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Water and related chemistry in the solar system. A guaranteed time key programme for Herschel

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ABSTRACT

"Water and related chemistry in the Solar System" is a Herschel Space Observatory Guaranteed-Time Key Programme. This project, approved by the European Space Agency, aims at determining the distribution, the evolution and the origin of water in Mars, the outer planets, Titan, Enceladus and the comets. It addresses the broad topic of water and its isotopologues in planetary and cometary atmospheres. The nature of cometary activity and the thermodynamics of cometary comae will be investigated by studying water excitation in a sample of comets. The D/H ratio, the key parameter for constraining the origin and evolution of Solar System species, will be measured for the first time in a Jupiter-family comet. A comparison with existing and new measurements of D/H in Oort-cloud comets will constrain the composition of pre-solar cometary grains and possibly the dynamics of the protosolar nebula. New measurements of D/H in giant planets, similarly constraining the composition of proto-planetary ices, will be obtained. The D/H and other isotopic ratios, diagnostic of Mars' atmosphere evolution, will be accurately measured in H_2O and CO. The role of water vapor in Mars' atmospheric chemistry will be studied by monitoring vertical profiles of H_2O and HDO and by searching for several

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other species (and CO and H_2O isotopes). A detailed study of the source of water in the upper atmosphere of the Giant Planets and Titan will be performed. By monitoring the water abundance, vertical profile, and input fluxes in the various objects, and when possible with the help of mapping observations, we will discriminate between the possible sources of water in the outer planets (interplanetary dust particles, cometary impacts, and local sources). In addition to these inter-connected objectives, serendipitous searches will enhance our knowledge of the composition of planetary and cometary atmospheres.

1. Introduction

The Herschel Space Observatory (HSO) (Genzel, 1997; Pilbratt, 2008) is a space-borne far-infrared observation facility of the European Space Agency which has been launched by an Ariane 5 rocket on 14 May 2009. The planned mission duration is 3–4 years. Herschel carries a 3.5 m telescope which will enable high sensitivity and high spatial resolution observations from 55 to 672 μm.

The initial key programme Announcement of Opportunity was issued in February 2007 and among others the guaranteed time key project "Water and related chemistry in the Solar System", also known as "Herschel Solar System Observations" (HssO) Key Programme,[1] has successfully undergone a peer-review process. It spends 293.7 h of guaranteed time. The time is provided by 10 countries, two mission scientists, and Herschel Science Centre members. The team consists of 50 individuals from 25 institutes in 10 countries, with internationally recognized expertise in cometary and planetary science and a larger number of publications and citations related to the research topics of this project.

In this paper, we aim at presenting the HssO Key Program. In Section 2, we will first briefly draw up the main characteristics of the payload instruments onboard the Herschel spacecraft. In Section 3, we will describe the HssO project and its main objectives. Then, the sub-programs dedicated to Mars (Section 4), to the outer planets, Enceladus and Titan (Section 5) and to the comets (Section 6) will be introduced more specifically. Afterwards, we will detail our data processing and analysis plan in Section 7. Finally, the project's objectives will be summarized in Section 8.

2. The HSO payload instruments

The Herschel spacecraft will carry three instruments: the Heterodyne Instrument for the Far-Infrared (HIFI) (de Graauw and Helmich, 2001; de Graauw et al., 2008), the Photodetector Array Camera and Spectrometer (PACS) (Poglitsch et al., 2001, 2008) and the Spectral and Photometric Imaging REceiver (SPIRE) (Griffin et al., 2001, 2008).

HIFI is composed of seven mixer bands that cover the 480–1250 GHz (bands 1–5) and the 1410–1910 GHz (bands 6–7) frequency ranges and of two spectrometers. The High Resolution Spectrometer (HRS) enables the instantaneous coverage of 250 MHz (up to 500 MHz in the low resolution mode) with spectral resolutions ranging from 0.14 to 0.54 MHz (1.1 MHz in the low resolution mode), while the Wide Band Spectrometer (WBS) will cover 4 GHz with a spectral resolution of 1.1 MHz. A summary of the sensitivities and beam sizes depending on the frequency range can be found in Table 1.

PACS is designed to perform either imaging photometry or line spectroscopy (Table 2). In photometry mode, the instrument will provide a field-of-view (FOV) of $1.75' \times 3.5'$ and will offer the possibility to observe two of the three available bands: 60−85 or 85−125 and 125−210 μm. In line spectroscopy mode, PACS will cover a FOV of $47'' \times 47''$ (with a 5×5 pixel array) between 57 and 210 μm. The spectral resolution of the spectrometer will be ~1700 in its highest resolution.

SPIRE is composed of a three-band camera at 250, 350 and 500 μm for photometry and a Fourier Transform Spectrometer (FTS) for spectroscopy that covers the 194−672 μm with two bands with a resolving power of 20–1000. The camera has a FOV of $4' \times 8'$ whereas the FTS has a 2.6' in diameter circular FOV. More details are given in Table 3.

The Herschel Space Observatory will enable us to observe water (among many other molecules) in one of the last unexplored region of the electromagnetic spectrum with unprecedented sensitivity, spatial and spectral resolution without obscuration by the atmosphere of the Earth (that occurs at most

Table 1
The Heterodyne Instrument for the Far Infrared.

Bands	Spectral bands (GHz)	T_{sys} (K)	Beam size (")
1	480–640	160	33−44
2	640–800	320	26−33
3	800–960	480	22−26
4	960–1120	730	19−22
5	1120–1250	1250	17−19
6	1410–1710	2500	12−15
7	1710–1910	2500	11−12

Notes: T_{sys}: system temperature. Reference: de Graauw et al. (2008).

Table 2
The Photodetector Array Camera and Spectrometer.

Observing mode	Spectral band (μm)	FOV
Imaging	60−85	$1.75' \times 3.5'$
dual	85−125	$1.75' \times 3.5'$
photometry	125−210	$1.75' \times 3.5'$
Integral-field	55−73	$47'' \times 47''$
line	73−98	$47'' \times 47''$
spectroscopy	102−210	$47'' \times 47''$

Notes: FOV: field-of-view. Reference: Poglitsch et al. (2006, 2008).

Table 3
The Spectral and Photometric Imaging REceiver.

Observing mode	Spectral band (μm)	N_d	FOV	Beam size (")
Photometric	250	139	$4' \times 8'$	19
imaging	350	88	$4' \times 8'$	24
	500	43	$4' \times 8'$	35
Spectral	194–324	37	2.6′	16
imaging	316–672	19	2.6′	35

Notes: N_d: number of detectors; FOV: field-of-view; Sensitivity: values given for typical observations. Reference: Griffin et al. (2008).

[1] Webpage: http://www.mps.mpg.de/projects/herschel/HssO/index.htm.

Table 4
Planets and moons in the Solar System to be observed by this project.

Object	Apparent size (″)
Mars	5–10
Jupiter	36–45
Saturn	16.5–19.5
Titan	0.75
Enceladus	0.08
Uranus	3.5
Neptune	2.5

Table 5
Principal molecular lines to be observed or searched for in planetary and cometary atmospheres with HIFI.

Molecule	Transition	Frequency	Target	HIFI band
CO	5–4	576.3	Mars	1
	6–5	691.5	Mars	2
	8–7	921.8	Mars	3
$C^{17}O$	7–6	786.3	Mars	2
$C^{18}O$	7–6	768.3	Mars	2
^{13}CO	7–6	771.2	Mars	2
H_2O	$1_{10}-1_{01}$	556.9	Mars, outer planets, Titan, comets	1
	$2_{11}-2_{02}$	752.0	Mars, comets	2
	$2_{02}-1_{11}$	987.9	Comets	4
	$3_{12}-3_{03}$	1097.4	Mars, outer planets	4
	$1_{11}-0_{00}$	1113.3	Comets	4
	$2_{21}-2_{12}$	1661.0	Comets	6
	$2_{12}-1_{01}$	1669.9	Outer planets, comets	6
$H_2^{17}O$	$1_{10}-1_{01}$	552.0	Mars	1
$H_2^{18}O$	$1_{10}-1_{01}$	547.7	Mars, comets	1
HDO	$1_{10}-1_{01}$	509.3	Comets	1
HDO	$2_{11}-2_{02}$	599.9	Mars	1
NH_3	1_0-0_0	572.5	Comets	1
H_3O^+	$0_0^- - 1_0^+$	984.6	Comets	4
O_2	54–34	773.8	Mars	2
H_2O_2		1898.1	Mars	6
HCl	3–2	1876.2	Mars	6
CH_4		1882	Outer planets	6

Note: Frequencies are given in GHz.

of the observable wavelengths). The telescope will explore a wider frequency range with a better sensitivity than other submillimeter space telescopes like SWAS and Odin, which bands were mostly centered around 550 GHz. To illustrate the gain in sensitivity we compare the SWAS (Gurwell et al., 2000) and Odin (Biver et al., 2005) observations of Mars with what we expect from HIFI. In both cases more than 24 h of observation time were required in order to get an absorption spectrum of the rotational ground-state of water with a signal-to-noise ratio (S/N) of ~10. HIFI needs about 10 min of observation time for a S/N of 100 (nominally only a few seconds for an S/N of 10). A S/N of 100 is required for retrieving the vertical profile of water (e.g., Hartogh and Jarchow, 2004) and it is a unique feature of Herschel. Herschel will also have much better sensitivity and spectral resolution than ISO. Therefore, the vertical profiles of molecules in planetary atmospheres will not only be retrieved from line shapes, but also for instance from multi-line analysis of PACS spectra (Rengel et al., 2009). The Herschel spacecraft has been put into orbit at the Lagrangian point L2. Thus, the telescope is at a very good position to observe most of the Solar System objects. However, the HSO can only observe objects with solar elongations in the range 60–120°. This precludes the observation of Venus and is a strong penalty for cometary studies. Especially, Target of Opportunity (TOO) comets will not be observable when their solar distance is smaller than ~1 AU. In Table 4, we present the planets and satellites of the Solar System that will be observed, along with their apparent sizes during the telescope operations.[2] As its instruments are versatile, Herschel is well suited for planet and satellite observations as well as for comet observations (spectral lines and continuum).

3. The HssO project

This project proposes to observe water and related chemical molecules in a variety of objects of the Solar System (see Table 5 for the species looked for with HIFI, for example). Indeed, water is ubiquitous in the Solar System and throughout the Universe. It is present in gaseous form in all planetary and cometary atmospheres (e.g., Biver et al., 2005; Feuchtgruber et al., 1997). We find it in the form of ice on the surface and subsurface of Mars (Boynton et al., 2002; Bibring et al., 2004; Bandfield, 2007), comets, most outer satellites and distant bodies. So far, liquid water has been found only on Earth, but it was most likely present in the past history of Mars, and it could also presently exist under the icy surface of Europa (Squyres et al., 1983), Enceladus (Manga and Wang, 2007), and possibly other outer satellites.

Water has played a key role in the formation of Solar System planets. Indeed water, made of two atoms with high cosmic abundances, must have been a relatively abundant molecule in the protosolar disk (Pollack et al., 1994). As water is the first hydrogenated molecule to condense as the temperature decreases, it actually determines the position of the "snow line" which separates the region of terrestrial planet formation from that of the giant planets (e.g., Encrenaz, 2008, for a review). Beyond the snow line, in the outer Solar System, most of the satellites and small bodies contain a significant fraction of water ice; in the case of comets, this fraction is as high as 80% in the icy phase (Bockelée-Morvan et al., 2005). Water also played a major role in the diverging evolution of the terrestrial planets, by being in gaseous form on Venus (Ingersoll, 1969; Grinspoon, 1993; Gurwell et al., 2007), mostly in liquid form on Earth, and preferentially in solid form on Mars (Boynton et al., 2002; Bibring et al., 2004; Bandfield, 2007).

Studying water and its isotopologues in Solar System bodies provides key information about their formation and evolution. A crucial parameter, in particular, is the deuterium/hydrogen (D/H) ratio measured in water (Robert et al., 2000). It is known from laboratory experiments, and confirmed by observations in the interstellar medium (ISM), that deuterium is enriched in ices, due to ion-molecule and grain-surface reactions at low temperature, and the D/H ratio is known to increase as the temperature decreases (e.g., Watson, 1974; Brown and Millar, 1989). The D/H ratio in Solar System objects (see Fig. 1) provides information about the physico-chemical conditions under which the water formed (Gautier and Hersant, 2005; Owen et al., 1999). As an example, the D/H value in comets, presently measured for six comets originating from the Oort-cloud (Weaver et al., 2008; Altwegg and Bockelée-Morvan, 2003; Hutsemékers et al., 2008; Villanueva et al., 2009), none of them a Jupiter-family short period comet from the Kuiper Belt, appears to be twice the Standard Mean Ocean Water (SMOW) value, which seems to imply that the terrestrial water did not entirely come from cometary bombardment; an important measurement will be the determination of D/H in comets coming from the Kuiper belt reservoir. In giant planets, the D/H in Jupiter and Saturn represents the protosolar gas value (Lellouch et al., 2001), while Uranus and Neptune appear to be enriched in D (Feuchtgruber

[2] The comets that will be observed are presented in Table 6 (see Section 6).

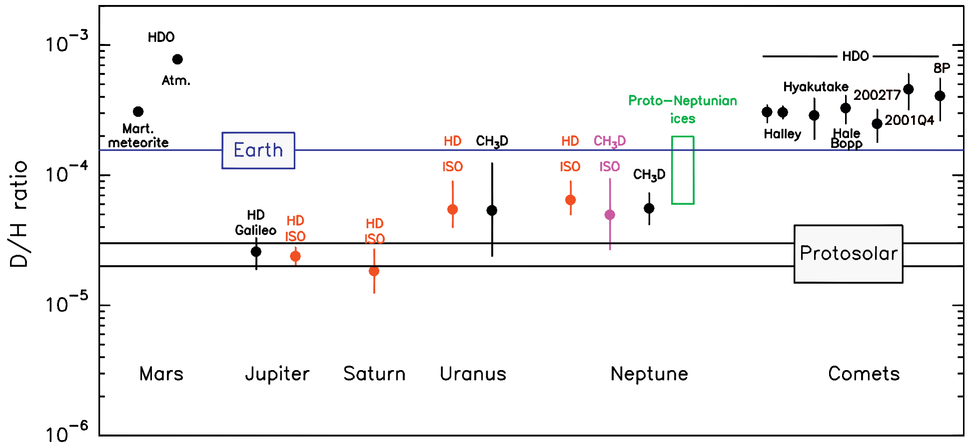

Fig. 1. D/H ratios in the Solar System.

et al., 1999) due to the mixing of their atmospheres with D-rich grains present in their cores (see Fig. 1). Comparing the D/H ratio in the four giant planets therefore provides a key insight into the composition of the protoplanetary grains, and their possible link to cometary grains (Hersant et al., 2001). The exact knowledge of the current D/H ratio in the Martian atmosphere is a key parameter in understanding the pre-Jeans escape water reservoir which is believed to be characterized by a D/H value about twice the terrestrial D/H ratio (Owen et al., 1988; Krasnopolsky et al., 1997), i.e. consistent with (Oort-cloud) cometary values. Whether cometary material is the best choice for the dominant source of Martian water or if differences in the Martian accretion history (i.e. heterogeneous versus homogeneous accretion in connection with hydrodynamic escape) can explain this enrichment, is an open question. Knowledge about the exact D/H ratios of the present Martian atmosphere and in Kuiper belt comets (from HDO/H_2O) will be milestones in constraining not only the thermal escape flux, but also the currently remaining water reservoirs on Mars. Herschel will also allow us to determine the origin of the external sources of water on the giant planets and Titan (Feuchtgruber et al., 1997; Coustenis et al., 1998). These measurements will be used to better constrain the production of water and dust in the outer Solar System. Specific aspects of water studies of this programme concerning the terrestrial and outer planets on the one hand and comets on the other hand will be described in the following sections.

4. Mars

HIFI will be able to determine vertically resolved D/H profiles from H_2O and HDO vertical profiles in the Martian atmosphere. The accuracy of the D/H determination will be an order of magnitude higher compared to former column abundances measurement (Krasnopolsky et al., 1997) (enrichment by 5 ± 2 compared to SMOW), i.e. it will not only constrain the water reservoir (Leshin, 2000; Lunine et al., 2003) and Jeans escape (e.g., Yung et al., 1988; Owen et al., 1988) of Mars, but also has the potential to find isotopic fractionation as a function of altitude and season (see Montmessin et al., 2005). Regarding oxygen, slightly non-terrestrial values have been reported for $^{18}O/^{16}O$ and $^{17}O/^{16}O$, respectively, 13% and 7% lower than their telluric counterpart (Krasnopolsky et al., 1996). Neither confirmed by Encrenaz et al. (2005) nor by Krasnopolsky et al. (2007), this surprising result (obtained with CO_2) needs confirmation by measuring the oxygen isotopic ratios in both CO and H_2O. Thus, specific observations of $C^{17}O$, $C^{18}O$, $H_2^{17}O$ and $H_2^{18}O$ will be performed. Understanding water isotopic ratios requires understanding of the Martian atmosphere as a whole, but there are still many unsolved questions related to the past climate of Mars and, in particular, the history of the H_2O and CO_2 reservoirs. In order to address these problems, we first need to better understand the present aeronomy of Mars and, more precisely, the water cycle. The composition of the Martian atmosphere is largely governed by the photochemistry of carbon dioxide and water (Nair et al., 1994), since water is the gas source of hydrogen radicals. The latter have been identified as the predominant catalytic drivers of carbon and oxygen chemistry and explain the rather low amounts of CO and O_2 in the Martian atmosphere (Parkinson and Hunten, 1972; Sonnemann et al., 2006). Quasi-simultaneous measurements of the vertical distribution of H_2O along with CO, O_2, H_2O_2 and temperature of the lower and middle atmosphere of Mars are a powerful tool for constraining these models. Regarding the Martian atmospheric composition, few gaseous molecular species have been spectroscopically identified so far: CO_2, CO (Kaplan et al., 1969), H_2O (Kaplan et al., 1964), O_2 (Carleton and Traub, 1972), O_3 (Lane et al., 1973) and recently H_2 (Krasnopolsky and Feldman, 2001), H_2O_2 (Clancy et al., 2004). Yet, photochemical models do predict the presence of a number of additional compounds, such as OH, HO_2, NO, etc. (Nair et al., 1994; Lefèvre et al., 2004; Sonnemann et al., 2009). A number of minor species in the Martian atmosphere are intimately related to water and are expected to vary in correlation (e.g., H_2O_2, HO_2, OH) or anti-correlation (O_3). They play an important role in the comparative planetology context (e.g., Seele and Hartogh, 1999; Hartogh et al., 2004; Sonnemann et al., 2007).

The water cycle is a key aspect of the Martian atmosphere/surface system. Temporal and spatial variations of the column-integrated amount of water have been characterized by space missions such as Viking (Jakosky and Farmer, 1982), Mars Global Surveyor, (Smith, 2002), and Mars Express (Fouchet et al., 2007). However, it was not possible to retrieve the vertical profile of water from these observations due to their low spectral resolution, except recent solar infrared occultation observations with Mars Express of Fedorova et al. (2009). HIFI observations should enable retrievals with an accuracy at least better by a factor of 5. So, extremely limited information is available on the vertical profile of water. So far only ground-based heterodyne observations using the weak H_2O 22 or 183 GHz and HDO 226 GHz lines (Clancy et al., 1992; Encrenaz et al., 1995, 2001) SWAS and Odin observations which both targeted the ground state transition of water (Gurwell et al., 2000; Biver et al., 2005) have provided results, but they have generally lacked in sensitivity to retrieve precisely the vertical profile of water. The most significant finding was the "variable hygropause level" between 10 km (aphelion) and ~50 km (perihelion). With its outstanding sensitivity and spectral resolution, Herschel will enable precise retrievals of disk-averaged vertical profiles of water as a function of solar longitude L_s (i.e. season). Thus, it will look for a confirmation and better characterization for the "variable hygropause level" asymmetry. If confirmed, this asymmetry is expected to drive a strong unbalance in the meridional transport from the source region in the North to the South and to influence strongly the water cycle. Due to its potential importance, a better observational characterization of this phenomenon is needed. It will be a strong constraint for models, describing the general circulation of the Martian atmosphere (e.g., Forget et al., 1999; Hartogh et al., 2005) and in particular its meridional transport (e.g., Medvedev and Hartogh, 2007).

For all topics (variable hygropause, chemistry, oxygen/hydrogen isotopic ratios and spectral scans), we will monitor the temporal behavior over the largest possible L_s coverage, because water controls chemistry and thus composition (line scans). Isotopic fractionation, especially of D/H, may be determined as a function of altitude and, due to its link to the chemistry, it may be seasonally variable as well. Most observations are planned at the beginning and the end of the first two observation windows (August–December 2009, $L_s = 323-22^\circ$ and March–July 2010, $L_s = 67-116^\circ$). Mars' apparent diameter will vary between 5 and 10 arcsec during both windows.

Vertical temperature profiles, derived from CO, will be obtained for accurate retrievals. The accuracy of a temperature profile depends on the knowledge of the vertical CO profile. Both can be retrieved simultaneously from observations of ^{12}CO and ^{13}CO lines. The quasi-simultaneous observation of higher-J lines of CO and its isotopes with S/N of 100 will extent the vertical coverage of the retrieved CO and temperature vertical profiles and increase the accuracy compared to lower-J line ground-based observations (since the lines are stronger).

5. Outer planets, Titan and Enceladus

A major discovery of ISO was the detection of water in the upper atmospheres of the four giant planets and Titan (Feuchtgruber et al., 1997; Coustenis et al., 1998), implying the existence of external sources of water. The associated fluxes are roughly estimated to broadly span the 1×10^4 to $1 \times 10^7\,\mathrm{mol\,cm^{-2}\,s^{-1}}$ range. This oxygen supply, which manifests itself also through the presence of CO_2 and CO in these atmospheres, may have several sources: (i) a permanent flux from interplanetary dust particles (IDP) produced from asteroid collisions and from cometary activity (Prather et al., 1978), (ii) local sources from planetary environments (rings, satellites) (Strobel and Yung, 1979; Prangé et al., 2006), (iii) cometary "Shoemaker-Levy 9 (SL9) type" impacts (Lellouch et al., 1995). Disentangling the various sources is a key objective. It bears implications on a variety of poorly understood phenomena such as (i) the production of dust at large heliocentric distances (Kidger, 2003) (ii) the transport and ionization of solid and gaseous material from satellites and rings in planetary magnetospheres (Connerney, 1986; Kempf et al., 2008) (iii) the frequency of cometary impacts in the outer Solar System today (Bottke et al., 2002; Levison et al., 2000).

In the current picture, most of the water present in Jupiter's upper atmosphere was delivered by the SL9 impacts in 1994, as determined from ISO, SWAS and Odin observations (Lellouch et al., 2002; Cavalié et al., 2008), and the permanent flux into Jupiter is at least 30 times less than in Saturn (Lellouch et al., 2002) and even lower than in Uranus and Neptune (Feuchtgruber et al., 1997). This scenario would suggest (i) an important role of the local sources (notably the rings) at Saturn (Prangé et al., 2006) and (ii) a large dust production in the Kuiper Belt. In addition, the input flux into Titan, although very uncertain, seems to be as high as in Saturn (Coustenis et al., 1998), which seems odd, given that gravitational focussing and ring contribution at Saturn are not available at Titan. A possibility could be that Hyperion is an effective source of icy dust (Banaszkiewicz and Krivov, 1997) that feeds the atmosphere of Titan. The overall picture of the source of oxygen has gained even more in complexity in recent years with important results on the origin of CO in Jupiter (Bézard et al., 2002), Saturn (Cavalié et al. 2009a, b), Titan (Hörst et al., 2008) and Neptune (Lellouch et al., 2005) and its first detection in Uranus (Encrenaz et al., 2004). Indeed, an external source seems to be active in all planets, possibly being due to regular large comet impacts in Jupiter, Saturn and Neptune. However, the entire picture remains tentative and demands confirmation, and the problem needs to be entirely re-addressed with new data.

For each of the five targets (the four giant planets and Titan), the proposed observations will consist of a combination of: (i) high signal-to-noise ratio ($S/N = 100$), spectrally resolved observations of one or a few water lines with HIFI, (ii) full-range spectra with SPIRE (except at Jupiter and Saturn, which are too bright) and (iii) dedicated, very high S/N (>100) observations of selected water lines with PACS. With the observations of this programme, we will:

- Improve the accuracy of the water abundances measured by ISO (Feuchtgruber et al., 1997; Lellouch et al., 2002), SWAS (Bergin et al., 2000) and Odin (Cavalié et al., 2008).
- Determine the vertical profile of water in the atmospheres of the outer planets and Titan. The water distribution is not only diagnostic of its origin (e.g., cometary impact vs. permanent dust deposition), but also of the rate at which it is transported within and removed from the atmosphere. This rate has to be known to estimate properly the input fluxes which are key in discriminating between the possible sources. The vertical profile of water will be determined from (i) line-shape measurements with HIFI, (ii) multi-line observations with PACS and SPIRE, or (iii) using a combination of the two approaches. Both methods have been applied on Jupiter from ISO, SWAS and Odin observations, by Bergin et al. (2000), Lellouch et al. (2002) and Cavalié et al. (2008), respectively. However, as (except in Titan's case) line widths are mostly due to rotational broadening (10–20 $\mathrm{km\,s^{-1}}$), measuring the line shape requires a high S/N, typically 100 at 4 MHz resolution, which might not be possible at Uranus and Neptune. There and at Titan, we will perform line scans with PACS on a variety of lines with very high S/N (>100) to obtain the vertical profile from a global modelling of the unresolved line contrasts. An accurate analysis of the H_2O line observations requires a good knowledge of the stratospheric thermal profile. Thermal information will be provided from simultaneous ground-based observations at 8 μm and from observations of CH_4 at 1882 GHz by HIFI (Jupiter and Saturn) and at 119.7 μm with PACS (including dedicated PACS line scans at Uranus and Neptune). The WBS of HIFI will enable the observation of the broad tropospheric absorption of the 1882 GHz line of CH_4 as well as its stratospheric emission core. The observation of CH_4 in Uranus and Neptune is interesting in itself as the stratospheric abundance of methane in Uranus and Neptune remains very uncertain.[3]

[3] We will combine Herschel observations with ISO CH_4 ν_4 band observations and/or ISO and Spitzer H_2 observations to get the thermal profile for these planets.

- Search for latitudinal variability of H_2O on Jupiter and Saturn from rough mapping with HIFI (only for Jupiter) and PACS (for both planets). An SL9 origin could still be visible as a hemispheric asymmetry in Jovian water, like in Jovian CO_2 (Lellouch et al., 2006). On both planets, a larger abundance at $40-60^\circ$ would be the signature or ring/satellite material preferentially infalling at high latitudes (Connerney, 1986).
- Search for temporal variability of all the above parameters. We will monitor the abundance of water about every 1.5 years (three visits to each object). This is a reasonable compromise between the Herschel lifetime and the variability timescales: (i) the vertical and horizontal mixing times are of the order of several years (ii) over a timescale of a few years, outer planets may get in or out of major cometary trails, which may modulate the H_2O/dust influx rates. If variations are found, we will search for correlations with the position of the planets with respect to the major cometary trails.
- Measure other species besides H_2O, including at least NH_3, PH_3 and CH_4 in Jupiter and Saturn, HCN and CO in Neptune, and CH_4, HCN, CO, and their isotopes in Titan, in full-range spectra with PACS and SPIRE. We will also explore serendipitously the spectra in search of yet undiscovered molecules. We anticipate the first detection of PH_3 in Uranus and Neptune.
- Observe HD with PACS in Jupiter, Saturn, Uranus and Neptune, permitting a new and consistent determination of the D/H ratio in H_2 in all four giant planets. The need for high precision justifies a dedicated PACS line scan of HD on Uranus and Neptune.

Water-driven cryo-volcanism was discovered by Cassini on Enceladus (Hansen et al., 2006) and maybe Titan (Lopes et al., 2007), but remains to be better characterized (temperature, surface extent, nature). A possible method is to monitor the continuum flux of these bodies and search for a hot-temperature component. We will search for a volcanic component from repeated, high S/N, 3-band PACS photometric measurements. The fact that each observation will give three exposures in the $130-210\,\mu m$ band means that we will have sufficient measurements to carry out reliable statistics with the photometry and use the $130-210\,\mu m$ band to fix our photometric baseline. Measurements in the $60-85\,\mu m$ band will be our prime detectors of cryovolcanic plumes. We wish to take nine observations at approximately 8 day intervals through the visibility window, with some flexibility permissible in the separation (from 6 to 10 days is acceptable). Our primary aim will be the detection of time variability in the $60-85\,\mu m$ flux (that samples the peak of the Planck function) that may be attributable to cryovolcanic activity. To minimize confusion with scattered emission from the rings, particularly for Enceladus, with its rather small elongation, and to still include the Southern polar regions in the beam, it is essential to carry out the observations during the 2010 ring plane crossing with the Saturnian ring system almost edge-on. This limits the observations to the visibility window from 19 May 2010 to 22 July 2010.

6. Comets

Having retained and preserved pristine material from the Solar Nebula at the moment of their accretion, comets contain unique clues to the history and evolution of the Solar System. Their study assesses the natural link between interstellar matter and Solar System bodies and their formation (Irvine et al., 2000; Bockelée-Morvan et al., 2000, 2005). Ironically, although being the most abundant cometary volatile, water is one of the most difficult species to observe. Since cometary gas is cold (10–100 K) and water is rotationally relaxed at fluorescence equilibrium, the rotational transitions between the lowest energy states are the most intense. The $1_{10}-1_{01}$ water line at 557 GHz is expected to be among the strongest lines of the radio spectrum of comets (Bockelée-Morvan, 1987). Its observation by the SWAS (Neufeld et al., 2000; Chiu et al., 2001; Bensch et al., 2004) and Odin (Lecacheux et al., 2003; Biver et al., 2007) satellites in several comets is very promising for Herschel.

Besides current in situ explorations and comet nucleus sample return missions in a more distant future, remote sensing is presently the best way to investigate the chemical and isotopic composition of cometary material. Recent observations resulted in a dramatic progress in our knowledge of cometary volatiles, where spectroscopy at radio wavelengths got the lion's share (Bockelée-Morvan et al., 2000, 2005). Other significant results came from infrared spectroscopy, either from space with ISO or from the ground at high spectral resolution (e.g., Crovisier et al., 1997; Mumma et al., 2003). By providing a sensitive access to a still poorly explored spectral domain, the three instruments of Herschel are expected to contribute significantly to these investigations (Bockelée-Morvan and Crovisier, 2001; Crovisier, 2005).

6.1. Water excitation and coma thermodynamics

Water plays an important role in the thermal balance of cometary atmospheres, as a cooling agent via emission in its rotational lines. This role is crucial in determining the expansion velocity and temperature of the atmosphere, which are two fundamental parameters for the physical description of this medium (Combi, 2002; Bensch and Bergin, 2004; Zakharov et al., 2007). Indeed, cooling becomes effective only in the outer coma where the transitions become optically thin. The observations of several water lines with Herschel will provide insights into the excitation of this molecule and optical depth effects. Observations of H_3O^+ will constrain the excitation by ionic collisions. This will lead us to more realistic models of the thermodynamics of the atmosphere.

6.2. The D/H ratio

Simultaneous observations of HDO and H_2O determine D/H in cometary water. This ratio was first measured in situ in comet 1P/Halley, then from ground-based observations in four other comets from the Oort-cloud (Altwegg and Bockelée-Morvan, 2003; Hutsemékers et al., 2008; Villanueva et al., 2009) and also from space-based observations in one more comet from the Oort-cloud (Weaver et al., 2008). A ratio D/H $\sim 3\times10^{-4}$ was derived in these six comets, none of them a Jupiter-family short period comet. This corresponds to an enrichment factor of $\sim$12 with respect to the protosolar D/H value in H_2, inexplicable by isotopic exchanges between H_2O and H_2 in the Solar Nebula. Fractionation effects through ion-molecule or grain surface reactions in the presolar cloud or the protosolar nebula have been invoked (Mousis et al., 2000; Ceccarelli et al., 2007). This ratio, however, is significantly below that of dense molecular clouds. This suggests that comets incorporated material reprocessed in the inner Solar Nebula, which was transported outwards by turbulent diffusion. This deuterium measurement was used by Hersant et al. (2001) to constrain evolutionary solar nebula models. Measurements of the D/H ratio in a larger sample of comets with HIFI, including short-period comets coming from the Kuiper Belt, would provide further constraints for Solar Nebula models. Short-period comets from the Kuiper Belt could have formed outside the turbulent Solar Nebula and may thus exhibit higher D/H ratios, as expected for unprocessed material. Comets formed close to the orbit of Jupiter are expected to have lower D/H ratios.

6.3. Full spectral scans

Full spectral scans with PACS and SPIRE will provide us with the simultaneous measurement of a number of water lines, the serendipitous observations of other volatiles, and the determination of the comet spectral energy distribution (SED). Observations of the thermal emission of the dust is a powerful tool for studying the mineralogy, the PACS spectral range being well adapted for searches for hydrous silicates (Mutschke et al., 2008). In the broader framework of the formation of planetary systems, cometary dust observation will provide important clues for interpretation of the evolution of dusty disks around young stars and should be a key tool for interpretation of Herschel observations of circumstellar media (Ehrenfreund et al., 2005).

6.4. Selected comets

The best short-period comets with returns in 2009–2012 have been selected according to their observing conditions and expected water outgassing. The figure of merit, roughly proportional to the signals, is the quantitative parameter we used for this selection. It is the ratio between $Q[H_2O]$ and Δ, where $Q[H_2O]$ is the expected production rate of water as derived from observations and models and Δ is the distance between Herschel and the comet.

103P/Hartley 2 is the best opportunity due to its close approach to Earth in October 2010. We wish to observe an unexpected comet as a TOO. We will aim at the first comet with $Q[H_2O]/\Delta > 10^{29}\,s^{-1}\,AU^{-1}$ occurring in the Herschel observing window (i.e., figure of merit larger than 103P/Hartley 2). On the average, one such comet is expected each year. The atypical comet 29P/Schwassmann-Wachmann 1 is also in our programme. It has a nearly circular orbit at $r_h \sim 6$ AU and two observing windows each year. At the time of the proposal acceptance, three other, weaker, comets had been selected: 22P/Kopff, 81P/Wild 2 and 144P/Kushida. Due to launch delays, this list has been revised (see Table 6). 22P/Kopff and 144P/Kushida were removed. Instead, C/2006 W3 Christensen is to be observed during the Science Demonstration Phase, and 45 P/Honda-Mrkos-Pajdušáková or another comet at a later stage of the mission.

With a very close Earth approach of 0.12 AU in October 2010, 103P/Hartley 2 will provide us with the opportunity of measuring weak lines not detectable in the other short-periodic comets and of mapping the water emission in the coma with the highest resolution achievable with Herschel. In particular, we expect that these observations will yield the first measurement of the HDO/H_2O ratio in a Jupiter-family comet. Observations of the $1_{10}-1_{01}$ ortho water ground-state transition provides the largest S/N ratio for a given integration time and these lines are used for mapping the water vapor in the coma and monitoring the overall cometary activity. The water excitation is constrained using dedicated observations of H_3O^+ (constraining the electron density) and higher-excited water rotational transitions made with HIFI as well as the SPIRE spectrometer and PACS line scans. While PACS and SPIRE allows for the quasi-simultaneous measurement of strong water lines, only HIFI can resolve the narrow line profiles and thus provide key information on water excitation and the kinematics of the outgassing.

With observations of comets C/2006 W3 Christensen, 81P/Wild 2 and 45P/Honda-Mrkos-Pajdušáková, we expand the water excitation studies to a small sample of comets and answer the question to what extent the result for 103P/Hartley 2 and the TOO comet are typical. With the line intensities in these targets being weaker by a factor of 8–12, the water excitation study will use a sub-set of lines observed in 103P/Hartley 2. High-resolution line profiles will also be measured to study asymmetric outgassing

Table 6
List of comets to be observed.

Date	r_h (AU)	Δ (AU)	θ (deg)	m_1	$Q[H_2O]$ ($10^{28}\,s^{-1}$)	*FM* Q/Δ	
C/2006 W3 Christensen (perihelion: 6 July 2009 at $r_h = 3.13$ AU)							
14 September 2009	3.20	2.56	120		4.0	1.6	Window begins
11 November 2009	3.36	3.74	60		4.0	1.1	Window ends
[Comet active far from the Sun; $m_1 = 10$ at $r_h = 3.7$ AU pre-perihelion; $Q[H_2O]$ extrapolated from unpublished OH observations with the Nançay radio telescope in February–April 2009]							
81P/Wild 2 (perihelion: 23 February 2010 at $r_h = 1.60$ AU)							
13 October 2009	2.08	2.40	60	13.6	0.5	0.2	Window begins
13 November 2009	1.88	1.84	77	12.4	0.8	0.4	
13 December 2009	1.75	1.45	89	11 4	1.0	0.7	
13 January 2010	1.65	1.12	103	10.4	1.2	1.1	
13 February 2010	1.60	0.86	120	9.7	1.3	1.5	Window ends
103P/Hartley 2 (perihelion: 28 October 2010 at $r_h = 1.06$ AU)							
23 October 2010	1.06	0.12	120	3.8	1.2	10.	Window begins
[$\Delta = 0.15\,AU$ on 3 November, 0.20 AU on 15 November]							
45P/Honda-Mrkos-Pajdušáková (perihelion: 28 September 2011 at $r_h = 0.53$ AU)							
14 August 2011	1.03	0.063	60	8.0	0.5	8.	Window begins
18 August 2011	0.98	0.071	120				Window ends
[$\Delta = 0.060$ AU on 15 August 2001]							
29P/Schwassmann-Wachmann 1							
07 April 2010	6.20	5.62	120				Window begins
12 June 2010	6.22	6.66	60				Window ends
10 November 2010	6.24	6.66	60				Window begins
11 January 2011	6.24	5.70	120				Window ends
[only windows in 2010 are listed]							
TOO comet							
TBD	[1.00]	[1.00]			[10]	>10	

Notes: r_h : distance to Sun; Δ : distance to Earth; θ : solar elongation angle; m_1 : expected total visual magnitude (taken from JPL/HORIZONS ephemerides); $FM = Q[H_2O]/\Delta$: figure of merit in units of $10^{28}\,s^{-1}\,AU^{-1}$.

and velocity offsets, as well as self-absorption effects. Differences in orbital and therefore thermal history of the chosen comets will be reflected in variable and specific outgassing patterns.

A shorter PACS SED scan will be made, focusing on the global dust emission (constraining the dust production and size distribution). We exploit the relatively large visibility windows of up to 6 months for these comets to study not only the spatial but also the temporal variation of the water vaporization using the ground-state transition of ortho-water. Finally, observations of water and ammonia will be made for 29P/Schwassmann-Wachmann 1. CO (with $Q{\sim}2\times10^{28}\,s^{-1}$) is mainly responsible for its activity, but cometary grains could be a source of water. We wish to conduct a sensitive search for water outgassing in this comet, at the limit $Q{\sim}10^{27}\,s^{-1}$.

7. Data processing and analysis plan

The data obtained within the framework of this Key programme will be processed using the standard Herschel data pipeline to produce calibrated brightness temperature spectra of individual objects. All reduced spectra will be individually inspected by the experts from the HIFI, SPIRE, and PACS consortia involved in the programme, who will assess the quality of the data and decide whether any additional post-processing, outside of the Herschel pipeline, is required before the data can be released to the public. If needed, additional data reduction tools will be developed at this point and the final, corrected spectra will then be made available for inclusion in the ESA Herschel Science Archive. The subsequent analysis and dissemination will proceed in three steps, as described below. The software tools needed for the analysis and interpretation of the data within each subprogramme are already well developed.

The immediate science goal of our programme is to extract a set of vertical profiles and isotopic ratios in individual objects. The detailed analysis will vary depending on the object. For Mars, vertical profiles will be retrieved using the MPS radiative transfer and retrieval model (e.g., Hartogh and Jarchow, 2004; Hartogh et al., 2007), which has recently been matched to a 3-d general circulation/chemistry transport (GCM/CTM) model of the Martian atmosphere, in that it is based on the same grid pattern. The model takes into account nadir and limb contributions. For each observation sequence, we will first retrieve the vertical temperature profile from observations of CO, and use it as an input parameter for the retrieval of other molecules. A number of these vertical profiles will either be derived for the first time, or with a much higher accuracy than before, including the vertical profiles of the isotopic ratios (D/H, $^{16}O/^{17}O$, and $^{16}O/^{18}O$). This will be done in a timely fashion, after the calibrated observations are delivered to the team. For the outer planets, calibrated spectra will be calculated using standard radiative transfer models. The computer codes, already in place at various institutions (Observatoire de Paris, Laboratoire d'Astrophysique de Bordeaux, MPS Lindau), include all relevant physical and geometrical aspects (rotational smearing, integration over viewing angles, etc.) and have been validated on ISO (Lellouch et al., 2002), SWAS (Bergin et al., 2000) and Odin (Cavalié et al., 2008) observations. For each planet, the atmospheric thermal profile will first be determined from the CH_4 observations, and then used to retrieve the H_2O vertical profile. As the data come in, we will rapidly release the resulting vertical profiles of water vapor in each planet and its horizontal distribution in Jupiter and Saturn. In this initial analysis, the vertical profiles may be described in a simple, heuristic fashion (e.g., the vertical gradient of concentration with pressure). Furthermore, we will analyze the spectral scans carried out with HIFI, PACS, and SPIRE, discussing new results on the atmospheric composition. Topical papers, especially on the CH_4 abundance in Uranus and Neptune and in the D/H ratio in all four giant planets will also be written. For comets, water excitation and the D/H ratio will be analyzed in individual targets. The data will be used for refining the existing cometary excitation models (Bensch and Bergin, 2004; Bockelée-Morvan, 1987; Zakharov et al., 2007), which include collisions within the coma (with water and electrons), solar pumping and photo-dissociation within a flexible framework (e.g., Monte Carlo simulations). A 3-D model, that can handle any coma density and velocity distribution as input, is already available to analyze the H_2O spectral maps. Reliable water production rates will then be provided for supporting ground-based observations (IRAM, CSO, APEX) conducted by the members of our team, as well as other groups.

In the second phase of the data analysis, we will compare the derived vertical profiles with predictions of more sophisticated models. In the case of Mars a comparison with the GCM/CTM predictions will provide information about variable hygropause, water cycle and meridional transport, HO_x-chemistry, stability of the Martian atmosphere, detailed studies on ozone chemistry, etc. Depending on the outcome of the observations, we may involve external experts in this step. For outer planets, photochemical models, in which the essential free parameters are the atmospheric eddy diffusion coefficient profile and the input flux of water, will be computed to match the observations. Such models are already available or in development at several of our institutes (e.g., Laboratoire d'Astrophysique de Bordeaux, Ollivier et al., 2000; Cavalié et al., 2008; Instituto de Astrofisica de Andalucia, Lara et al., 1996). The strength of combining expertise in radiative transfer and photochemical modelling is that we will be able to directly test physically based profiles of water against the actual data.

At the end of the mission, with all observational data at hand, we will be able to present monitoring studies of water in several Solar System sources. We will also synthesize all our observational results and draw an overall picture of the origin of water in the outer Solar System and the variation of D/H in the Solar System. This last step may involve external experts (e.g., in dust production from cometary trails or asteroid collisions). We will also carry out a comparison of water abundance and isotopic ratios in the Solar System objects with those in the ISM, in collaboration with the "Water In Star-forming regions with Herschel" (WISH) Key Programme.

8. Conclusion

Much of the observing time of this Key Programme will be used to observe strong water lines, in which the atmosphere of the Earth is completely opaque. For other molecules, the line transitions in the Herschel bands are much stronger than those accessible from Earth, i.e. high S/N observations are provided. These are required in order to:

- Retrieve vertical profiles of H_2O, its isotopes, O_2, and H_2O_2 in the Martian atmosphere.
- Retrieve vertical profiles of water in the stratospheres of the outer planets and Titan.
- Determine the water excitation and D/H ratio in comets.
- Perform line surveys. Retrievals of vertical profiles without a priori assumptions require S/N of 100, unachievable from the ground.

In addition to these inter-connected objectives, serendipitous searches will enhance our knowledge of the composition of planetary and cometary atmospheres.

The observations proposed in this programme will result in a comprehensive set of sensitive and well-calibrated spectra of water, its isotopologues, and chemically related species in Solar System objects. Our immediate science goal is extracting vertical profiles and isotopic ratios in individual objects. This will be done using sophisticated radiative transfer and retrieval models that have been developed by the members of the team. The tools needed for this task are already at hand for Mars (Lindau, Paris), outer planets (Paris, Bordeaux, Lindau), and comets (Paris, Bonn) and have been validated by previous ground-based and space-borne observations. In the second stage of the data analysis, the derived vertical profiles and mixing ratios will be compared with predictions of circulation/chemistry transport and photochemical models. In the final stage, the results for individual sources will be synthesized to produce a unified picture of the origin and evolution of water in the Solar System objects. A comparison with ISM sources, in collaboration with the WISH Key Programme, will also be carried out.

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