Constraints from deuterium on the formation of icy bodies in the Jovian system and beyond

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Abstract

We consider the role of deuterium as a potential marker of location and ambient conditions during the formation of small bodies in our Solar system. We concentrate in particular on the formation of the regular icy satellites of Jupiter and the other giant planets, but include a discussion of the implications for the Trojan asteroids and the irregular satellites. We examine in detail the formation of regular planetary satellites within the paradigm of a circum-Jovian subnebula. Particular attention is paid to the two extreme potential subnebulae – “hot” and “cold”. In particular, we show that, for the case of the “hot” subnebula model, the D:H ratio in water ice measured from the regular satellites would be expected to be near-Solar. In contrast, satellites which formed in a “cold” subnebula would be expected to display a D:H ratio that is distinctly over-Solar. We then compare the results obtained with the enrichment regimes which could be expected for other families of icy small bodies in the outer Solar system – the Trojan asteroids and the irregular satellites. In doing so, we demonstrate how measurements by Laplace, the James Webb Space Telescope, HERSCHEL and ALMA will play an important role in determining the true formation locations and mechanisms of these objects.

Key words: Solar system formation; Deuterium; Jupiter; Satellites: Regular; Satellites: Irregular; Asteroids: Main Belt; Asteroids: Trojan; Spacecraft.

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1 Introduction

The physical and chemical characteristics of the proto-planetary nebula from which our solar system formed can be inferred through the analysis of “primitive” objects such as meteorites, comets, and the giant planets themselves. We can obtain useful constraints on these processes by examining the degree to which fossil deuterium contained within the water in some of these objects is enriched when compared to the protosolar abundance, which can be measured in various objects within the Solar system. Within the Solar nebula, the main reservoir of deuterium was molecular hydrogen. However, isotopic exchange occurred between this hydrogen and other deuterated species, resulting in the formation of secondary reservoirs of deuterium. As a result of the high cosmic abundance of oxygen, the most important secondary reservoir in the nebula is water (HDO), either in gaseous or solid phase.

Calculations of the temporal and radial evolution of the D:H ratio in the primitive nebula (Drouart et al., 1999; Mousis et al., 2000) have been performed in order to reproduce existing data on comets (Balsiger et al., 1995, Eberhardt et al., 1995; Bockelée-Morvan et al., 1998; Meier et al., 1998; see Horner et al., 2007), and measurements taken from meteorites (Deloule et al., 1998). One particularly interesting result of these calculations is that the D:H ratio in water ice produced in the nebula varies by a significant amount as a function of the distance from the Sun at which the ice was formed. This variation can be seen clearly in the compilation of measurements given by Drouart et al. (1999), in Fig.1 of that work. Such results led Horner et al. (2007) to discuss how measurements of the D:H ratio in cometary bodies might prove helpful in answering the question of whereabouts in the Solar system the different cometary populations had formed. The study of D:H extends beyond the study of cometary bodies, however.

In order to consider the measured D:H enrichment within an object to be the direct result of its formation, it is clear that the deuterated reservoir incorporated within that object must have undergone little or no alteration since its formation within the nebula. Therefore, despite the fact that deuterium enhancement has been measured on the Earth, Venus and Mars, it is obvious that we cannot consider the resulting value to be primordial. Indeed, the value measured on the Earth could be the result of the combination of volatile material from a number of sources (Dauphas et al., 2000). Furthermore, the values measured on Venus and Mars are believed to be the result of strong atmospheric fractionation, which has occurred throughout the history of the planets (Donahue, 1999; Bertaux & Montmessin, 2001).

Even further from the Sun, observations of Titan reveal an unexpectedly high D:H ratio within the methane of the satellite’s atmosphere (Bézard et al.,
The cause of this enhancement is still under some debate. It could be the result of isotopic exchange between methane and molecular hydrogen within the early Solar nebula, prior the formation of the icy planetesimals that were ultimately accreted by Titan (e.g. Mousis et al., 2002a). Alternatively, it could result from a photochemical process occurring within the atmosphere of the satellite (Lunine et al., 1999).

A number of ambitious projects, such as the proposed Laplace\(^1\) mission and the James Webb Space Telescope (scheduled for launch in 2013), will allow us to revisit the Jovian satellite system, and provide new measurements of the satellites of the giant planet in the coming years. As such, the time seems right to revisit the question of how these satellites formed, and what effect their formation would have on the quantities that could be observed by such a mission. In light of these proposed missions, such work takes on an interesting new aspect. How would the D:H ratio in the Jovian (or Saturnian) satellites be affected by their formation? Could measurements of deuterium in these satellites help us to understand the final stages of the formation of their parent bodies? Furthermore, it is important to examine such ideas during the period over which the missions are designed, to enable the construction of instruments which are fully capable of answering the questions posed.

In this work, we aim to detail the various properties which would have affected the regular satellites during their formation, highlighting how the fractionation of deuterium within their ices may represent a vital window into their formation. We also examine the benefits that observations of the degree of deuteration in the irregular satellites and the Trojan asteroids would have for our understanding of the origin of the volatiles they contain, together with presenting a discussion of how and when such observations may be made.

The simple picture portrayed for the comets, although applicable for other objects which formed freely in the Solar nebula (such as the asteroids), becomes more complicated when one wishes to understand the formation of the satellites of the giant planets. For the regular satellites, it is possible that material from the Solar nebula underwent a significant amount of additional processing within the planetary sub-nebula. In section 2, we will review the main results of prior discussions and calculations involving the D:H ratio in the Solar nebula, while in section 3 we show how further processing within planetary sub-nebulae would eventually lead to a reduction in the D:H ratio incorporated in the satellites forming therein when compared to gas at an equivalent distance in the Solar nebula. In section 4, we examine the cases of the irregular planetary satellites and the Jovian Trojan asteroids, two groups of object for which the study of deuteration may help untangle the minutiae of their formation. The measurement of the D:H ratio in satellites and other

\(^{1}\) http://jupiter-europa.cesr.fr/
objects by future space missions is discussed in section 5, and, in section 6, we conclude with a summary and discussion of our ideas, along with their implications for future missions to, and observations of, the giant planets and their satellite systems.

2 Temporal and Radial evolution of D:H in the Solar nebula – previous work

Here, we summarise the works of Drouart et al. (1999), Mousis et al. (2000), Hersant et al. (2001), Mousis (2004a) and Horner et al. (2007) who described the evolution of the deuterium enrichment factor, $f$, in H$_2$O within the Solar nebula. The calculations of these authors were based on the fact that the main reservoir of deuterium in the Solar nebula was molecular hydrogen (HD vs. H$_2$), and that ion-molecule reactions in the interstellar medium (see e.g. Brown & Millar, 1989) resulted in the fractionation of deuterium between deuterated species. Consequently, in the pre-solar cloud, such fractionation was present, resulting in heavier molecules being enriched. Water was the second most abundant hydrogen bearer in the Solar nebula, as it is in our current Solar system, and therefore became the second largest deuterium reservoir.

In the Solar nebula, the isotopic fractionation of deuterium between water and hydrogen followed the reversible reaction (Geiss & Reeves, 1981):

$$\text{H}_2\text{O} + \text{HD} \rightleftharpoons \text{HDO} + \text{H}_2$$

At low temperatures, this reaction favors the concentration of deuterium in HDO, but the reaction kinetics at such temperatures tend to inhibit the enrichment of deuterium in water. The enrichment factor, $f$, which results from the exchange between HD and HDO is defined as the ratio of D:H in the considered deuterated species to that in molecular hydrogen (the protosolar value). As a result, for water we have:

$$f = \frac{\text{HDO}/\text{H}_2\text{O}}{\text{HD}/\text{H}_2}$$

The afore-mentioned authors physically interpreted the measurements of the D:H ratio in the LL3 meteorites, along with measurements taken of comets 1P/Halley, C/1996 B2 (Hyakutake), and C/1995 O1 (Hale-Bopp) (all three of which share a similar value of D:H in H$_2$O). Time dependent turbulent models of the Solar nebula were then applied which depend on three physical parameters: the initial mass of the nebula $M_{D0}$, its initial radius $R_{D0}$, and the viscosity parameter $\alpha$ (derived from the prescription of Shakura & Sunyaev,
They calculated $f$ in water with respect to the protosolar value in molecular hydrogen by integrating an equation of diffusion in the Solar nebula, as a function of the heliocentric distance and time. The comparison of the obtained value of $f$ to observations allowed a range of possible values for $M_{D0}$, $R_{D0}$, and $\alpha$ to be determined.

This diffusion equation takes into account the isotopic exchange between HDO and $H_2$ in the vapor phase, and turbulent diffusion throughout the Solar nebula (see Sec. 3 for details). The isotopic exchange between HDO and $H_2$ occurs as long as $H_2O$ remains in the vapor phase. This implies that the value of the enrichment in microscopic ices is the one fixed at the time and at the location of the condensation of the water vapor. As soon as the grains reach millimetre size, they begin to decouple from the gas as they grow further, leading to the formation of planetesimals. Whatever the subsequent evolution of these bodies, their D:H ratio is that of the microscopic grains from which they formed. In this paper, we consider the case where the solids that grew in the Solar nebula were accreted only from icy grains formed locally. This means that the D:H ratio in the deuterated ices within these planetesimals is that which was present at the time and location at which they condensed.

Figure 1 shows the variation of $f$ for water trapped within icy grains, as a function of their distance from the Sun, in the case of the minimum-mass and maximum-mass models of the Solar nebula employed by Mousis (2004a) (see Table 1). Here, as in previous work, we assume that $f(R) = 31$ at $t = 0$ for D:H in water. This value corresponds to that measured in the highly enriched component (where D:H = $(73 \pm 12) \times 10^{-5}$) found in LL3 meteorites (Deloule et al., 1998) compared to a protosolar value assumed to be $(2.35 \pm 0.3) \times 10^{-5}$ (Mousis et al., 2002).

As discussed by Mousis (2004a), assuming that Jupiter and Saturn were formed at their current locations in the Solar system (Pollack et al., 1996), the plausible range of values of $f$ in the solids produced in the feeding zones of both giant planets is covered by the vertical error bars in Fig.1. The value of $f$ in $H_2O$ in ices produced in the feeding zone zone of Jupiter is thus between 3.8 and 4.7 times the Solar value. In the case of ices produced in the feeding zone of Saturn, the value of $f$ in $H_2O$ is ranging between 4.8 and 6.8 times the Solar value. Note that these calculations do not consider the formation of planetesimals from a mixing of grains coming from all over the nebula, due to turbulent mixing. In such a case, the global enrichment factor in the inner regions should be somewhat higher, while it would be expected to be a little lower in the outer regions, as the mixing “smears” the distribution. This effect is discussed in more detail in Horner et al. (2007), and will not be considered further in this work.
3 Deuterium enrichment in the regular icy satellites

In the core-accretion model, the formation process of giant planets can be separated in two phases, depending on the physical phenomenon governing the rate of gas accretion. Indeed, during the first epoch of formation, the large cooling timescale (which is necessary to allow the release of the accretion energy of the planetesimals that build the core) prevents the accretion of substantial amounts of gas. The total radius of the planet is therefore equal to its Hill radius (the region over which the planet’s gravity exerts a stronger pull on objects than that of the Sun). Once the planet reaches a certain mass, the second epoch of its formation begins. At this point, the cooling timescale becomes low enough to allow a far greater gas accretion rate, which may even be larger than that which can be supported by the protoplanetary disk\(^2\). At this stage, the total radius of the planet shrinks, and it becomes significantly smaller than its Hill radius. Matter flowing from the Solar nebula to the forming planet forms a circum-planetary disk, known as a subnebula, in which regular satellites are believed to form (Lubow et al., 1999; Magni and Coradini, 2004).

The structure and evolution of the subnebula is therefore linked to both the formation of the giant planet and the behaviour of the Solar nebula, which supplies the gas and gas-coupled solids that may ultimately take part in the formation of satellites (Canup & Ward, 2002 & 2006). The calculation of the structure and evolution of the subnebula has been the subject of much scrutiny (see e.g. Canup & Ward, 2002 & 2006; Mousis et al., 2002; Mosqueira & Estrada, 2003; Mousis & Gautier, 2004; Alibert et al., 2005). Depending on the precise structure of the subnebula, two scenarios can be invoked for the formation of the regular satellites.

In this work, we only discuss the evolution of the gas phase within the Jovian subdisk, though the results are also likely to be applicable to the Saturnian system. In both scenarios discussed below, we follow Canup & Ward (2002) in assuming the accretion of the satellites during large scale migration within the subdisk.

In the first scenario, solid particles which are dynamically coupled to the gas (ranging in size from tens of centimeters to a few meters) are accreted from the Solar nebula to the subnebula, which is initially warm enough to vaporise them (or, at least, the ices they contain). In this case, chemical reactions in the gas phase may lead to the destruction/production of some volatile species (Prinn & Fegley, 1981 & 1989). More importantly, high temperature gas phase isotopic exchanges between molecular hydrogen and hydrogen-bearing molecules

\(^2\) The maximum accretion rate that can be supplied by the disk is governed by its surface density and viscosity.
may alter the deuterium concentration from that which was acquired by the
infalling material during its formation in the Solar nebula. When the subneb-
ula cools, the icy particles re-condense and start to grow. As a result, the D:H
ratios trapped within the icy components of the planetesimals, and therefore
within the regular satellites themselves, are likely to be different from the
original values acquired in the Solar nebula.

In the second scenario, the regular satellites are formed later, from a cold
subnebula, in which the temperature is too low to cause the vaporisation
of the volatile components of infalling particles. The regular satellites would
therefore be expected to have D:H ratios which reflect the Solar nebula at
their epoch of formation, as discussed in section 3.2.

Between these two extreme scenarios, a wide variety of setups are possible,
such that the regular satellites could have been formed from a combination
of re-vaporised and un-vaporised material. In other words, the two scenarios
discussed represent the two end-members of a continuum of models, through
which the modified and un-modified fractions of the material incorporated
within the regular satellites vary with the initial conditions. The following two
sections discuss these extremes in more detail, allowing us to draw conclusions
on how the measurement of the $f$-value within the regular satellites will shed
light on the details of the formation.

Note that the evolution and structure of the subnebula, as presented above, is
directly linked to the final stages of planetary formation. In particular, a con-
tinuous flow of material from the solar nebula to the subnebula occurs during
the first epoch of the subnebula’s evolution. This inflowing material, which has
a D:H value which was acquired in the solar nebula, will therefore alter the
evolution of the deuterium enrichment in the subnebula. Such considerations
need to be taken into account when one attempts to determine the formation
of satellites in such a system. In the diffusion equation presented below (Eq.
6), a source term would be needed to describe the vaporisation of these high-$f$
planetesimals.

However, since it is difficult to formulate and incorporate such an expression
in the diffusion equation, we did not consider the source term in this initial
work. We intend to examine the problem in much more detail in the near
future, and will address the influence of the vapourisation of high-$f$
planetes-
imals on the evolution of the global value of $f$ in the subnebula gas phase at
that stage. Here, then, we will concentrate solely on the two extreme closed
subnebula models, described above, saving a more precise calculation of D:H
ratio evolution for future work.
3.1 The formation of satellites in a warm subnebula

In this section, we consider the formation of regular satellites from icy planetesimals produced in the Jovian subnebula. This hypothesis implies that the Jovian subdisk was initially warm enough to vaporise all the icy solids which formed in the solar nebula before being fed into the disk. In order to provide a description of the thermodynamic structure of the disk, we use the one-dimensional analytical turbulent model developed by Dubrulle (1993) and Drouart et al. (1999).

3.1.1 The Jovian subnebula model

Our turbulent model of the Jovian subnebula is based on the work of Shakura & Sunyaev (1973), who characterise the turbulent viscosity $\nu_t$ as

$$\nu_t = \alpha \frac{C_S^2}{\Omega},$$

(3)

where $C_S$ is the local sound velocity, $\Omega$ the Keplerian rotation frequency and $\alpha$ the dimensionless viscosity parameter. Since the physical origin of turbulence in accretion disks is still not well established, this model is useful since it allows us to describe the qualitative influence of whichever process is responsible for the transport of angular momentum through the disk. Our model also incorporates the opacity law developed by Ruden & Pollack (1991; see e.g. Drouart et al., 1999 for details). The temporal evolution of the disk temperature, pressure and surface density profiles depends upon the evolution of the accretion rate, $\dot{M}$, which we define (following Makalkin & Dorofeeva (1991)

to be:

$$\dot{M} = \dot{M}_0(1 + \frac{t}{t_0})^{-s}.$$  

(4)

$\dot{M}$ decreases with time following a power law which is determined by the initial accretion rate $\dot{M}_0$ and the accretion timescale $t_0$. In this work, we adopt $s = 1.5$, a value that allows our law to be consistent with that derived from the evolution of accretion rates in circumstellar disks (Hartmann et al., 1998). The accretion timescale $t_0$ is calculated by Makalkin & Dorofeeva (1991) to be:

$$t_0 = \frac{R_D^2}{3\nu_D},$$

(5)

where $\nu_D$ is the turbulent viscosity at the initial radius of the subdisk, $R_D$. Three parameters constrain $\dot{M}_0$ and $t_0$: the initial mass of the disk $M_{D0}$, the
3.1.2 Thermodynamic conditions within the subnebula

Table 2 summarises the thermodynamic parameters used in our turbulent model of the Jovian subnebula. The outer radius of the subnebula is taken as $150 R_J \sim 1/5 \times R_{Hill}$, a value close to that calculated by Magni & Coradini (2004) using a 3D hydrodynamical model of the final stages of Jupiter’s formation. The initial accretion rate chosen in our model is a high value, namely $10^{-5} \text{M}_\odot/\text{yr}$, allowing us to describe a highly viscous disk in which temperature and pressure conditions are elevated, particularly at early epochs. The final parameter, $\alpha$, which governs the viscosity, is, at best, poorly constrained by observational data. However, in an attempt to reproduce the ice/rock fractions of the Jovian satellites, Alibert et al. (2005) derived a range of possible values for the viscosity parameter. In this model, we use their favoured value, namely $2 \times 10^{-4}$.

Figures 2–4 show radial profiles of temperature $T$, pressure $P$ and surface density $\Sigma$, respectively, at various epochs during the evolution of the subnebula. Water is in the vapour phase at $t = 0$ throughout the subnebula, and $T$, $P$, and $\Sigma$ decrease over time and as a function of the distance to Jupiter. At $t \sim 4000$ yr, water starts to crystallise at the outer edge of the subdisk. The cooling of the subnebula results in the inward migration of the water condensation front, which reaches the orbits of Callisto ($26.6 R_J$), Ganymede ($15.1 R_J$), Europa ($9.5 R_J$) and Io ($6 R_J$) at $t = 0.06$ Myr, 0.14 Myr, 0.27 Myr and 0.6 Myr, respectively.

3.1.3 Isotopic exchange

In the warm Jovian subnebula, the evolution of $f$ is governed by the equation of diffusion previously detailed by Drouart et al. (1999) and Mousis et al. (2000), which is:

$$\partial_t f = k(T)P(A(T) - f) + \frac{1}{\Sigma R} \partial_R (\kappa R \Sigma \partial_R f).$$

The first term in the right-hand side of Eq. 6 describes isotopic exchange between HDO and H$_2$. Function $A(T)$ is the isotopic fractionation at equilibrium, $k(T)$ is the rate of the isotopic exchange between HDO and H$_2$, and $P$ is the total pressure. $A(T)$ is derived from the tables given in Richet et al. (1977), and the rate $k(T)$ is taken from experiments carried out by Lécluse and Robert (1994). The second term on the right-hand side of Eq. 6 describes turbulent diffusion throughout the subnebula. This term is a function of the local surface density $\Sigma(R,t)$, and on the diffusivity $\kappa$. Following
Drouart et al. (1999), $\kappa$ is assumed to be the ratio of the turbulent viscosity to the Prandtl number $P_R$, the value of which is always close to the unity.

As in the case of the Solar nebula, Eq. 6 is valid as long as $\text{H}_2\text{O}$ does not condense in the Jovian subdisk. This implies that the final value of deuterium enrichment in the microscopic ices incorporated within the regular satellites is that obtained at the time and at location at which the vapour condenses. As soon as the grains become millimeter-sized, they begin to decouple from the gas, and continue to grow, eventually forming planetesimals. Whatever the subsequent evolution of these solids, however, the D/H ratio within them will be that of these microscopic grains.

The enrichment factor, $f(R, t)$, can then be obtained by integrating Eq. 6, which requires the determination of spatial and temporal boundary conditions. The spatial boundary conditions are obtained by setting $\partial f/\partial R = 0$ at both $R = 1 R_J$ and $R = R_D$. When condensation occurs within $R_D$, we set $\partial f/\partial R = 0$ at the radius of condensation. Since the vapor phase of the Jovian subnebula initially consisted of both gas and vaporized ices falling in from the Solar nebula, the initial D:H ratio in water vapor within the subdisk is that of the water ice produced in the feeding zone of Jupiter. As mentioned in Sec. 2, the value of $f$ in $\text{H}_2\text{O}$ ice produced in the feeding zone of Jupiter is between 3.8 and 4.7 times the Solar value. Setting $f(R) = 3.8$ at $t = 0$ when integrating Eq. 6 reveals that, as shown on Fig. 5, $f(R, t)$ rapidly decreases and reaches values lower than $\sim1.2$ throughout the entire gas phase of the Jovian subnebula. Setting $f(R) = 4.7$ at $t = 0$ when integrating Eq. 6 leads to the same result. Once this material has condensed within the formation zone of the regular satellites, at late epochs, the water ice will keep this low deuterium enrichment value.

The value reaches $f \sim1$ very rapidly, well before the water condenses, at which point a stable equilibrium has been reached between the two deuterium reservoirs ($\text{H}_2$ and $\text{H}_2\text{O}$). As a result, regular icy satellites accreted from icy planetesimals produced in situ will also retain this value of $f$ in their water ice.

Note that CO to $\text{CH}_4$ and CO$_2$ to $\text{CH}_4$ gas phase conversions may occur within a warm and dense Jovian subdisk via the following reversible reactions (Prinn & Fegley, 1981; Mousis & Alibert, 2006):

\[
\text{CO} + 3\text{H}_2 = \text{CH}_4 + \text{H}_2\text{O},
\]

\[
\text{CO}_2 + 3\text{H}_2 = \text{CH}_4 + 2\text{H}_2\text{O}.
\]

Such gas phase reactions would lead to the production of additional water in the Jovian subnebula from hydrogen with a Solar D:H ratio. Since the D:H
ratio in the water produced via these reactions would then exhibit Solar D:H, our conclusion that the regular icy satellites would exhibit \( f \) of order unity would not be affected.

Finally, it should be noted that, although the calculations shown above have been carried out in the context of the Jovian subnebula, they would be equally valid within the Saturnian disk.

3.2 The formation of satellites in a cold subnebula

In the previous sections, we have considered the case where material entering a planetary subnebula would be vaporised and undergo a period during which further reactions are possible. In the opposite scenario, however, where the planetary subnebula is sufficiently cold that the material is never revaporised, the situation is far simpler. The material which is used to form the regular satellites of the planet would be representative of that making up the subnebula, which would, in turn, be the same as that in the general vicinity of the planet within the Solar nebula. As a result, one would expect that, for the “cold subnebula” hypothesis, the regular planetary satellites would exhibit D:H ratios identical to that present in the Solar nebula at the heliocentric formation distance of their parent planet.

However, should that planet has migrated a significant distance between its formation and the formation of its satellites, we would expect that the satellites would display \( f \)-values representative of the regions through which the planet migrated as they formed. Hence, if some satellites formed earlier in the migration than others, they could display some variation in their incorporated deuterium content, and individual satellites may have values which result from the combination of deuterated ice from various locations in the planetary migration. However, unless the planets migrated over a very large distance, these variations should be fairly minor.

It is clear, therefore, that there would be expected to be a significant difference in the measured D:H values for the regular icy planetary satellites between these two models (the “hot” and “cold” subnebula approaches). This means that measurements of the D:H value in these satellites are critical in helping our understanding of subnebula processes and the general conditions present at the time of the formation of the regular icy satellites.

At a first glance, it appears that the idea of a “cold” subnebula is, at the very least, at odds with the volatile-poor compositions of both Io and Europa. Indeed, it could be argued that these bodies argue for a “hot” subnebula - at least in the inner regions closest to Jupiter. However, when one considers the temporal evolution of the subnebula, that is, the way in which the subnebula
cools over time, it is quite possible that the two innermost Galilean satellites formed early, while the nebula was still hot enough to vaporise the volatile content of inbound planetesimals, whilst the outer moons would form later, after the nebula has cooled sufficiently that the remaining infall of planetesimal material remains frozen throughout. This “hybrid” model has previously been discussed (e.g. Mousis & Gautier 2004, and Alibert et al. 2005). In other words, it is possible that the various satellites formed in different thermodynamic regimes, typified by our two extreme cases.

4  Deuterium enrichment in the irregular satellites and beyond

Beyond the case of the regular planetary satellites, the study of deuterium could offer insights into the formation mechanisms for other populations of icy bodies. Horner et al. (2007) made a study of the way that \( f \) measured in icy planetesimals (particularly the comets we observe today) would be affected by their formation location in the Solar nebula. It is clear that the application of these ideas need not be limited to the study of cometary bodies, and so we here extend our arguments to the other icy bodies in the outer Solar system, an ever increasing number of which have been discovered in recent years. One family of icy bodies whose numbers have grown rapidly in the last decade are the irregular satellites of the outer planets. Ongoing surveys (e.g. Sheppard et al., 2006) have now found many such bodies orbiting around Jupiter, Saturn, Uranus, and Neptune, with a roughly equivalent number in each case. This is a somewhat unexpected result when one considers the huge range of semi-major axes and mass that is covered from Jupiter to Neptune. The satellites themselves seem to gather in discrete dynamical families - which suggests that a much smaller population of objects has slowly been collisionally shattered to provide that we see today. The satellites orbit far further from their parent planets than the regular satellites discussed earlier, with a much wider range of eccentricities and inclinations. Indeed, many of the irregular satellites orbit their parent planets in a retrograde fashion. These orbits are believed to the result of the parent bodies of the irregular families having been captured during the final stages of planet formation.

Whilst the catalogue of icy Solar system objects has been growing rapidly, a number of authors have been looking into methods by which these various populations of object could be formed (e.g. Morbidelli et al., 2005, on the permanent Jovian Trojans; Horner & Evans, 2006, on the capture of Centaurs onto Trojan orbits and Jewitt et al., 2007 on the capture of the irregular satellites). From the various formation mechanisms proposed for the different reservoirs, it is clear that these bodies could have formed from material sourced from throughout the outer Solar system, and hence would be expected to display \( f \)-values significantly different to those expected from objects which
formed at 5 AU. Indeed, the first measurements of the mass and density of a binary object within the Jovian Trojan population (Patroclus, found to have $\rho \sim 0.8 \pm 0.15 \text{g/cm}^3$ (Marchis et al., 2006)) have shown that at least some of these objects are similar in nature to objects in the outer Solar system (binary Edgeworth-Kuiper belt objects, for example), rather than being dense rocky or metallic objects.

Given that these families of icy bodies are likely to be captured members of these parent populations, we can apply the same arguments to them as applied by Horner et al. (2007) to the comets. Studies of $f$ in the ice of a particular irregular satellite, for example, could then give information on its formation region within the Solar nebula - with chaotic scattering of the icy bodies in the disk, it is quite possible that the irregular satellites formed throughout the outer Solar system, and thus that they will exhibit a wide range of $f$-values. That said, if the bodies within a family of irregular satellites truly represent the remains of a single, collisionally fractured parent body, then we would expect that the $f$-value measured for all objects within a family would be the same. Different families would have a different $f$, reflecting their different formation regions, but all bodies in given family would have the same $f$. It is also clear that, given their different formation mechanism, the irregular satellites should display $f$-values that are greatly different to those that would be observed in the regular family - not only did they likely form at different heliocentric distances, but the material from which they formed was also not reprocessed in the planetary subnebula, and as such would be expected to contain significantly more deuterium within their water than is present in the regular satellites.

Next, consider the various theories of Jovian Trojan formation. From the above, it is clear that, had the Trojan asteroids formed in situ, then they would display $f$-values typical of objects forming at $\sim 5$ AU from the Sun. If, however, the Trojans were captured late in the development of the Solar system (for example, during the Late Heavy Bombardment, e.g. Morbidelli et al., 2005), it is possible that the bulk of the material which formed between the orbits of Jupiter and Neptune would have been cleared, and thus that the Trojans could primarily have originated in the youthful Edgeworth-Kuiper belt. This would, in turn, mean that the bulk of the objects would display similar, high values of $f$. Had the Trojans instead been captured at an earlier epoch, one might expect them to display a far wider range of $f$-values, representative of those for objects forming in the whole outer Solar system.
5 The future of extra-terrestrial deuterium enrichment measurements

Observations of the D:H ratio in water have been carried out for the terrestrial planets (e.g. Encrenaz et al., 1995, Makrides et al., 2006 etc.), together with comets Hyakutake (Bockelée-Morvan et al., 1998), Hale-Bopp (Meier et al., 1998) and Halley (Balsiger et al., 1995). Additionally, the D:H ratio in molecular hydrogen has been measured for the giant planets (e.g. Feuchtgruber et al., 1999, Lellouch et al., 2001), while the value of the D:H ratio within CH$_4$:CH$_3$D in the atmosphere of Titan has been measured from the Earth (e.g. Coustenis et al., 2003) and by Cassini (e.g. Bézard et al., 2007). However, beyond this restricted set of measurements, little is known about the amount of deuterium incorporated in the bodies of our Solar system. Fortunately, in the forthcoming years, a number of new instruments should shed new light on the deuteration of the Solar system.

Since they cover the far infrared/millimeter range, the Herschel Space Observatory and Atacama Large Millimeter Array (ALMA) will both provide an opportunity for observers to measure $f$ in the atmospheres of the planets, and comae of comets. We will have access to the Centaurs and short-period comets, and any object that could exhibit a tenuous atmosphere. It is now well understood that the short-period comets are the daughter population of the Centaurs (e.g. Horner et al., 2004). Therefore, it is clear that, even if no Centaur is active enough to be studied with these instruments, additional measurements of deuterium in such comets will provide new constraints on the range of $f$-values which exist in these bodies (as discussed in Horner et al., 2007). In turn, this will allow us to place better constraints on the formation regions of the various cometary reservoirs. For a more detailed review of the measurements which will be possible with these instruments, we direct the reader to Encrenaz et al. (2005).

Rosetta will rendezvous with comet 67P/Churyumov-Gerasimenko in 2014. Onboard the main spacecraft is a near-infrared spectrometer, VIRTIS, that will provide spectra in the near infrared (2-5 microns) at spectral resolutions R between 300 and 1000. Detection of deuterated species such as HDO and CH$_3$D on the nucleus will be possible (Coradini et al., 1998). The MODULUS Ptolemy experiment on the Roland lander will obtain isotopic ratios of the major volatiles in situ by ion trap mass spectrometry and gas chromatography (Biele et al. 2002). These measurements, offering us the chance to look at a Jupiter family comet close up, will allow us further information on the $f$-value in Jupiter-family comets, and their parents, the Centaurs.

The James Webb Space Telescope (hereafter JWST) will allow the D:H ratio in many solar system objects to be probed beginning in 2014. This will
be possible thanks to two instruments, the Mid-IR Instrument (MIRI) and the multi-object spectrometer (NIRspec). MIRI will provide broadband field imagery and medium resolution spectroscopy (up to R = 3000) between 5 and 27 microns (29 microns for the spectroscopy), while NIRspec will allow simultaneous spectroscopic observations at comparable spectral resolution, of up to 100 objects at wavelengths between 0.6 and 5 microns. It will be possible to examine the inner comae of active comets with NIRSpec, allowing high precision measurements of the degree of deuterium enrichment. For the largest and closest KBOs, it will also be possible to obtain spectra, allowing the identification of major molecules and isotope ratios (including deuterated species) for objects such as Triton, Pluto, Quaoar and Varuna (Gardner et al., 2006). It should therefore also be possible to measure the value of D:H in the water ice on the surface of the Jovian satellites, together with taking advantage of the outgassing from Enceladus to measure the $f$-value for the Saturnian satellite in some detail.

It has been suggested that the dust clouds recently discovered in the vicinity of the Galilean satellites in the Jovian system are the result of hypervelocity impacts of interplanetary micrometeorites upon their surface (e.g. Krivov et al. 2002; Krüger et al. 2003, 2006). Collection of this dust by a spacecraft would therefore enable us to study the $f$-value present in the ices of these worlds. For this reason, looking still further into the future, it is vital that the proposed Laplace mission, scheduled to launch in 2017 at the earliest, includes instruments dedicated to the analysis of both the chemical and isotopic composition of dust particles collected while in the Jovian system. In particular, we believe that the mission should make a priority of the collection of dust in the vicinity of the icy satellites during close fly-bys. In order that the value of $f$ in these grains can be measured, the mission will need to incorporate a dust collector with an ablation system which would vaporise them. A high resolution mass spectrometer would then allow the measurement of D:H in hydrogen bearing volatiles. It is important to note that such an instrument would need to have a significantly higher resolution than the Ion and Neutral Mass Spectrometer on Cassini. That instrument, although it has obtained many exciting results, sadly lacks the resolution necessary to separate different species with the same atomic weight, having a resolution of just 1 amu. Therefore, the identification of deuterated species is not possible due to the presence of other molecules of the same weight (e.g. HD$^{16}$O vs. H$_2^{17}$O; NH$_3$ vs. CH$_3$D).

With regard to the irregular satellites, it may be that a close approach by a mission (such as Laplace) en-route to Jupiter may reveal traces of outgassing from one of these icy bodies, allowing a direct measurement of the $f$-value within the body to be made. However, it is more likely that such a close approach would allow such a mission to collect dust and ice sputtered from the surface of these satellites in the same way as with the regular satellites.
We suggest that such a flyby would be of great value to the scientific community as a whole, and hope that the proposed missions can find room in their schedules for a visit to the irregular regime.

6 Summary and discussion

In previous work (Horner et al., 2007), we examined the role that variations in the D:H ratio through the Solar nebula would have on cometary objects observed to originate from different reservoirs in the outer Solar system. The goal of that work was to highlight that observations of the D:H ratio in such objects could prove a cornerstone in helping our understanding of the different regions in which the various cometary populations formed.

Here, we have extended our arguments to include the other populations of hydrated objects in the outer Solar system - the icy planetary satellites (both regular and irregular), and the Jovian and Neptunian Trojans. We have shown that, since these objects cover a wide range of formation scenarios, the study of the D:H incorporated in their water ice provides a useful tool to answer questions on their origin. Did the regular satellites form in a hot or cold subnebula? Do the irregular planetary satellites truly represent a captured and then shattered population of objects? If so - from where were they captured? What was the origin of the Jovian and Neptunian Trojans?

We focus, in particular, on the formation of regular satellites in a circumplanetary disk of gas and dust around Jupiter – the Jovian subnebula. Current theories which describe the formation of such satellites cover a wide range of initial conditions. However, the two extreme cases are the “hot” and “cold” subnebula models. In the former, the entire subdisk is sufficiently warm that icy material falling into the subnebula from the Solar nebula is entirely vaporised, allowing the exchange of deuterium between molecular hydrogen and water to continue in the gas phase, when the water involved would otherwise already be trapped as ice. The other extreme, the “cold” model, assumes that the subnebula was sufficiently cold that none of the infalling volatiles were vaporised prior to their accretion in the planetesimals which went on to form the satellites. Although the true formation scenario for the regular satellites undoubtedly lies somewhere between these extremes, they allow us to constrain the behaviour of the ices which went on to form the satellites we currently observe. In the case of the “hot” subnebula model, we have shown that the effect of the re-vaporisation of the infalling water ice allows gas phase reactions between HDO and $H_2$ to occur, leading to the gradual depletion of deuterium within the initially D-rich water. As a result, satellites which formed in this way would be expected to exhibit D:H ratios in their ice which are close to the Solar value. By contrast, in the case where the satellites form in a “cold”
subnebula, since vaporisation of the volatiles does not occur, the D:H ratio within the satellite ices would be significantly higher, representative of material within the Solar nebula at the heliocentric distance at which the satellite’s parent planet formed. The measurement of the D:H ratios within the regular satellites therefore provides a key constraint for the discussion of their formation. Although we do not go into specific detail, the models described above are equally applicable for satellites forming in the Saturnian subnebula.

In the future, new observatories and space missions will allow us to measure $f$ with a greater accuracy, and in many more objects, than ever before. HERSCHEL, ALMA, Rosetta, and the JWST will allow the measurement of deuterium in objects as diverse as KBOs, comets, and the satellites of the giant planets, while the proposed Laplace Jupiter orbiter offers a unique opportunity to measure deuterium in-situ, through use of a dust collector/ablation system, allowing the direct comparison of the regular and irregular Jovian satellites, and offering new insights into their formation. Early discussion of the type of measurements required is vital for those involved in the planning stages of these projects, in order that appropriate instrumentation is constructed to make the required measurements.

Another factor which may have influenced the final value of $f$ obtained by objects (particularly the giant planets and their regular satellites) is that the giant planets are thought to have migrated over a significant distance during their formation and subsequent evolution. In the most extreme examples, it has even been suggested that Uranus and Neptune formed between the orbits of Jupiter and Saturn (Levison et al., 2004)!

In these cases, it is likely that the value of $f$ shown by the regular satellites of these planets will provide a doubly useful tool in determining the true history of the outer Solar system, even though it seems likely that these satellites have been destroyed and reassembled since their formation (e.g. Banfield & Murray, 1992). If it is the case that Uranus and Neptune formed far closer to the Sun than their current location, then it seems likely that the material incorporated in their regular satellites could reflect their formation and migration. It must be pointed out, here, that current measurements of the $f$-value in the giant planets themselves provides no useful constraint on their formation location, due to the fact that the measured value is heavily affected by the gaseous hydrogen incorporated during their formation, in addition to water obtained from planetesimals. Given a sufficiently good interior model (e.g. Feuchtgruber et al. 1999), it may be possible to extract the native $f$-value of the accreted icy fraction of the planet, which would clearly prove very useful in the study of the planetary migration. However, the satellites currently offer a simpler solution to the problem, since they formed solely from the accretion of planetesimals. Studies of these objects could provide detailed information on their $f$-values, which can constrain their migration and formation histories. Were the satellites present prior to the migration? Did they form afterward, or during the process? Similarly, should
it turn out that the “cold subnebula” model is the fairest representation of
the formation of the regular Jovian and Saturnian satellites, then it is possible
that these objects contain, trapped within their ices, a record of the migration
of their parent planets through the Solar nebula. Clearly, such measurements
could even be used to place constraints on the distance over which the planets
migrated.

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Table 1
Initial radius $R_{D0}$, mass $M_{D0}$ and viscosity parameter $\alpha$ of the minimum-mass and maximum-mass solar nebula models used by Mousis (2004).

|                      | $R_{D0}$ (AU) | $M_{D0}$ ($M_\odot$) | $\alpha$ |
|----------------------|--------------|----------------------|---------|
| Maximum mass solar nebula | 27           | 0.3                  | 0.003   |
| Minimum mass solar nebula | 15           | 0.06                 | 0.003   |
Table 2
Thermodynamic parameters adopted for the warm sub nebula.

| Thermodynamic parameters                  | Value               |
|-------------------------------------------|---------------------|
| Mean mol. weight (g/mole)                 | 2.4                 |
| $\alpha$                                  | $2 \times 10^{-4}$  |
| Disk’s radius ($R_J$)                     | 150                 |
| Initial disk’s mass ($M_J$)               | $3 \times 10^{-3}$  |
| Initial accretion rate ($M_J$/yr)         | $1 \times 10^{-5}$  |
| Accretion timescale (yr)                  | 140                 |
Fig. 1. Deuterium enrichment factor $f$ calculated at the epochs of the condensation of water for the minimum mass and maximum mass solar nebula models (see e.g. Mousis 2004). The vertical bold solid lines correspond to the range of values of $f$ inferred in the icy solids produced in Jupiter and Saturn’s feeding zones.
Fig. 2. Temperature profiles at different epochs in the midplane of the Jovian sub-nebula, at times (from top to bottom) $t = 0$, 100 yr, 300 yr, $10^3$ yr, $2 \times 10^3$ yr, $5 \times 10^3$ yr and $10^4$ yr.
Fig. 3. Pressure profiles at different epochs in the midplane of the Jovian subnebula. Times are the same as in Fig. 2.
Fig. 4. Surface density profiles at different epochs in the midplane of the Jovian subnebula. Times are the same as in Fig. 2.
Fig. 5. Enrichment factor $f$ of the D:H ratio in H$_2$O with respect to the protosolar value in the Jovian subnebula midplane, as a function of the distance to Jupiter, at times (from top to bottom) $t = 1$ yr, 5 yr, 10 yr, 50 yr, 100 yr and $10^3$ yr. Calculations are made for the deuterium exchange between water and hydrogen in the vapor phase. They are stopped when water is condensed, a process that occurs closer and closer to Jupiter when time increases. The value for $f$ at $t = 0$ is taken to be equal to 3.8 (the minimum deuterium enrichment value in water ice condensed at 5.2 AU in the solar nebula – see e.g. Fig. 1), whatever the distance to Jupiter in the subdisk.