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Ortho-to-para ratio of interstellar heavy water*


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LETTER TO THE EDITOR

ABSTRACT

Context. Despite the low elemental deuterium abundance in the Galaxy, enhanced molecular D/H ratios have been found in the environments of low-mass star forming regions, and in particular the Class 0 protostar IRAS 16293-2422.

Aims. The CHESS (Chemical HErschel Surveys of Star forming regions) Key Program aims at studying the molecular complexity of the interstellar medium. The high sensitivity and spectral resolution of the HIFI instrument provide a unique opportunity to observe the fundamental $\nu_1 - \nu_0$ transition of the ortho-D$_2$O molecule, inaccessible from the ground, and to determine the ortho-to-para D$_2$O ratio.

Methods. We have detected the fundamental transition of the ortho-D$_2$O molecule at 607.35 GHz towards IRAS 16293-2422. The line is seen in absorption with a line opacity of $0.62 \pm 0.11$ (1σ). From the previous ground-based observations of the fundamental $\nu_1 - \nu_0$ transition of para-D$_2$O seen in absorption at 316.80 GHz we estimate a line opacity of $0.26 \pm 0.05$ (1σ).

Results. We show that the observed absorption is caused by the cold gas in the envelope of the protostar. Using these new observations, we estimate for the first time the ortho to para D$_2$O ratio to be lower than 2.6 at a 3σ level of uncertainty, to be compared with the thermal equilibrium value of 2.1.

Key words. astrochemistry – ISM: individual (IRAS 16293-2422) – ISM: molecules
1. Introduction

Among all molecules in interstellar space, water is a special one because of its dominant role in the cooling of warm gas and in the oxygen chemistry as well as for its role in the chemistry of the atmospheres of exoplanets and its potential connection with life. Water abundance in cold molecular gas is very low because it is frozen onto the interstellar grains and forms icy mantles around them. Although water can form theoretically via gaseous reactions which first form H2O and H3O+ (e.g. Rodgers & Chantley 2002), no observational evidence has been collected so far. It is believed that the major mechanism of water formation is on grain surfaces. One observable that helps to discriminate between the various formation mechanisms is the abundance of single and double deuterated water with respect to the normal isotopologue. Another potential discriminant can be the ortho-to-para ratio (OPR), namely the ratio between water molecules with different nuclear spins. In fact, since radiative and inelastic collisional transitions between the two ortho and para states are strongly forbidden, the OPR is set at the moment of the water formation and it is changed by nuclear spin reactions exchange later on. This can occur either in the gas phase by reactions with ions in which actual nuclei change places, or on the grain surfaces by interaction with electron spins or, perhaps, even other nuclear spins (e.g. Le Bourlot et al. 2000, Limbach et al. 2006). Although little is known on the spin exchange in the gas phase, it is usually assumed that this is a slow process and that the OPR is likely to keep memory of the moment of its formation. Emprechtinger et al. and Lis et al. in this volume report determinations of the water OPR in several environments based on new Herschel observations. The doubly deuterated isotopologue of water, D2O, consists of two species, ortho and para with a nuclear spin statistic weight 2:1. So far D2O has only been detected towards the solar type protostar IRAS 16293-2422 (hereafter IRAS16293), via the observation of the fundamental transition of the para-D2O transition at 316.8 GHz (see our Figure 1; Butner et al. 2007). The observed line profile (see Figure 2) shows a component in emission with a deep absorption at the cloud velocity (~ 4 km s⁻¹). The emission component has been attributed to heavy water in the hot corino of this source where the grain ices are sublimated and released into the gas phase (Cecarelli et al. 2000; Bottinelli et al. 2004), based on the detailed analysis of several HDO lines observed in IRAS16293 (Parise et al. 2005). The absorption component, whose linewidth is 0.5 km s⁻¹, is likely due to the foreground gas (molecular cloud and cold envelope). Therefore, the absorption component provides a straightforward measure of the column density of para-D2O in the cold gas surrounding IRAS16293.

Fig. 1. Energy levels for the detected fundamental lines of D2O.
Table 1. Derived parameters of the ortho and para D$_2$O fundamental lines. Note that the parameters are in T* for ortho-D$_2$O and T_{mb} for para-D$_2$O (see text).

<table>
<thead>
<tr>
<th>Species</th>
<th>Transition</th>
<th>Frequency</th>
<th>Telescope</th>
<th>T_{o}dv (mK km/s)</th>
<th>T_{abs} = T_{C}-T_{L} (mK)</th>
<th>AV (km/s)</th>
<th>V_{LSR} (km/s)</th>
<th>T_{C} (mK)</th>
<th>τ</th>
</tr>
</thead>
<tbody>
<tr>
<td>ortho-D$_2$O</td>
<td>1_{1,0}-0_{0,0}</td>
<td>607.34945</td>
<td>Herschel</td>
<td>77 ± 17</td>
<td>108 ± 11</td>
<td>0.57 ± 0.09</td>
<td>4.33 ± 0.04</td>
<td>234 ± 19</td>
<td>0.62 ± 0.11</td>
</tr>
<tr>
<td>para-D$_2$O</td>
<td>1_{1,0}-1_{0,1}</td>
<td>316.79981</td>
<td>JCMT</td>
<td>120 ± 49</td>
<td>220 ± 30</td>
<td>0.55 ± 0.15</td>
<td>4.15 ± 0.04</td>
<td>850 ± 35</td>
<td>0.26 ± 0.05</td>
</tr>
</tbody>
</table>

3. Determination of the D$_2$O OPR

Crimier et al. (2010) have used the JCMT SCUBA maps of IRAS16293 at 450 μm and 850 μm (and other data) to reconstruct the structure of the IRAS16293 envelope. From this work, one can compute the expected continuum in the HIFI beam at 607 GHz (o-D$_2$O line). Using the SED of Crimier et al. (Fig. 1 panel d) and their Table 1, the IRAS16293 flux is 270 ± 108 Jy at 450 μm and the HIFI beam contains approximately 80% of the total source flux (Fig 1, panel b). One can note that the SED steep slope yields the flux at 607 GHz to be smaller than the one at 450 μm (~ 660 GHz) by about 30%, making the expected flux at 607 GHz to be about 0.7 ± 0.8 × (270 ± 108) Jy i.e. (0.34 ± 0.14) K, using the HIFI Jy to K conversion factor (C. Kramer : Spatial response, contribution to the HIFI framework document), in perfect agreement with the observed continuum value (~ 0.33 K in main beam temperature). Most of the continuum, more than 70% (resp. 80%) of its peak emission at 316 GHz (resp. 607 GHz) is emitted from a region of about 900 AU in radius (~ 15″ in diameter). The absorption of the continuum by heavy water is most likely due to the cold envelope surrounding IRAS16293 as well as the parent cloud, much more extended than the continuum emitting region. Note that, as far as the sizes of the absorbing layer are larger than the sizes of the region emitting the continuum, the line-to-continuum ratio does not depend on the sizes of the telescope beam used for the observations. Therefore, we can compute the D$_2$O OPR directly from the line-to-continuum ratios of the JCMT and Herschel observations, with no further correction. Note also that the para-D$_2$O line has an emission component that Butner et al. (2007) attributed to the hot corino region, whereas here we are dealing with an absorption component only. On the contrary, the ortho-D$_2$O line reported here shows an absorption only as the emission component is very likely diluted in the 35″ HIFI beam, much larger than the 15″ JCMT beam at 316 GHz.

Adopting the density and temperature profiles of the envelope of IRAS16293 (Crimier et al. 2010), the gas at a distance larger (in radius) than 900 AU has a temperature lower than 30 K and a density lower than about 5 × 10$^{-6}$ cm$^{-3}$ (see Figure 3). Thus, given the temperature of the gas absorbing the D$_2$O lines, we only consider the first two levels of each D$_2$O form. We use the recently computed collisional rates for the two fundamental deexcitation transitions of ortho- and para-D$_2$O with para-H$_2$ in the 10-30 K range: 2.3 × 10$^{-11}$ and 3.8 × 10$^{-11}$ cm$^3$ s$^{-1}$ respectively (Wiesenfeld, Faure & Scribano, in preparation).
the low temperatures found in the cold envelope, it is likely that H$_2$ is mainly in its para form (Pagani et al. 2009, Trocmont et al. 2009). With the collisional rates given above, the critical densities of the ortho- and para-D$_2$O fundamental transitions are $1 \times 10^9$ and $2 \times 10^7$ cm$^{-3}$ respectively, and the upper levels of the two transitions are only moderately sub-thermally populated for a density of $5 \times 10^6$ cm$^{-3}$. For a two-level system, the species column density can be computed as follows:

$$N_{\text{tot}} = \frac{8\pi r^2}{A_{\text{coll}}} \frac{\sqrt{\pi}}{2} \frac{\Delta V}{\ln 2} \frac{Q(T_{\text{exc}})}{g_{\text{o}}} \exp\left(\frac{E_{\text{u}}}{kT_{\text{exc}}}ight) \exp\left(\frac{h\nu}{kT_{\text{exc}}} - 1\right)$$

(1)

where $A_{\text{coll}}$ is the Einstein coefficient (2.96 x 10$^{-3}$ s$^{-1}$ for the ortho transition and 6.3 x 10$^{-4}$ s$^{-1}$ for the para transition), $E_{\text{u}}$ is the upper level energy ($E_{\text{u}}/k$=15.2 K for the para transition and =29.2 K for the ortho transition), $g_{\text{o}}$ is the upper statistical weight (3 for the ortho transition, 6 for the para transition), $\nu$ is the frequency (316.79981 GHz for the para transition and 607.349449 GHz for the ortho transition), $\lambda V$ is the linewidth (cm s$^{-1}$) and $r$ is the opacity at the line center. $T_{\text{exc}}$ is the excitation temperature and $Q(T_{\text{exc}})$ is the corresponding partition function. In the approximation of the escape probability formalism, $T_{\text{exc}}$ is defined by the equation:

$$T_{\text{exc}} = \frac{h\nu/k}{h\nu/kT_{\text{c}} + \ln(1 + A_{\text{coll}}/C_{\text{coll}})}$$

(2)

where $C_{\text{coll}} = \gamma_{\text{coll}} \times n_{\text{collision}}, n_{\text{collision}}$ being the density of the collision partner (in this case para-H$_2$) and $\gamma_{\text{coll}}$ being the collisional rate in cm$^3$ s$^{-1}$ (values given above). The $\beta$ parameter represents the probability that a photon at some position in the cloud escapes the system. For a static, spherically symmetric and homogeneous medium, Osterbrock and Ferland (2006, Appendix 2) derives this parameter as a function of the optical depth $\tau$ in the direction of the observer. The opacity at the line center is expressed as a function of the line depth ($T_{\text{abs}} = T_{\text{c}} - T_L$) and the continuum ($T_C$):

$$\tau = -\ln\left(\frac{T_{\text{sh}}}{T_C} + J_0(T_{\text{c}}) + J_1(T_{\text{c}})\right)$$

(3)

Where $J_0(T_{\text{c}}) = (h\nu/k)/((\exp(h\nu/k) - 1)$ and $T_{\text{c}}$ is the cosmic microwave background radiation temperature (2.73 K). In the limit of $\tau \gg 1, T_C \approx T_{\text{abs}} \approx J_0(T_{\text{c}})$ and $T_{\text{c}} \approx 5K$. Since the D$_2$O transitions are probably optically thin, we can reasonably assume that $T_{\text{exc}}$ is lower than 5 K and $J_0(T_{\text{c}}) - J_1(T_{\text{c}})$ is negligible.

As discussed above, we assume that the absorbing layer is much larger than the continuum emitting region. Considering the uncertainty in the H$_2$ density (lower than $5 \times 10^6$ cm$^{-3}$) and the kinetic temperature (lower than 30 K), we applied the method described above to determine the column densities with $n_{\text{H}_2} = 10^6$ cm$^{-3}$ and $T_{\text{c}} = 20 K$. Table 1 lists the computation of the optical depths for both lines as well as the corresponding uncertainties. Since $\tau = -\ln(T_{\text{c}}/T_L)$ the uncertainty in the line optical depth is given by $\Delta \tau = \exp(\tau) \times \sigma(T_{\text{c}}/T_L)$. Our computation yields an OPR equal to 1.1 $\pm$ 0.4 with the corresponding column densities: $N_{\text{ortho}} = (8.7 \pm 2.1) \times 10^{11}$ cm$^{-2}$ and $N_{\text{para}} = (7.8 \pm 2.6) \times 10^{11}$ cm$^{-2}$. All errors here are 1 $\sigma$. Both lines are optically thin and their $T_{\text{c}}$ are lower than 5 K. Note that decreasing the density and/or the kinetic temperature doesn’t change the OPR by more than 10%. Therefore, the OPR is lower than 2.4 at a 3 $\sigma$ level of uncertainty (where we added the 3 $\sigma$ statistical error and the mentioned 10% to the 1.1 value). We assumed (see section 2) that the relative gains on the lower and upper side-bands are equal. Since we do not have any information concerning the sideband ratio at the frequency of the D$_2$O line, we can only introduce a maximum uncertainty of 16%, corresponding to the overall calibration budget for band 1b. The resulting upper limit on the OPR is therefore increased to about 2.6. Figure 4 shows the measured OPR interval and the thermal equilibrium as a function of the gas temperature.

4. Conclusions

A discussed in §3, the gas absorbing the D$_2$O line lies at more than 900 AU from the center and has a temperature lower than 30 K. The comparison between the upper value of the measured D$_2$O OPR and the thermal equilibrium value shows that they are consistent with a gas at a temperature larger than about 15 K (at a 3 $\sigma$ level of confidence), and, therefore, with the assumed absorbing gas location. On the other hand, the D$_2$O gas could have formed in a previous phase, where the gas was colder, and, in this case, it means that it had the time to thermalise to the Boltzmann value. Unfortunately, given the poor knowledge of the mechanisms that can exchange the D$_2$O spins (see the Introduction), it is difficult to infer here the timescale for this change and, consequently, to give a lower limit to the object age. On the other hand, the relatively large uncertainty in the OPR derived here does not allow either to exclude a non-thermal equilibrium situation. Higher S/N observations will be needed to lower the uncertainty on the OPR value and give a more robust result.

Using the density and temperature profiles of the envelope of IRAS16293 by Cramer et al. (2010), the column density of the gas colder than 30 K is about $1 \times 10^{23}$ cm$^{-2}$. Therefore, the D$_2$O abundance (with respect to H$_2$) is about $2 \times 10^{-11}$. An estimate of the water abundance profile will soon be available with the HIFI observations with a much higher spatial and spectral resolution than the one provided by the ISO observations (Ceccharelli et al. 2000). D$_2$O molecules might form with one OPR, but then could freeze out on grains surfaces that could modify the ratio and then get desorbed. Due to the high uncertainty in the H$_2$O abundance, we cannot at the time being completely exclude or confirm formation through grain surface chemistry. A modeling of the OPR evolution is beyond the scope of the present letter. With an improved calibration and better understanding of the instrumental effects, a more accurate determination of the D$_2$O OPR in this source and potentially other sources will be possible. Also,
ALMA may hopefully yield an answer in a near future with the observation of cold D$_2$O with a higher spatial resolution.

In summary, this Letter presents the first tentative to estimate the OPR for the D$_2$O molecule, demonstrating the outstanding capabilities of the HIFI instrument. The poor knowledge of the mechanisms of exchange of the nuclear spins and the relatively large error in the derived OPR prevent to drawing firm conclusions on the formation of heavy water at that time.

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