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LETTER

Detection of HD in the atmospheres of Uranus and Neptune: a new determination of the D/H ratio*

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Abstract. Observations with the Short Wavelength Spectrometer (SWS) onboard the Infrared Space Observatory (ISO) have led to the first unambiguous detection of HD in the atmospheres of Uranus and Neptune, from its R(2) rotational line at $37.7\,\mu$m. Using S(0) and S(1) quadrupolar lines of H_2 at 28.2 and 17.0 μm as atmospheric thermometers, we derive D/H ratios of $5.5(^{+3.5}_{-1.5}) \times 10^{-5}$ and $6.5(^{+2.5}_{-1.5}) \times 10^{-5}$ on Uranus and Neptune respectively. This confirms that compared to Jupiter and Saturn, Uranus and Neptune have been enriched in deuterium by the mixing of their atmospheres with D-rich protoplanetary ices. Assuming complete mixing of the planets, the D/H ratio in these ices is however found to be lower than in cometary ices.

Key words: planets and satellites: general – planets and satellites: individual: Neptune – planets and satellites: individual: Uranus – solar system: formation – infrared: solar system

1. Introduction

The determination of the D/H ratio in the Giant planets has long been recognized as a powerful tool to understand the formation of the Solar System from the primitive nebula (recent reviews in Owen 1992; Lécluse et al. 1996). The common view is that the giant planets accreted from the collapse of the surrounding protosolar nebula around an icy core of about 10-15 terrestrial masses. In the case of Jupiter and Saturn, whose core is a small fraction of their total mass, the D/H ratio is expected to reflect its protosolar value in H_2. In contrast, Uranus and Neptune which have more than half of their total mass contained in their core, are expected to be enriched in deuterium by the mixing of their hydrogen envelopes with D-rich icy grains (Hubbard & McFarlane 1980). Thus, comparing the D/H ratio in the four Giant Planets may allow to evaluate the composition of the protoplanetary ices embedded in the outer nebula.

The D/H ratio in Uranus and Neptune has been measured so far only from CH_3D in the near and mid-infrared (de Bergh et al. 1986, 1990; Orton et al. 1992). However, determining the bulk (i.e. in H_2) deuterium abundance from CH_3D requires the knowledge of the isotopic enrichment factor $f = (D/H)_{CH_4}/(D/H)_{H_2}$, which is uncertain (see Lécluse et al. 1996). In this respect, determining D/H from HD (i.e. $D/H = 1/2\ HD/H_2$) is more straightforward. Detections of HD at visible wavelengths have been reported on Uranus in the past (Trafton & Ramsay 1980), but such observations are difficult and, in the case of Uranus and Neptune, can probably provide only upper limits (Smith et al. 1989). On the other hand, in the far infrared range, HD possesses pure rotational lines at 112 μm (R(0)), 56 μm (R(1)) and 37.7 μm (R(2)) (Ulivi et al. 1991). While these lines were not detected in any of the Giant Planets by the Voyager/IRIS observations because of lack of spectral resolution and sensitivity, Bézard et al. (1986) predicted that most of them would be observable with ISO (Kessler et al. 1996). On this basis, HD rotational lines were systematically searched for on the four Giant Planets, both with SWS (de Graauw et al. 1996) and LWS (Clegg et al. 1996) onboard ISO. Preliminary reports on some of these observations have been presented (Griffin et al. 1996; Encrenaz et al. 1996; Lellouch et al. 1996; Feuchtgruber et al. 1997a). In this paper, we present the complete analysis of the SWS observations of HD at Uranus and Neptune and associated determinations of D/H.

2. Observations and data reduction

Observations were carried out in SWS grating modes AOT02 or AOT06 (de Graauw et al. 1996) at spectral resolutions of 1500-2200. Since the instrument covers the 2.36-45.2 μm range, observations were targeted at the R(2) rotational line of HD. In addition, the quadrupolar rotational lines of H_2 at 17.0 μm (S(1)) and 28.2 μm (S(0)) were observed. As detailed below, these lines can be used as thermometers of the lower and mid-stratosphere of Uranus and Neptune. Table 1 gives observational details for each measurement. All observations represent hemispheric av-

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Table 1. Summary of observations

Target	Date	T_{int} [min.]	Mode	Line[a]
Neptune	09-Oct-1996	83	S06[b]	HD R(2)
Neptune	26-Oct-1996	84	S06[b]	HD R(2)
Neptune	26-Mar-1997	83	S06[b]	HD R(2)
Neptune	12-Nov-1997	33	S02[c]	H_2 S(0)
Neptune	12-Nov-1997	21	S02[c]	H_2 S(1)
Uranus	22-Nov-1997	65	S02[c]	HD R(2)
Uranus	22-Nov-1997	21	S02[c]	H_2 S(0)
Uranus	22-Nov-1997	56	S02[c]	H_2 S(1)

[a] Wavelengths and SWS spectral resolutions ($\lambda/\delta\lambda$):
HD R(2): $37.7015\,\mu$m (1700); H_2 S(0): $28.2188\,\mu$m (1500);
H_2 S(1): $17.0348\,\mu$m (2200);
[b] Spectral range: $27 - 45.2\,\mu$m
[c] Spectral range: $\sim 10 - 12$ resolution elements

erages, since the SWS aperture size was $14" \times 27"$ or larger. Data were processed within the SWS interactive analysis system, based on standard ISO pipeline OLP V7.0 products. The data reduction adhered to the recommendations of Salama et al. (1997). Raw data were rebinned to a resolution of 4000. In order to improve the S/N, the three HD observations of Neptune were averaged after scaling to a common diameter ($2.24"$). As shown in Fig. 1, all observed lines are clearly detected. Our observations represent the first unambiguous detection of HD in Uranus and Neptune, and the first detection of the quadrupolar rotational lines of H_2 in Uranus (the S(1) line at Neptune has been observed by Orton et al. 1992).

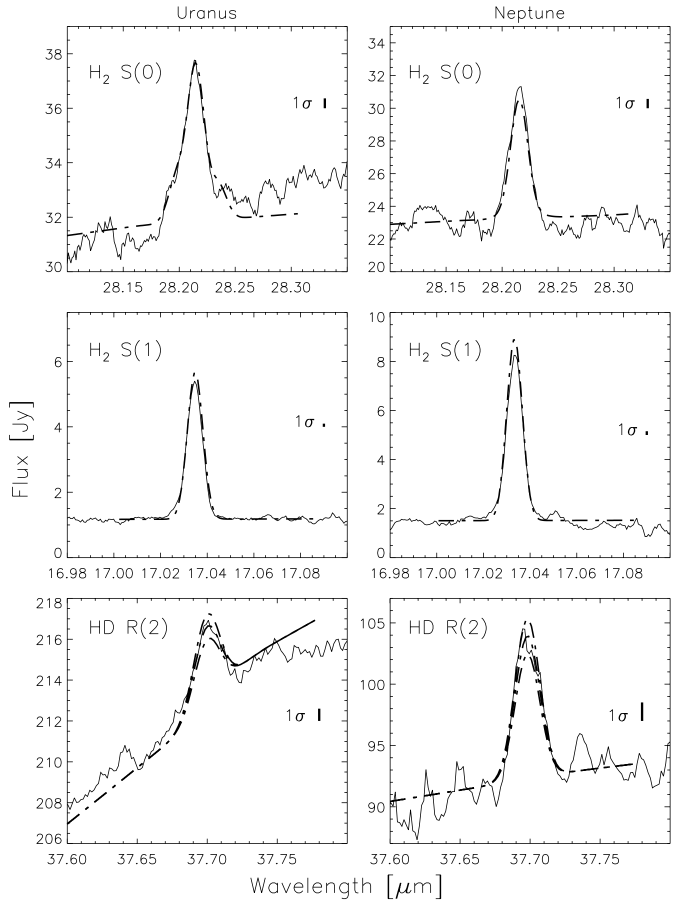

Fig. 1. H_2 and HD observations (solid lines) with best models fits (dashed-dotted lines). The HD mixing ratios are $9, 11, 13 \times 10^{-5}$ for Uranus and $11, 13, 15 \times 10^{-5}$ for Neptune. The thermal profiles used are the "nominal" profiles of Fig. 3.

3. Modelling

The observations were analyzed by means of a multilayer radiative transfer model in which the HD/H_2 mixing ratio, assumed to be uniform with altitude, is a free parameter. The synthetic spectra were calculated monochromatically, integrated over all viewing angles of the planets and then convolved with the instrumental profile at the respective wavelengths. Monochromatic contribution functions, calculated at line centers and in adjacent continua, illustrate (Fig. 2) that the continuum in the vicinity of the H_2 S(0) (resp. S(1)) line is formed in the $0.2 - 0.008$ bar (resp. $0.02-0.002$ bar) range. H_2 line centers probe broad atmospheric pressure ranges extending from $\sim 10^{-2}$ bar to $\sim 3\times10^{-4}$ bar for S(0) and from $\sim 4\times10^{-3}$ bar to $\sim 2\times10^{-5}$ bar for S(1). The continuum of the HD line is formed at 200-700 mbar, and the line core sounds the 10^{-4} - 3×10^{-3} bar. This demonstrates that the H_2 lines provide useful constraints on the thermal profile for modelling HD.

Starting with the pressure-temperature profiles determined by the Voyager 2 radio-occultation experiment (Lindal et al. 1987 and Lindal 1992 for Uranus and Neptune, egress profiles), we adjusted these profiles in order to fit both H_2 lines (continuum and contrast) and the continuum in the vicinity of the HD line. Note that H_2O lines, with mixing ratios from Feuchtgruber et al. (1997b) were included in the model since their contribution, at least for Uranus, is not negligible in the vicinity of the H_2 S(0) line. The accuracy of this method is driven by the absolute calibration uncertainties of the SWS data. We adopted a nominal $\pm 20\%$ uncertainty, appropriate in average longwards of $\sim 15\,\mu$m (Salama et al. 1997). The calibration procedure of the observations is such that this uncertainty applies independently on one hand on the S(1) line, and on the other hand on both the S(0) and R(2) lines. This means that the fits to the H_2 lines and HD continuum translate into a family of five thermal profiles (Fig. 3) representing nominal and extreme cases tolerated by the calibration errors. Specifically, in Fig. 3, "nominal" refers to the thermal profile retrieved for best guess calibration; in "maxmax" (resp. "minmin"), all lines are multiplied by 1.2 (resp. 0.8); in "maxmin", S(0) and R(2) are multiplied by 1.2 and S(1) by 0.8; and vice-versa for "minmax". The nominal thermal profiles show some differences with the radio-occultation profiles. In the case of Neptune, our best (disk-averaged) profile is $\sim$ 2-3 K warmer than the radio-occultation profile at 0.1-0.01 bar and 6 K at 0.001 bar. This is to be expected as the occultation egress profile occured at 42 S, a region of minimum temperatures in both the upper troposphere and the stratosphere (see e.g. Conrath et al. 1991 and Bézard et al. 1991). In the

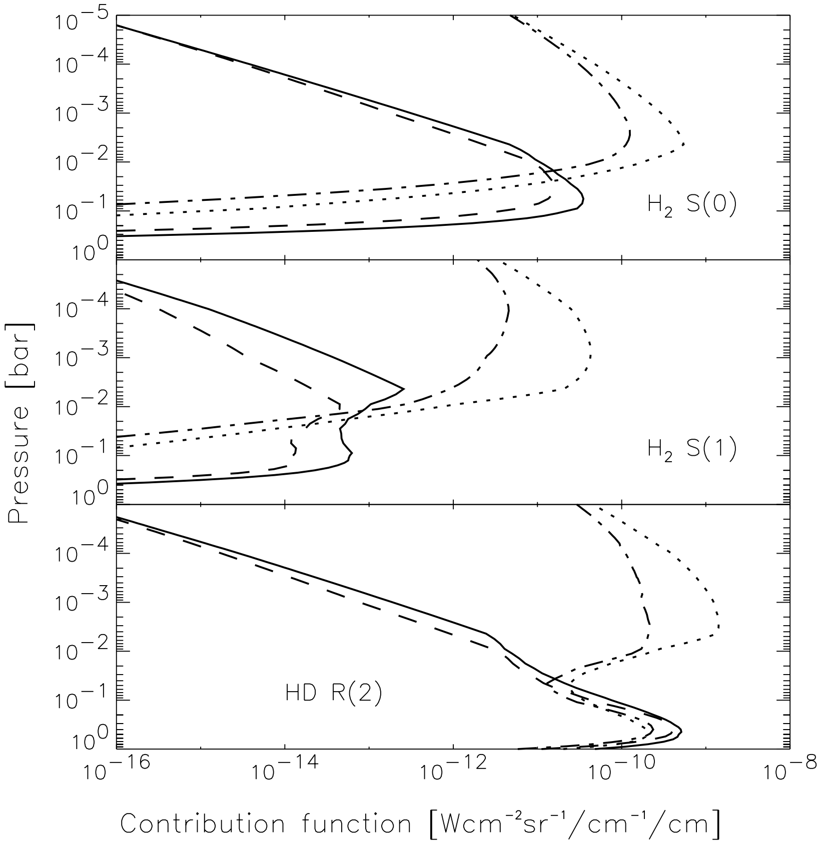

Fig. 2. Contribution functions $(B_\nu d(exp(-\tau_\nu))/dz)$ at infinite spectral resolution in $\mathrm{H_2}$ and HD line centers and in nearby continuum. Solid line: Neptune, continuum. Dashed line: Uranus, continuum. Dotted line: Neptune, line center. Dashed-dotted: Uranus, line center.

case of Uranus, our best profile is warmer than the occultation (equatorial) profile by 2 K at 1 bar and 4-6 K at 0.01-0.001 bar, and colder by 3 K at the tropopause. This is more difficult to interpret, although the latter feature is consistent with the fact that Voyager observed Uranus' mid-latitudes to be colder than the Equator and the Poles in the tropopause region (Flasar et al. 1987).

In each case, the HD R(2) line was then modelled with the associated thermal profile. HD line parameters were calculated from Ulivi et al. (1991) and Drakopoulos & Tabisz (1987a,1987b). $\mathrm{H_2}$ line parameters are from Jennings et al. (1987) and Poll & Wolniewicz (1978). Best fits to the lines with the nominal calibration are overplotted to the data in Fig. 1. Nominal $\mathrm{HD/H_2}$ mixing ratios are therefore 11×10^{-5} and 13×10^{-5} for Uranus and Neptune respectively. As illustrated in Fig. 1, the uncertainty due to noise on the resulting D/H is less than $\pm 1 \times 10^{-5}$. However, including calibration and associated thermal profile uncertainties, the $\mathrm{D/H}$ ratios are finally found to be equal to $5.5(^{+3.5}_{-1.5}) \times 10^{-5}$ for Uranus and $6.5(^{+2.5}_{-1.5}) \times 10^{-5}$ for Neptune.

Our results compare well with previous results from $\mathrm{CH_3D}$. For Uranus, de Bergh et al. (1986) infer $\mathrm{(D/H)_{CH_4}}$ = $9.0(^{+9.0}_{-4.5}) \times 10^{-5}$. Using f=1.68±0.23 from Lécluse et al. (1996) gives $\mathrm{(D/H)_{H_2}}$ = $5.4(^{+7.0}_{-3.0}) \times 10^{-5}$, fully consistent with our value but less accurate. For Neptune, adopting f = 1.61 ± 0.21 (Lécluse et al. 1996) the results of de Bergh et al. (1990) and Orton et al. (1992) from $\mathrm{CH_3D}$ respectively provide $\mathrm{D/H}$ = $9(^{+12}_{-6}) \times 10^{-5}$ and $5.6(^{+1.7}_{-1.4}) \times 10^{-5}$. Note also that observations of $\mathrm{CH_3D}$ at 8.66 μm on Neptune, obtained simultaneously in the short wavelength section of ISO SWS during our AOT06 observations (Bézard et al. 1997), give $\mathrm{D/H}$ = $5(^{+4.4}_{-2.3}) \times 10^{-5}$. The consistency of all these values is therefore excellent, although the various measurements, including ours, are not accurate enough to allow an observational determination of f.

4. Discussion

Our measurements confirm that the $\mathrm{D/H}$ ratio in Uranus and Neptune is larger than in Jupiter and Saturn. Indeed, the most recent values for $\mathrm{D/H}$ in Jupiter are $1.8(^{+1.1}_{-0.5}) \times 10^{-5}$ (from a preliminary analysis of the same R(2) line observed with ISO/SWS; Lellouch et al. 1996) and $(2.6 \pm 0.7) \times 10^{-5}$ (from the Galileo descent Probe; Mahaffy et al. 1998). In the case of Saturn, ISO/LWS indicates a preliminary value of $(1.5 - 3.5) \times 10^{-5}$ (Griffin et al. 1996). The deuterium enrichment expected on Uranus and Neptune is thus confirmed by the ISO observations. Following Lécluse et al. (1996), we can now estimate the $\mathrm{D/H}$ ratio in the protoplanetary ices forming the cores of these planets by:

$$\mathrm{(D/H)_{ices}} = \frac{\mathrm{(D/H)_{planet}} - \mathrm{x_{H_2}(D/H)_{proto}}}{(1 - \mathrm{x_{H_2}})}$$

where $\mathrm{x_{H_2}}$ is the per volume ratio of $\mathrm{H_2}$ in the planet, $\mathrm{(D/H)_{proto}}$ is the prosolar value. $\mathrm{(D/H)_{planet}}$ is the bulk $\mathrm{D/H}$ ratio in the planet, taken as its value in the fluid envelope

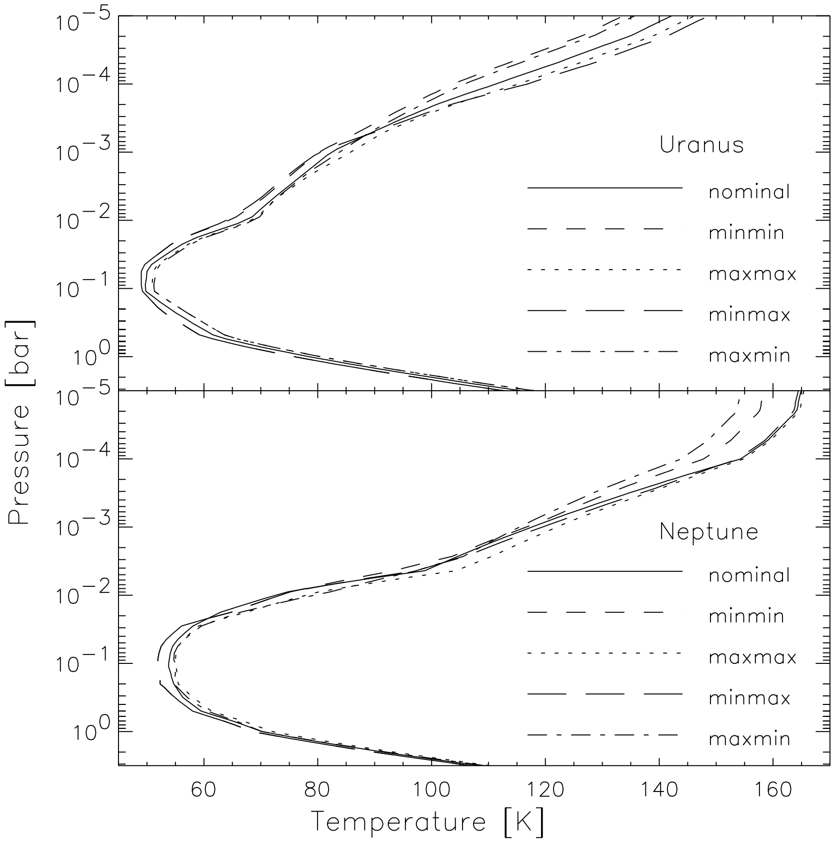

Fig. 3. Family of temperature profiles used in the modelling. See text for description of the various profiles.

$(\mathrm{D/H})_{\mathrm{envelope}}$. This assumes that the atmospheres and planetary interiors of Uranus and Neptune were fully mixed at least once in their history (i.e. equilibration of water and molecular hydrogen $(\mathrm{D/H})_{\mathrm{H_2O}} = (\mathrm{D/H})_{\mathrm{H_2}}$) (Lécluse et al. 1996). We take $x_{\mathrm{H_2}}$ from the interior models of Podolak et al. (1995). (The models by Marley et al. (1995) give somewhat different internal mass distributions, but essentially the same ice/gas ratios). For the protosolar D/H, we use the Jupiter values determined either by Galileo or by ISO. An intermediate and more accurate value of $(\mathrm{D/H})_{\mathrm{proto}} = (2.0 \pm 0.35) \times 10^{-5}$ can be determined from the He measurement of the Galileo probe and the ^{3}He/^{4}He ratio in the solar wind (Gautier & Morel 1998, private communication). However, as indicated in Table 2, the uncertainty on $(\mathrm{D/H})_{\mathrm{ices}}$ is more driven by interior models uncertainties than by the value of $(\mathrm{D/H})_{\mathrm{proto}}$.

The above approach implicitly assumes that $(\mathrm{D/H})_{\mathrm{envelope}}$ = $(\mathrm{D/H})_{\mathrm{H_2}}$. This is not true if the fluid envelope is heavily enriched in D-rich volatiles. This scenario is actually proposed by Lodders and Fegley (1994) for Neptune, for which they invoke a 440 times solar water abundance (which is in fact inconsistent with the Podolak et al. models). In this case, $(\mathrm{D/H})_{\mathrm{envelope}}$ = 1.24 $(\mathrm{D/H})_{\mathrm{H_2}}$ and the values for the proto-neptunian ices in Table 2 have to be raised by 25–30%.

In all these cases, we conclude that the D/H ratio in protoplanetary ices is significanly lower than in cometary ices (Halley: $31.6 \pm 3.4 \times 10^{-5}$, Eberhardt et al. 1995; Hyakutake: $29 \pm 10 \times 10^{-5}$, Bockelée-Morvan et al. 1998; Hale-Bopp: $33 \pm 8 \times 10^{-5}$, Meier et al. 1998) by a nominal factor of about 3. This result bears implications on the origin of comets (Bockelée-Morvan et al. 1998, Gautier 1998, Drouart et al. 1999, preprint). We stress that this conclusion is based on the hypothesis, supported by the Pollack & Bodenheimer (1989) evolutionary models, of complete mixing between planetary atmospheres and interiors. If mixing has been incomplete, the protouranian and prototneptunian ices may still hold the same D/H ratio as comets (Hubbard et al. 1995).

Table 2. D/H in protoplanetary ices

Model[a]	$x_{\mathrm{H_2}}$	$(\mathrm{D/H})^{\mathrm{b}}_{\mathrm{ices}}$ [$\times 10^{-5}$]	$(\mathrm{D/H})^{\mathrm{c}}_{\mathrm{ices}}$ [$\times 10^{-5}$]
Neptune 1	0.57	$12.8(^{+6.5}_{-5.0})$	$11.7(^{+6.8}_{-4.4})$
Neptune 2	0.33	$8.9(^{+4.0}_{-2.8})$	$8.5(^{+4.1}_{-2.7})$
Uranus	0.51	$9.4(^{+7.6}_{-4.2})$	$8.5(^{+8.0}_{-3.8})$

(a) Models from Podolak et al. (1995); $(\mathrm{D/H})_{\mathrm{proto}}$ from (b) ISO/SWS and (c) Galileo

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