Deciphering the Protostellar Disk Evolution Recorded by Cometary Deuterated Water

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1 Executive summary

Certain aspects of the physical and chemical evolution of protostars are difficult to address with astrophysical observations. Measurements of the deuterium abundance D/H in comets provides an opportunity to fill this knowledge gap. We propose dedicated efforts (e.g., a spaceborne Comet Survey Telescope) to ensure D/H comet observations reach their full astrophysical potential.

2 Comets help us understand protostars

The formation of stars and circumstellar disks is a complex phenomenon. The evolution of gas pressure and temperature during the cloud collapse, and the associated processing of organics and volatiles necessary for habitability, are largely unknown. The deuteration of water is a sensitive gauge of the physical conditions during protostellar contraction. Comet nuclei, that preserve presolar and processed ices, are treasure troves of information but the exploration of their D/H abundance is in its infancy. We call for a dedicated effort to harvest this information with the purpose of better understanding the protostar formation process.

In Sec. 3, we first recapitulate the physical evolution sequence of protostars. We then describe the formation of water and key changes to its deuteration level along this time sequence. The formation and dynamical evolution of comets are described (Sec. 4) and previous D/H measurements are summarized (Sec. 5). Based on this context we define a number of important questions about protostar formation that comet water D/H measurements can help answering (Sec. 6) and we provide recommendations on how to substantially expand the current state of knowledge (Sec. 7).

3 Water deuteration in collapsing protostars

The star–forming process starts with filament production in molecular clouds because of supersonic turbulence (Mac Low and Klessen 2004). Filaments break up into starless cores because of self–gravity (e.g., Klessen and Burkert 2000; Heitsch *et al.* 2001; Boss 2005). Starless cores typically have masses of 0.5–$5\,\mathrm{M}_{\odot}$, dimensions of $6\cdot10^{3}$–$4\cdot10^{4}\,\mathrm{AU}$, densities $n=10^{4}$–$10^{5}\,\mathrm{cm^{-3}}$, temperatures $T=8$–$12\,\mathrm{K}$ (Bergin and Tafalla 2007), and lifetimes of 0.3–$1.6\,\mathrm{Myr}$ (Lee and Myers 1999; Visser *et al.* 2002). Collapsing starless cores develop a central $\sim10\,\mathrm{AU}$ condensation with $n=10^{12}$–$10^{16}\,\mathrm{cm^{-3}}$ that heats up to $\sim2000\,\mathrm{K}$ (Masunaga *et al.* 1998; Machida *et al.* 2006). Such Class -I protostars live only $\sim10^{3}\,\mathrm{yr}$ and are rarely observed (Enoch *et al.* 2010). The dissociation of H_2 at the very center marks the transition to a Class 0 protostar. During their $\sim10^{4}\,\mathrm{yr}$ lifetime (André and Montmerle 1994) the central condensation grows to $\sim0.1\,\mathrm{M}_{\odot}$ and is fed by accretion from a few times more massive disk with dimensions $\sim100\,\mathrm{AU}$, in turn fed by infall from the $\sim10^{4}\,\mathrm{AU}$ envelope that still carries the majority of the mass (Froebrich *et al.* 2006; Machida *et al.*

2010; Machida and Matsumoto 2011). Accretion is driven by gravitational instabilities in the massive disk and angular momentum conservation triggers strong bipolar outflows (Bachiller 1996). The inner few AU of the accretion disk experiences a brief period of $T > 1000\,\mathrm{K}$ during the most intense accretion (Tscharnuter *et al.* 2009) that is needed for the production of Calcium–Aluminum–rich Inclusions or CAI (MacPherson *et al.* 1995; 2005). Therefore the "time zero" of the Solar System defined as the formation of CAI radiometrically dated to 4.567 Gyr ago (Amelin *et al.* 2002) likely coincides with the Class 0 stage (Tscharnuter *et al.* 2009). The disk temperature falls with distance to $\sim 100\,\mathrm{K}$ at $\sim 100\,\mathrm{AU}$ and the envelope remains much colder (Masunaga and Inutsuka 2000). The central object continues to accrete at a reduced rate during the Class I stage that lasts for a few times $10^5\,\mathrm{yr}$ (André and Montmerle 1994), the infall stream from the envelope impacts the protostellar disk at increasingly large radial distances under decreasing levels of shock heating (Visser *et al.* 2009) and the central object reaches its final stellar mass near the end of the Class I stage. At this point the envelope is gone, the remaining disk has a mass of order $10^{-2}\,\mathrm{M}_\odot$ and midplane densities and temperatures of $\{n,\, T\} = \{10^{15}\,\mathrm{cm}^{-3},\, 380\,\mathrm{K}\}$ at 1 AU, $\{10^{12}\,\mathrm{cm}^{-3},\, 120\,\mathrm{K}\}$ at 10 AU, and $\{10^{9}\,\mathrm{cm}^{-3},\, 40\,\mathrm{K}\}$ at 100 AU (Hayashi 1981) for a typical luminosity $\sim 3.5\, L_\odot$ ($L_\odot$ is the current solar luminosity) (Palla and Stahler 1993). Such Class II protostars, where the central object is observable at visual wavelengths for the first time (often referred to as a *T Tauri star*) and where the disk is referred to as the *Solar Nebula* in Solar System science, typically lasts for $\sim 3\,\mathrm{Myr}$ (Zuckerman *et al.* 1995; Haisch *et al.* 2001; Sicilia-Aguilar *et al.* 2006) until the gas component is dispersed. Gas giants necessarily need to form within that time frame, whereas terrestrial planets grow slower: the lunar–forming impact that provided the last $\sim 10\%$ of Earth's mass (Canup and Asphaug 2001) is radiogenically determined to have occurred $60 \pm 10\,\mathrm{Myr}$ after CAI (Barboni *et al.* 2017).

Production of presolar water takes place during the starless core stage and is highly deuterated because of the following mechanism (see, e.g., van Dishoeck *et al.* 2014). Cosmic rays ionize H_2 and H, leading to H_3^+ production. With CO removed from the gas phase through its condensation onto dust grains at the extremely low temperatures within a starless core, the major destroyer of H_3^+ is gone and the ion accumulates. Through the reaction $H_3^+ + HD \rightarrow H_2D^+ + H_2$ it becomes heavily deuterated because the reverse reaction is inhibited at low temperatures. When H_2D^+ is neutralized by colliding with negatively charged dust or by reaction with electrons, deuterium atoms are released and the atomic D/H ratio is increased. The D and H atoms freezeout and react with oxygen atoms or O_2 on the surface creating water molecules and transferring the high atomic D/H ratio to the water ice. Using the presolar nebula average $D/H = 2.1 \cdot 10^{-5}$ for reference (enhancement factor $f = 1$) the water deuterium abundances measured in Class 0 protostars (inherited from the starless core phase) have $14 \leqslant f \leqslant 4 \cdot 10^3$ (Ceccarelli *et al.* 2014).

During the Class I stage sublimated deuterated water may interact with the hydrogen reservoir and lose deuterium through the reaction $HDO + H_2 \rightarrow H_2O + HD$. At high temperature ($T > 500\,\mathrm{K}$) this quickly leads to $f = 1$ and at $200 < T < 500\,\mathrm{K}$ it leads to

$1 \leqslant f \leqslant 3$ on time–scales in the 10^2–10^5 yr range that depend strongly on temperature and pressure (Yang *et al.* 2013). The final radial distribution of D/H in the Solar Nebula at the time of planetesimal and planet formation therefore depends crucially on the following highly uncertain conditions; 1) the fraction of the ice in the Solar Nebula that manages to avoid sublimation and deuterium loss during earlier phases (models suggest up to 60%; Visser *et al.* 2011); 2) the quantity of new $f = 1$ water that is being produced in the gas phase near the central object and the extent to which f lowered in sublimated ice before it recondenses (this is extremely sensitive to the evolution of gas pressure and temperature with time at different heliocentric distances at the Class 0 and I stages; Yang *et al.* 2013); 3) the extent to which low–f water processed near the central object is diffusing out to larger distances (the discovery of high–temperature particles like CAI and chondrules in the *Stardust* sample–return from Comet 81P/Wild 2 suggest such disk mixing was substantial; Brownlee *et al.* 2012). We do not know if the D/H ratio in the Solar Nebula increased monotonically with heliocentric distance or had a more elaborate distribution (Yang *et al.* 2013). The prospect of reconstructing this complex chain of development increases when considering D_2O/H_2O as well as HDO/H_2O ratios (Furuya *et al.* 2016; 2017).

4 Comet formation and dynamical evolution

The giant planets of our Solar System likely formed at 5–15 AU from the Sun. Icy planetesimals formed primarily at 15–30 AU (Gomes *et al.* 2004) and to a substantially smaller extent at 30–45 AU (Parker and Kavelaars 2010; Parker *et al.* 2011). To first order, the D/H ratio of planetesimals in this so–called *Primordial Disk* was inherited from that in the Solar Nebula. The detailed composition depends on whether they formed rapidly from localized material through gravitational collapse of pebble–swarms created by streaming instabilities (Youdin and Goodman 2005; Johansen *et al.* 2007) or gradually from sub–units originating from different localities through hierarchical agglomeration (Weidenschilling 1997; Davidsson *et al.* 2016). In either case, certain mixing may have occurred later during collisional evolution between dynamically excited objects (Morbidelli and Rickman 2015). The giant planets are believed to have experienced substantial migration. Inward Type I and II migration of Jupiter and Saturn followed by a mutual resonant coupling that reversed the drift outwards may have brought Jupiter as close as to the Mars orbit at 1.5 AU from the Sun, as in the Grand Tack scenario (Walsh *et al.* 2011). If so, high–f planetesimals would be brought to the inner Solar System and low–f originating closer to the Sun would be mixed out into the Primordial Disk. The Nice model (Tsiganis *et al.* 2005; Levison *et al.* 2008) envisions a gravitational instability between Jupiter and Saturn that initiated a Type III migration of Saturn, Uranus, and Neptune outward toward their current orbits that disrupted the Primordial Disk. If this event is responsible for the Late Heavy Bombardment (Gomes *et al.* 2005) it took place about 400 Myr after CAI (Morbidelli *et al.* 2012; Marchi *et al.* 2013).

The disruption of the Primordial Disk created the Kuiper belt at 30–50 AU (Levison *et al.*

2008), superimposed on a small fraction of objects formed *in situ* known as the dynamically cold trans–neptunians. Some of the Kuiper belt objects have experienced close encounters with Neptune that created a related dynamical structure known as the Scattered Disk. Dynamical studies show that the Scattered Disk is the source region of objects that continuously are being transported to small heliocentric distances (Levison and Duncan 1997) where they are observed as *Jupiter–family comets* or JFCs. The disruption of the Primordial Disk also created the Oort cloud (e.g., Brasser and Morbidelli 2013) located $\sim 10^4$ AU from the Sun. Galactic tides and stellar encounters regularly cause some of these objects to enter nearly–parabolic orbits with perihelia close to the Sun, where they are observed as *Oort cloud comets*, or OCCs.

Any given Primordial Disk object has equal probabilities of ending up in the Scattered Disk and in the Oort cloud – it is essentially a random process. Therefore, both JFCs and OCCs should display the same distributions of D/H values that sample variability within the entire original 15–30 AU region. This simple view is complicated by the possibility that dynamically cold objects formed *in situ* at 30–45 AU may infiltrate the Scattered Disk and show up as JFCs, while objects captured from other stars may infiltrate the Oort cloud and show up as OCCs (Levison *et al.* 2010).

5 Observations of deuterated water in comets

Measuring the D/H ratio in comets is extremely challenging. It has only been done *in situ* by mass spectroscopy for two comets (1P/Halley and 67P/Churyumov–Gerasimenko) and by groundbased spectroscopy at a variety of wavelength regions for eight other comets (see compilations by Bockelée-Morvan *et al.* 2015 and Altwegg *et al.* 2015). The two JFCs have the lowest ($f = 7.8$ for 103P/Hartley 2, comparable to that of Earth's water, $f = 7.1$) and the highest values ($f = 25.2$ for 67P/Churyumov–Gerasimenko), while the range for OCCs is $9.8 \leqslant f \leqslant 21.9$. The sample is too small to determine if there are any statistically significant differences between JFCs and OCCs and we do not know if f changes over time for a given target because of chemical heterogeneity.

6 Astrophysical questions answered by comet D/H

Based on the review above we define the following important questions.

#1) What was the level of deuteration in water ice formed in the Solar System starless core? Astrophysical D/H observations rely on observing water in the gas phase that may have been processed already. Comets offer the possibility of accessing unprocessed ice formed in the starless core.

#2) To what extent is shock heating of envelope material falling onto protoplanetary disks avoided? This process takes place when the protostar is obscured by its thick envelope and is difficult to observed directly. Comets provide an opportunity to determine the fraction of preserved presolar ice, identified by unusually high D/H ratios.

#3) Is the initial radial distribution of D/H in a circumstellar disk monotonic? Comets can help reveal the radial distribution by coupling their D/H ratios with other potential indicators of formation distance (e.g., crystalline/amorphous silicate mass ratio, abundance of supervolatiles).

#4) To what extent do stars exchange weakly gravitationally bound material with each other? This question can be answered if the D/H ratio is measured for a sufficiently large sample of comets to determine if there is a systematic difference between JFCs and OCCs.

#5) Does the planetesimal growth process in circumstellar disks involve mergers between sub–units born at very different distances from the Sun? This question may be answered by measuring the level of chemical heterogeneity in comet nuclei on macroscopic size scales.

7 Recommendations

In order to address several of the questions in Sec. 6 it is necessary to measure the D/H ratio for a sample of JFCs and OCCs that is substantially larger than that of currently studied comets. This is needed in order to obtain the statistics required to reveal potential systematic differences between the populations, with implications for circumstellar disk dynamics and interactions between stellar systems. Ideally, measurements should be performed several times during the perihelion passage of each target, and occasionally the nucleus rotation period should be temporally resolved. This is needed in order to understand to what extent comet nuclei are chemically heterogeneous, with implications for circumstellar disk evolutionary processes, such as planetesimal formation.

The D/H ratio of comets can be measured remotely, in situ, and in returned samples. Remote observations utilize the fact that deuterated water and its photodissociation products are observable in many different wavelength regions – UV, IR, and microwaves. Because of the high level of extinction in the terrestrial atmosphere, and in order to reach the necessary number of observable targets, we propose a dedicated Comet Survey Telescope that could carry a range of detectors. In situ measurements can be done with mass spectrometers, and cryogenic sample return allows for high–precision laboratory measurements. Therefore, there is a multitude of technologies available in order to address the questions in Sec. 6, and comets have the potential to reveal important information about astrophysical environments that is difficult to obtain in other ways.

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