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1. Herschel Observations

The observations of comet 103P/Hartley 2 were carried out using the HIFI[31] instrument aboard the *Herschel Space Observatory*[32]. The observational sequence consisted of ten 32-min long observations of the HDO 1_{10}–1_{01} rotational line at 509.292 GHz, interleaved with simultaneous 6-min measurements of the H_2O and $H_2^{18}O$ 1_{10}–1_{01} lines at 556.936 and 547.676 GHz, respectively. The H_2O and $H_2^{18}O$ lines were observed in the upper and lower sideband of the HIFI band 1a receiver, respectively, tuned to a local oscillator (LO) frequency of 551.88 GHz. The HDO line was observed in the lower sideband of the band 1a receiver, with the LO frequency tuned to 514.092 GHz. In addition to these single point measurements, five on-the-fly maps of the H_2O 1_{10}–1_{01} transition, of 16-min duration, were acquired. All lines were observed in the two orthogonal HIFI polarizations. To achieve cancellation of the instrumental background, the HDO and $H_2O/H_2^{18}O$ single point observations were carried out in the frequency-switching observing mode, with a frequency throw of 94.5 MHz. Spectra were acquired with both the Wideband Spectrometer (WBS) and High Resolution Spectrometer (HRS), which provide spectral resolutions of 1.1 MHz and 140 kHz, respectively. The telescope beam sizes at the frequencies of the three lines are very similar (half power beam widths of 38.1″, 38.7″ and 41.6″ for the H_2O, $H_2^{18}O$, and HDO lines, respectively), so that the three molecules were observed in the same, ~6500 km diameter, region of the coma.

H_2O maps were used to place these single point measurements into context, by allowing a check of the telescope pointing accuracy and enabling an investigation of the morphology of the coma. In all maps, the H_2O 1_{10}–1_{01} line peaks approximately 10″ westward of the tracked nucleus position, toward the tail direction. The comet was tracked using an up-to-date ephemeris provided by the JPL Horizons system and the Herschel r.m.s. pointing accuracy is approximately 1″. Therefore, the excess emission westward of the nucleus, also observed in early November 2010 with the PACS and SPIRE instruments aboard Herschel, is likely explained by an asymmetric distribution of water molecules that may be related to a production from large icy grains accelerated in the anti-solar direction by non-gravitational forces[13].

2. HDO and $H_2^{18}O$ excitation models

The excitation models used in the interpretation of the data include collisions with H_2O and electrons, which dominate the excitation in the inner coma, as well as solar infrared pumping of vibrational bands followed by spontaneous decay, which establishes fluorescence equilibrium in the outer coma. Self-absorption effects are insignificant for HDO and $H_2^{18}O$ lines, except in the very inner coma, unresolved by the HIFI beam. The observed 1_{10}–1_{01} HDO and $H_2^{18}O$ transitions are optically thin. For $H_2^{18}O$, we used the same solar pumping rates as determined for the $H_2^{16}O$ isotopologue[29]. Solar excitation of HDO was modelled including excitation by collisions and absorption of the solar IR radiation[35]. With a beam diameter of ~6500 km projected on the comet, the HIFI measurements mostly sample molecules with an excitation state intermediate between Local Thermal Equilibrium (LTE) and fluorescence equilibrium. Hence their level populations depend on collisional rates involving water and electrons, as well as on the gas kinetic temperature. We used two approaches to model the collisional excitation. In model (1), water-water collisional cross-sections are modelled following commonly accepted methods[45] and water-electron cross-sections are derived from Itikawa's formulae[46]. The same model was used to interpret submillimetre HDO observations in comets C/1996 B2 (Hyakutake)[35] and C/1995 O1 (Hale-Bopp)[36]. Model (2) uses water-water and water-electron cross-sections according to[47,48,49]. Both models use electron density and temperature profiles based on in situ measurements in comet 1P/Halley, scaled to the activity of 103P/Hartley 2 at the time of the observations[49]. A scaling factor x_{ne} is further applied to the electron density. A value $x_{ne} = 0.2$ best fits the brightness radial profiles of the 557 GHz line observed in comets[50,51]. The distribution of water density is represented by the standard Haser distribution, which assumes isotropic outgassing at constant velocity. The water production rate in the calculations is taken equal to 1×10^{28} s^{-1}. We assumed an ortho-to-para ratio of 2.8 in the $H_2^{18}O$ model, consistent with infrared measurements[52,53] of comet 103P/Hartley 2.

3. Gas kinetic temperature

Constraints on the gas kinetic temperature in comet 103P/Hartley 2 at or near the time of the HIFI measurements are available. The rotational temperature of H_2O and other molecules was determined from ro-vibrational emission lines observed in the near-infrared at scales of 0.5–2″ (100–300 km at the distance of the comet)[53,54]. Values range from 70 to 85 K. In contrast, a gas kinetic temperature of 50 K is inferred from millimetre observations of methanol lines that probe outer regions of the coma (N. Biver, personal communication). A decrease of the gas kinetic temperature with increasing distance from the nucleus is consistent with a quasi-adiabatic expansion of cometary gases.

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Supplementary Table S1: D/H ratios in the solar system

Object	Species	D/H $\times 10^{-4}$	Reference
Earth (VSMOW)	H_2O	1.558 ± 0.001	33
103P/Hartley 2	H_2O	1.61 ± 0.24	this work
1P/Halley	H_2O	3.06 ± 0.34	34
C/1996 B2 (Hyakutake)	H_2O	2.90 ± 1.00	35
C/1995 O1 (Hale-Bopp)	H_2O	3.3 ± 0.8	36
153P/Ikeya-Zhang	H_2O	< 2.50	37
C/2002 T7 (LINEAR)	H_2O	2.5 ± 0.7	38
8P/Tuttle	H_2O	4.09 ± 1.45	39
Enceladus	H_2O	$2.5^{+1.5}_{-0.7}$	40
CI chondrites	H_2O	1.70 ± 0.10	41
Protosolar	H_2	0.21 ± 0.04	15
Interstellar medium	H	0.16 ± 0.01	15
Jupiter	H_2	0.225 ± 0.035	42
Saturn	H_2	$0.17^{+0.075}_{-0.045}$	42
Uranus	H_2	$0.55^{+0.35}_{-0.15}$	43
Neptune	H_2	0.45 ± 0.1	44

Compilation of the D/H ratios in the solar system following Figure 1: name of the object, species from which the D/H ratio was determined, D/H ratio with the corresponding uncertainty, reference to the measurement.