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Letter to the Editor

The ^{16}OH/^{18}OH and OD/OH isotope ratios in comet C/2002 T7 (LINEAR)[⋆]

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ABSTRACT

The ^{16}OH/^{18}OH and OD/OH isotope ratios are measured in the Oort-Cloud comet C/2002 T7 (LINEAR) through ground-based observations of the OH $A\,^2\Sigma^+ - X\,^2\Pi_i$ ultraviolet bands at 3063 Å (0, 0) and 3121 Å (1, 1) obtained with the Very Large Telescope (VLT) feeding the Ultraviolet-Visual Echelle Spectrograph (UVES). From the ^{16}OH/^{18}OH ratio, we find ^{16}O/^{18}O = 425 ± 55, equal within the uncertainties to the terrestrial value and to the ratio measured in other comets, although marginally smaller. We also estimate OD/OH from which we derive D/H = $2.5 \pm 0.7 \times 10^{-4}$ in water. This value is compatible with the water D/H ratios evaluated in other comets and is marginally higher than the terrestrial value.

Key words. comets: general – comets: individual: C/2002 T7 (LINEAR)

1. Introduction

The determination of the abundance ratios of the stable isotopes of light elements in different objects of the Solar System provides important clues for the study of their origin and history. This is especially true for comets, which carry the most valuable information regarding the material in the primitive solar nebula.

The ^{16}O/^{18}O isotopic ratio has been measured from space missions in a few comets. In-situ measurements with the neutral and ion mass spectrometers onboard the Giotto spacecraft gave ^{16}O/^{18}O = 495 ± 37 for H_2O in comet 1P/Halley (Eberhardt et al. 1995; Balsiger et al. 1995). A deep integration of the spectrum of the bright comet 153P/2002 C1 (Ikeya-Zhang) with the sub-millimeter satellite Odin led to the detection of the $H_2^{18}O$ line at 548 GHz (Lecacheux et al. 2003). Subsequent observations resulted in the determination of ^{16}O/^{18}O = 530 ± 60, 530 ± 60, 550 ± 75 and 508 ± 33 in the Oort-Cloud comets Ikeya-Zhang, C/2001 Q4, C/2002 T7 and C/2004 Q2 respectively (Biver et al. 2007). Within the error bars, these measurements are consistent with the terrestrial value (^{16}O/^{18}O (SMOW[1]) = 499), although marginally higher (Biver et al. 2007). More recently, laboratory analyses of the silicate and oxide mineral grains from the Jupiter family comet 81P/Wild 2 returned by the Stardust space mission provided ^{16}O/^{18}O ratios also in excellent agreement with the terrestrial value. Only one refractory grain appeared marginally depleted in ^{18}O (^{16}O/^{18}O = 576 ± 78) as observed in refractory inclusions in meteorites (McKeegan et al. 2006).

The D/H ratio has been measured in four comets. In-situ measurements provided D/H = $3.16 \pm 0.34 \times 10^{-4}$ for H_2O in 1P/Halley (Eberhardt et al. 1995; Balsiger et al. 1995), a factor of two higher than the terrestrial value (D/H (SMOW) = 1.556×10^{-4}). The advent of powerful sub-millimeter telescopes, namely the Caltech Submillimeter Observatory and the James Clerck Maxwell telescope located in Hawaii, allowed the determination of the D/H ratio for two exceptionally bright comets. In comet C/1996 B2 (Hyakutake), D/H was found equal to $2.9 \pm 1.0 \times 10^{-4}$ in H_2O (Bockelée-Morvan et al. 1998), while in comet C/1995 O1 (Hale-Bopp) the ratios D/H = $3.3 \pm 0.8 \times 10^{-4}$ in H_2O and D/H = $2.3 \pm 0.4 \times 10^{-3}$ in HCN were measured (Meier et al. 1998a,b), confirming the high D/H value in comets. Both Hyakutake and Hale-Bopp are Oort-Cloud comets. Finally, bulk fragments of 81P/Wild 2 grains returned by Stardust indicated moderate D/H enhancements with respect to the terrestrial value. Although D/H in 81P/Wild 2 cannot be ascribed to water, the measured values overlap the range of water D/H ratios determined in the other comets (McKeegan et al. 2006).

Among a series of spectra obtained with UVES at the VLT to measure the ^{14}N/^{15}N and ^{12}C/^{13}C isotope ratios in various comets from the 3880 Å CN ultraviolet band (e.g. Arpigny et al. 2003; Hutsemékers et al. 2005; Jehin et al. 2006; Manfroid et al. 2008), we found that the spectrum of C/2002 T7 appeared bright enough to detect the ^{18}OH lines in the $A\,^2\Sigma^+ - X\,^2\Pi_i$ bands at 3100 Å allowing – for the first time – the determination of the ^{16}O/^{18}O ratio from *ground-based* observations. We also realized that the signal-to-noise ratio of our data was sufficient to allow a reasonable estimate of the OD/OH ratio from the same bands.

The possibility of determining the ^{16}O/^{18}O ratio from the OH ultraviolet bands has been emphasized by Kim (2000). Measurements of the OD/OH ratio were attempted by A'Hearn et al. (1985) using high resolution spectra from the International

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[1] Standard Mean Ocean Water.

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Table 1. Observing circumstances.

Date (2004)	r (AU)	$\dot{r}$ (km s^{-1})	Δ (AU)	Offset (10^3 km)	t (s)	Airmass
May 6	0.68	15.8	0.61	1.3	1080	2.2–1.9
May 26	0.94	25.6	0.41	0.0	2677	1.3–1.8
May 26	0.94	25.6	0.41	0.0	1800	2.1–2.7
May 28	0.97	25.9	0.48	10.0	3600	1.3–1.7

r and $\dot{r}$ are the comet heliocentric distance and radial velocity; Δ is the geocentric distance; t is the exposure time; Airmass is given at the beginning and at the end of the exposure.

Ultraviolet Explorer and resulting in the upper limit D/H < 4×10^{-4} for comet C/1989 C1 (Austin). These observations now become feasible from the ground thanks to the high ultraviolet sensitivity of spectrographs like UVES at the VLT.

2. Observations and data analysis

Observations of comet C/2002 T7 were carried out with UVES mounted on the 8.2 m UT2 telescope of the European Southern Observatory VLT. Spectra in the wavelength range 3040 Å–10 420 Å were secured in service mode during the period May 6, 2004 to June 12, 2004. The UVES settings 346 + 580 and 437 + 860 were used with dichroic #1 and #2 respectively. In the following, only the brighest ultraviolet spectra obtained on May 6, May 26 and May 28 are considered. The 0.44 × 10.0 arcsec slit provided a resolving power $R \simeq 80\,000$. The slit was oriented along the tail, centered on the nucleus on May 26, and off-set from the nucleus for the May 6 and May 28 observations. The observing circumstances are summarized in Table 1.

The spectra were reduced using the UVES pipeline (Ballester et al. 2000), modified to accurately merge the orders taking into account the two-dimensional nature of the spectra. The flat-fields were obtained with the deuterium lamp which is more powerful in the ultraviolet.

The data analysis and the isotopic ratio measurements were performed using the method designed to estimate the carbon and nitrogen isotopic ratios from the CN ultraviolet spectrum (Arpigny et al. 2003; Jehin et al. 2004; Manfroid et al. 2005). We compute synthetic fluorescence spectra of ^{16}OH, ^{18}OH and ^{16}OD for the $A\,^2\Sigma^+ - X\,^2\Pi_i$ (0, 0) and (1, 1) ultraviolet bands for each observing circumstance. Isotope ratios are then estimated by fitting the observed OH spectra with a linear combination of the synthetic spectra of the two species of interest.

2.1. The OH model

We have developed a fluorescence model for OH similar to the one described by Schleicher and A'Hearn (1988). As lines of the OH(2–2) bands are clearly visible in our spectra we have included vibrational states up to $v = 2$ in the $A^2\Sigma^+$ and $X^2\Pi_i$ electronic states. For each vibrational state rotational levels up to $J = 11/2$ were included, leading to more than 900 electronic and vibration-rotation transitions. The system was then solved as described in Zucconi & Festou (1985).

Accurate OH wavelengths were computed using the spectroscopic constants of Colin et al. (2002) and Stark et al. (1994). OD wavelengths were computed using the spectroscopic constants of Abrams et al. (1994) and Stark et al. (1994). ^{18}OH wavelengths were derived from the ^{16}OH ones using the standard isotopic shift formula; they are consistent with the measured values of Cheung et al. (1995).

Electronic transition probabilities for OH and OD are given by Luque & Crosley (1998, 1999). We used the dipole moments of OH and OD measured by Peterson et al. (1984) to compute the rotational transition probabilities and the vibrational lifetimes computed by Mies (1974). Because of the very small difference in the structure of ^{18}OH and ^{16}OH the transition probabilities for ^{18}OH and ^{16}OH are the same.

The OH fluorescence spectrum is strongly affected by the solar Fraunhofer lines, especially in the 0–0 band, so a carefully calibrated solar atlas is required. We have used the Kurucz (2005) atlas above 2990 Å and the A'Hearn et al. (1983) atlas below.

The role of collisions in the OH emission, in particular those with charged particles inducing transitions in the Λ doublet ground rotational state, was first pointed out by Despois et al. (1981) in the context of the 18 cm radio emission and then also considered in the UV emission by Schleicher (1983) and Schleicher & A'Hearn (1988). Modeling the effect of collisions may be done by adding the collision probability transition rate between any two levels, i and j:

$$C_{i,j} = \sum_{\mathrm{c}} n_{\mathrm{c}}(\boldsymbol{r})\, v_{\mathrm{c}}(\boldsymbol{r})\, \sigma_{\mathrm{c}}(i, j, v_{\mathrm{c}})$$

where the sum extends over all colliders. n_{c} is the local density of the particles inducing the transition, v_{c} is the relative velocity of the particles and σ_{c} is the collision cross section. It also depends on the energy of the collision i.e. of v_{c}. The reciprocal transition rates are obtained through detailed balance:

$$C_{j,i} = C_{i,j} \frac{g_i}{g_j} \exp(E_{ij}/kT)$$

in which g_i is the statistical weight and E_{ij} is the energy separation between the states. In order to reduce the number of parameters required to model the collisions we have adopted a simplified expression of the form $C_{i,j} = q_\Lambda$ for the transition in the Λ doublet ground state. In order to better fit the OH spectra we have also found it necessary to take into account rotational excitation through a similar expression $C_{i,j} = q_{\mathrm{rot}}$ with q_{rot} different from 0 only for dipole transitions, i.e. when $\Delta J < 2$, which appeared to correctly fit the data. Furthermore, since OH and OD have similar dipole moments, we assumed that collisional cross-sections are identical for both molecules.

The model assumes that the ^{16}OH lines are optically thin. This is verified by the fact that it correctly reproduces both the faint and strong OH emission lines.

2.2. ^{16}OH/^{18}OH

Two ^{18}OH lines at 3086.272 Å and 3091.046 Å are clearly detected in the (0, 0) band. However these lines are strongly blended with the ~500 times brighter ^{16}OH emission lines and thus are not useful for an accurate flux estimate. The (1, 1) band at 3121 Å, while fainter, is better suited for the determination of ^{16}OH/^{18}OH since (i) the wavelength separation between ^{18}OH and ^{16}OH is larger ($\simeq$0.3 Å instead of 0.1 Å); and (ii) the sensitivity of UVES rapidly increases towards longer wavelengths while the atmospheric extinction decreases, resulting in a better signal-to-noise ratio.

Figure 1 illustrates a part of the observed OH (1, 1) band together with the synthetic spectrum from the model. Two ^{18}OH lines are clearly identified.

To evaluate ^{16}OH/^{18}OH we first select the 3 brighest and best separated ^{18}OH lines at λ = 3134.315 Å, 3137.459 Å and

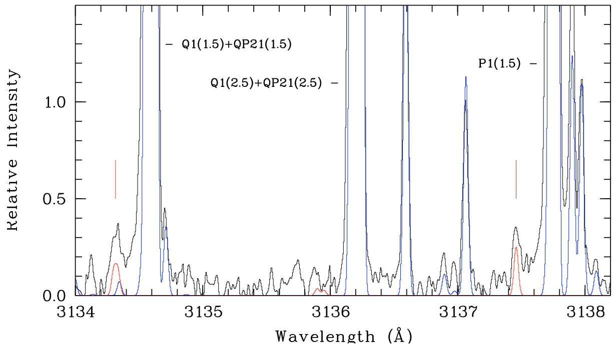

Fig. 1. A section of the May 6 spectrum of the OH (1, 1) band in comet C/2002 T7. Black: observed spectrum; blue: synthetic emission spectrum of ^{16}OH fitted to the observed one (the extended wings of the ^{16}OH lines are not modelled here; on the other hand, in this and all three other figures, the presence of prompt emission is taken into account); red: synthetic fluorescence spectrum of ^{18}OH with the typical ratio ^{16}OH/^{18}OH = 500. The position of the ^{18}OH lines at 3134.315 Å and 3137.459 Å is indicated.

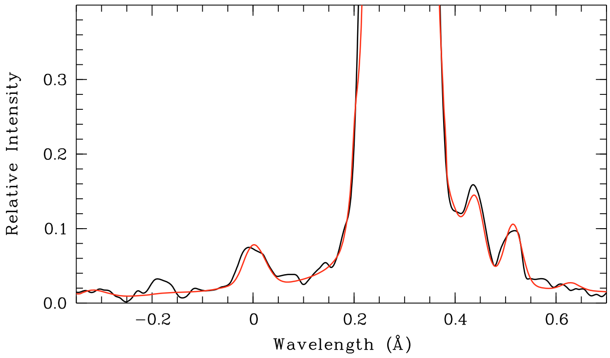

Fig. 2. Co-addition of the ^{18}OH lines at λ = 3134.315 Å, 3137.459 Å and 3142.203 Å from the May 6 spectrum after proper wavelength shifts. Co-added ^{18}OH is shifted to $\lambda = 0$ while ^{16}OH appears at $\lambda \simeq 0.3$. Black: observed spectrum; red: synthetic combined spectrum of ^{16}OH, ^{18}OH with ^{16}OH/^{18}OH = 410, and an empirical fit to the OH extended wings.

3142.203 Å. These lines are then Doppler-shifted and co-added with proper weights to produce an average profile which is compared to the ^{16}OH profile similarly treated (cf. Jehin et al. 2004, for more details on the method). We verified that the ^{16}OH faint wings and nearby prompt emission lines (to be analysed in detail in a forthcoming paper) do not contaminate the ^{18}OH lines nor the measurement of the isotopic ratios. The ratio ^{16}OH/^{18}OH is then derived through an iterative procedure which is repeated for each spectrum independently. For the spectra of May 6, 26 and 28 we respectively derive ^{16}OH/^{18}OH = 410 ± 60, 510 ± 130 and 380 ± 290. The uncertainties are estimated from the co-added spectra by considering the rms noise in spectral regions adjacent to the ^{18}OH lines, and by evaluating errors in the positioning of the underlying pseudo-continuum (i.e. the dust continuum plus the faint wings of the strong lines). The weighted average of all measurements gives ^{16}OH/^{18}OH = 425 ± 55.

Since OH is essentially produced from the dissociation of H_2O, ^{16}OH/^{18}OH represents the ^{16}O/^{18}O ratio in cometary water, with the reasonable assumption that photodissociation cross-sections are identical for $H_2^{18}O$ and $H_2^{16}O$.

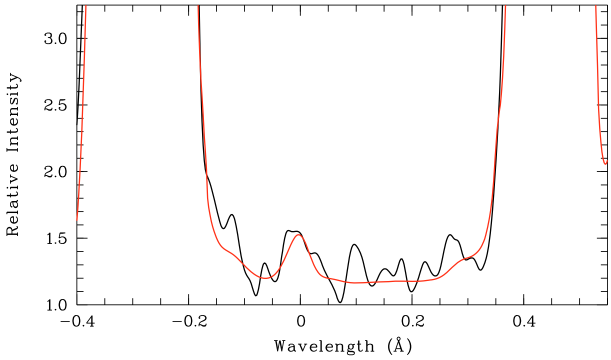

Fig. 3. Co-addition of 27 OD lines from the May 6 spectrum after proper wavelength shifts. Co-added OD is shifted to $\lambda = 0$. Black: observed spectrum; red: synthetic combined spectrum of OH, OD with OD/OH = 4×10^{-4}, and an empirical fit to the OH extended wings.

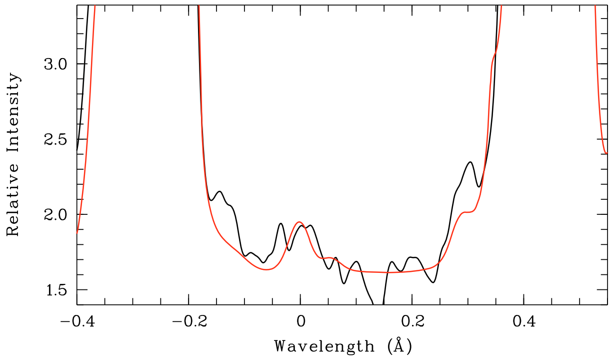

Fig. 4. Same as Fig. 3 for the May 26 spectrum.

2.3. OD/OH

The detection of OD lines is much more challenging since one may expect the OD lines to be a few thousand times fainter than the OH lines. Fortunately, the wavelength separation between OD and OH ($\gtrsim$10 Å) is much larger than between ^{18}OH and ^{16}OH such that both the (0, 0) and (1, 1) bands can be used with no OD/OH blending (apart from chance coincidences). Since no individual OD lines could be detected, we consider the 30 brighest OD lines (as predicted by the model) for co-addition. After removing 3 of them, blended with other emission lines, an average profile is built with careful Doppler-shifting and weighting as done for ^{18}OH. Only our best spectra obtained on May 6 and May 26 are considered, noting that the (0, 0) band – which dominates the co-addition – is best exposed on May 26 while the (1, 1) band is best exposed on May 6, due to the difference in airmass. The resulting OD line profiles are illustrated in Figs. 3 and 4 and compared to a synthetic spectrum computed with OD/OH = 4×10^{-4}. OD is detected as a faint emission feature which is present *at both epochs*. From the measurement of the line intensities, we derive OD/OH = $3.3 \pm 1.1 \times 10^{-4}$ and $4.1 \pm 2.0 \times 10^{-4}$ for the spectra obtained on May 6 and 26 respectively. The weighted average is OD/OH = $3.5 \pm 1.0 \times 10^{-4}$. The difference in the lifetime of OD and OH (van Dishoeck & Dalgarno 1984) does not significantly affect our results since the part of the coma sampled by the UVES slit is two orders of magnitude smaller than the typical OH scale-length. The uncertainties on OD/OH were estimated as for ^{16}OH/^{18}OH. Possible errors on the isotopic ratios related to uncertainties on the collision coefficients were estimated via simulations and found to be negligible. Even in the hypothetical case that collisions differently affect OD and OH, errors are much smaller than the other uncertainties, as expected since the contribution of collisions is small with respect to the contribution due to pure fluorescence.

To estimate the cometary D/H ratio in water, HDO/H_2O must be evaluated. While the cross-section for photodissociation of HDO is similar to that of H_2O, the production of OD+H is favoured over OH+D by a factor of around 2.5 (Zhang & Imre 1988; Engel & Schinke 1988). Assuming that the total branching ratio for HDO → OD + H plus HDO → OH + D is equal to that of $H_2O \rightarrow OH + H$, we find HDO/$H_2O \simeq 1.4$ OD/OH. With D/H = 0.5 HDO/H_2O, we finally derive D/H = $2.5 \pm 0.7 \times 10^{-4}$ in cometary water. The factor (OD+H)/(OH+D) = 2.5 adopted in computing the branching ratios for the photodissociation of HDO is an average value over the spectral region where the cross-sections peak. In fact (OD+H)/(OH+D) depends on the wavelength and roughly ranges between 2 and 3 over the spectral regions where absorption is significant (Engel & Schinke 1988; Zhang et al. 1989; Yi et al. 2007). Fortunately, even if we adopt the extreme ratios (OD+H)/(OH+D) = 2 or (OD+H)/(OH+D) = 3 instead of 2.5, the value of the D/H isotopic ratio is not changed by more than 6%.

3. Discussion

We have measured the oxygen isotopic ratio $^{16}O/^{18}O = 425 \pm 55$ from the OH $A\,^2\Sigma^+ - X\,^2\Pi_i$ ultraviolet bands in comet C/2002 T7. Although marginally smaller, our value do agree within the uncertainties with $^{16}O/^{18}O = 550 \pm 75$ estimated from observations by the Odin satellite (Biver et al. 2007), with the $^{16}O/^{18}O$ ratios determined in other comets, and with the terrestrial value (Sect. 1).

To explain the so-called “oxygen anomaly” i.e. the fact that oxygen isotope variations in meteorites cannot be explained by mass-dependent fractionation, models of the pre-solar nebula based on CO self-shielding were proposed, predicting enrichments, with respect to the SMOW value, of ^{18}O in cometary water up to $^{16}O/^{18}O \sim 415$ (Yurimoto & Kuramoto 2004). Recently, Sakamoto et al. (2007) found evidence for such an enrichment in a primitive carbonaceous chondrite, supporting self-shielding models. The value of $^{16}O/^{18}O$ we found in C/2002 T7 is also marginally smaller than the terrestrial value and compatible with these predictions. On the other hand, the measurement of $^{16}O/^{18}O = 440 \pm 6$ in the solar photosphere (Ayres et al. 2006; cf. Wiens et al. 2004, for a review of other, less accurate, measurements) indicates that solar ratios may deviate from the terrestrial ratios by much larger factors than anticipated, requiring some revision of the models. More observations are thus critically needed for an accurate value of $^{16}O/^{18}O$ in comets, assuming that cometary water is pristine enough and can be characterized by a small set of representative values. If self-shielding is important in the formation of the solar system, it is not excluded that significant variations can be observed between comets formed at different locations in the solar system, like the Oort cloud and Jupiter-family comets.

We also detected OD and estimated D/H = $2.5 \pm 0.7 \times 10^{-4}$ in water. Our measurement is compatible with other values of D/H in cometary water and marginally higher than the terrestrial value (Sect. 1). Our observations were not optimized for the measurement of OD/OH (or for ^{16}OH/^{18}OH) and one of our best spectra was obtained at airmass ~2 with less than 20 min of exposure time for a comet of heliocentric magnitude $m_r \simeq 5$ (for comparison, comet Hale-Bopp reached $m_r \simeq -1$). All these observing circumstances can be improved, including observations at negative heliocentric velocities to increase the OD/OH fluorescence efficiency ratio (cf. Fig. 1 of A’Hearn et al. 1985). This opens the possibility of routinely measuring both the $^{16}O/^{18}O$ and D/H ratios from the ground, together with the $^{12}C/^{13}C$ and $^{14}N/^{15}N$ ratios, for a statistically significant sample of comets of different types (e.g. Oort-cloud, Halley-type, and hopefully Jupiter-family comets although the latter are usually fainter). The measurement of D/H is especially important since it allows us to limit the contribution of comets to the terrestrial water, the high D abundance implying that no more than about 10 to 30% of Earth’s water can be attributed to comets (e.g. Eberhardt et al. 1995; Dauphas et al. 2000; Morbidelli et al. 2000). However, only a full census of D/H in comets could answer this question. In particular, if Jupiter-family comets, thought to have formed in farther and colder places in the Solar System, are characterized by an even higher D/H, closer to the ratio measured in the interstellar medium water, then the fraction of cometary H_2O brought onto the Earth could be even smaller.

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