering the above lines and also the lowest transition of para-H_2O at 270 µm. This will allow measurement of the ortho to para ratio, an important tracer of the origin of water as well as the D/H ratio in 100 comets over a 5-year mission lifetime, based on characteristics of known comets and an assumed water production/visual magnitude correlation. In addition to answering the key question posed above, this mission will enable study of the entire water trail from the interstellar medium to habitable planets.

A large survey of comets in the far-infrared, with a high spectral resolution and broadband spectrometer that covers H_2O, HDO, $H_2^{18}O$, as well as *ortho* and *para* lines simultaneously would be ideal. Sensitivity will be the limiting factor in a survey towards 100s of targets due to the generally shorter observation windows typically accessible with such telescopes (due to constraints such as moving target rate of motion, field-of-regard, and peak flux from short-lived apparitions). In order to achieve this, an estimate sensitivity of ~ 1×10^{-20} Wm^{-2} at 179 µm with a spectral resolution $R > 10^4$ and a cooled aperture would enable D/H measurements in hundreds of comets. The *Origins* mission concept has prioritized such studies in the Water Trail science goal and estimates D/H measurements in comets down to ~0.1 times VSMOW (for typical apparitions) with those requirements. Detections towards the brighter objects could/should be followed-up with heterodyne observations where detailed line profile analysis can be conducted to better constrain the physical parameters of the volatiles.

Recommendations

To accurately measure the D/H ratio in comets, we need near-simultaneous observations of both water and HDO, ideally with the same instrument, in the same field of view. SOFIA, with its GREAT spectrometer, or possible future heterodyne instrumentation, now allows such measurements in moderately bright comets, such as comet 46P/Wirtanen in December 2018. This will result in high-quality measurements of D/H ratio in up to a dozen comets over SOFIA's 15—20 years lifetime. However, a much larger sample, of order 100 comets, is needed to search for correlations with physical or orbital properties, to fully understand the underlying physics. Such measurements can only be carried out from space, with a far-infrared mission such as *Origins*, or a dedicated probe-class spectroscopic mission, targeting low-energy lines of water isotopologues. This is a high-priority goal for the next decade, required to fully understand Earth's habitability. Moreover, in order to derive precise D/H ratios from the observations, accurate excitation models are needed. This requires, in particular, computations of collisional excitation rates of water with water and HDO with water, which will have to be combined with spatially-resolved studies of the coma temperature distribution at far-infrared/millimeter wavelengths.

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