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 $A^2Σ^+ - X^2Π$ ultraviolet bands at 3063 Å (0,0) and 3121 Å (1,1) secured 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 ± 0.7 $10^{-4}$ in water. This value is compatible with the water D/H ratios evaluated in other comets and marginally higher than the terrestrial value.

Key words. Comets: general - Comets: individual: C/2002 T7 (LINEAR) - Solar system: general

1. Introduction

The determination of the abundance ratios of the stable isotopes of the light elements in different objects of the Solar System provides important clues into 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$_2$O in comet 1P/Halley (Eberhardt 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$_2$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) = 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 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 $^{13}$C/$^{12}$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 $A^2Σ^+ - X^2Π$ 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 already attempted by A’Hearn et al. (1985) using high resolution spectra from the International 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 throughput 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 8.2m UT2 telescope of the European Southern

* Based on observations collected at the European Southern Observatory, Paranal, Chile (ESO Programme 073.C-0525).
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1 Standard Mean Ocean Water
Table 1. Observing circumstances

| Date    | $r$ (AU) | $\dot{r}$ (km/s) | $\Delta$ (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; $\Delta$ is the geocentric distance; $t$ is the exposure time; Airmass is given at the beginning and at the end of the exposure.

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 $\Delta$ 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 and A'Hearn (1988). Modeling the effect of collisions may be done by adding the collision probability transition rate between any two levels, $i$ and $j$:

$$C_{i,j} = \sum_c n_c(r) v_c(r) \sigma_c(i, j, v_c)$$

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 $\sigma_c$ 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:

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

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 $C_{i,j} = q_{\Delta}$ for the transition in the $\Delta$ doublet ground state. In order to better fit the OH spectra we have also found necessary to take into account rotational excitation through a similar expression $C_{i,j} = q_{\text{rot}}$ with $q_{\text{rot}}$ 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.

2.1. 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 $A^2\Sigma^+ - X^2\Pi, (0,0)$ 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.

2.2. $^{16}$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 then not useful for an accurate flux estimate. In fact 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 ($\sim 0.3$ 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.

Fig. 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 actually evaluate $^{16}$OH/$^{18}$OH we first select the 3 brightest and best separated $^{18}$OH lines at $\lambda = 3134.315$ Å, 3137.459 Å and 3142.203 Å. These lines are then doppler-shifted and overlapped 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 (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 $= 410 \pm 60$, $510 \pm 130$ and $380 \pm 290$. 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 $= 425 \pm 55$.

Since OH is essentially produced from the dissociation of H$_2$O, $^{16}$OH/$^{18}$OH represents the $^{18}$O/$^{16}$O ratio in cometary water, with the reasonable assumption that photodissociation cross-sections are identical for H$_2^{16}$O and H$_2^{18}$O.

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 ($\geq 10$ Å) is much larger than between $^{16}$OH and $^{18}$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 brightest 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 $^{16}$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 Fig. 3 and 4 and compared to a synthetic spectrum computed with OD/OH $= 4 \times 10^{-4}$. 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 and 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
hypothesetical 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, HD/O/H$_2$O must be evaluated. While the cross-section for photodissociation of HDO is similar to that of H$_2$O, the production of OD+H is favoured over OH+D by a factor around 2.5 (Zhang and Imre 1988, Engel and Schinke 1988). Assuming that the total branching ratio for HDO → OD + H plus HDO → OH + D is equal to that of H$_2$O → OH + H, we find HDO/H$_2$O = 1.4 OD/OH. With D/H = 0.5 HD/H$_2$O, we finally derive D/H = 2.5 ± 0.7 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 and Schinke 1988).

Zhang et al. 1989, Yi et al. 2007. Fortunately, even if we adopt the extreme ratios (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 16O/18O = 425 ± 55 from the OH $A^2Σ^+ - X^2Π$, ultraviolet bands in comet C/2002 T7. Although marginally smaller, our value do agree within the uncertainties with 16O/18O = 550 ± 75 estimated from observations by the Odin satellite (Biver et al. 2007), with the 16O/18O 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 isotopic 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, of 18O in cometary water up to 16O/18O ~ 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 16O/18O 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 16O/18O = 440 ± 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 then critically needed to get an accurate value of 16O/18O in comets, assuming that cometary water is pristine enough and can be characterized by a small set of representative values. Namely, 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 Oort cloud and Jupiter-family comets.

We also detected OD and estimated D/H = 2.5 ± 0.7 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 (neither for 16OH/18OH) 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 $m_h$ ~ 5 (for comparison, comet Hale-Bopp reached $m_h$ = -1). All these observing circumstances can be improved, including observations at negative heliocentric velocities to increase the OD/OH fluorescence efficiency ratio (cf. figure 1 of A'Hearn et al. 1985). This opens the possibility to routinely measure both the 16O/18O and D/H ratios from the ground, together with the 12C/13C and 14N/15N 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 allow 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$_2$O brought onto the Earth could be even smaller.

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